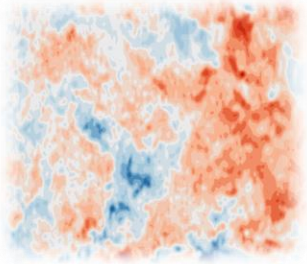
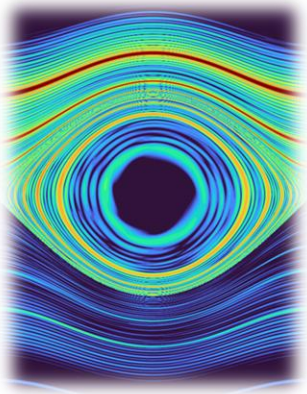




Polar Decompositions of Koopman Operators

Matthew Colbrook

University of Cambridge

29/02/2024

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

Motivation

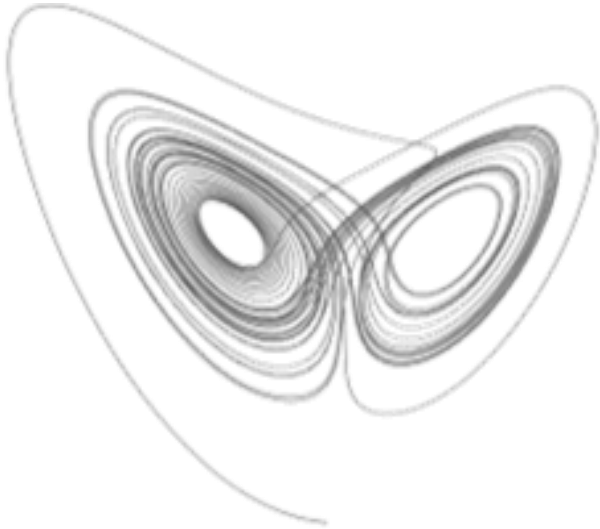
Data-driven dynamical systems

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

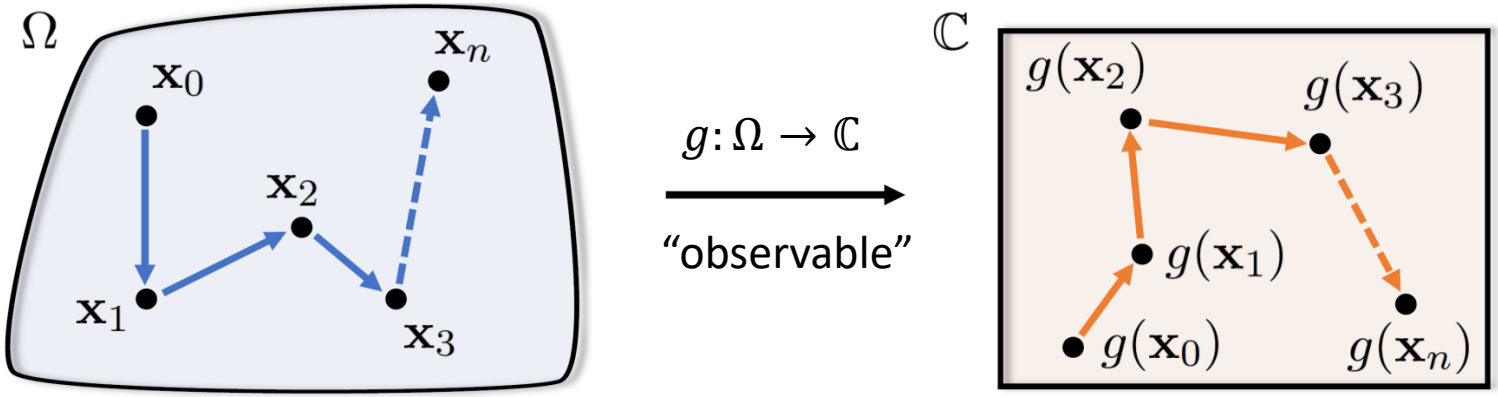
Unknown function $F: \Omega \to \Omega$ governs dynamics: $x_{n+1} = F(x_n)$

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

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

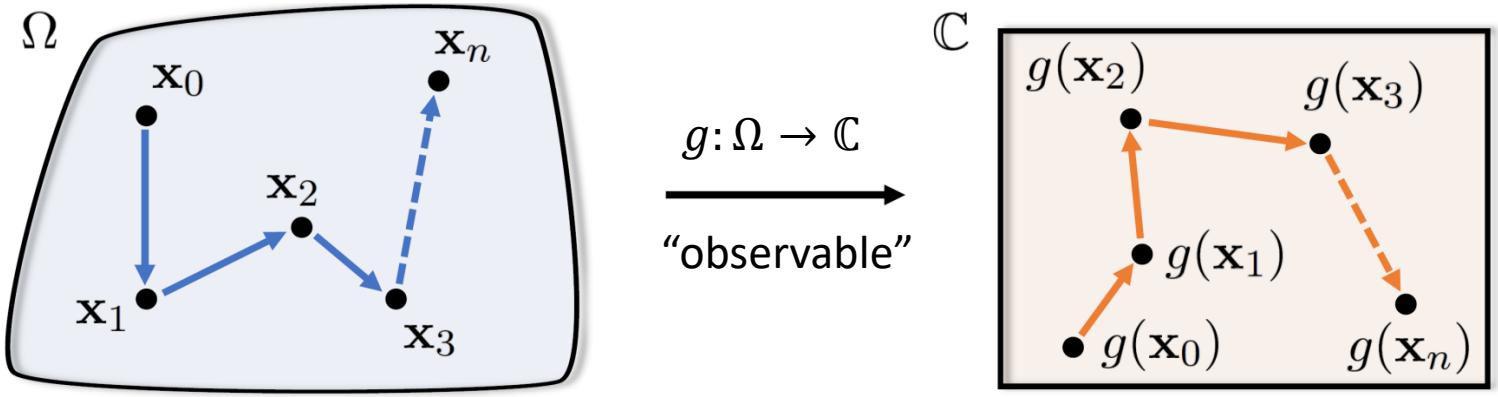


Koopman Operator $\mathcal{K}$: A global linearization



- 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.

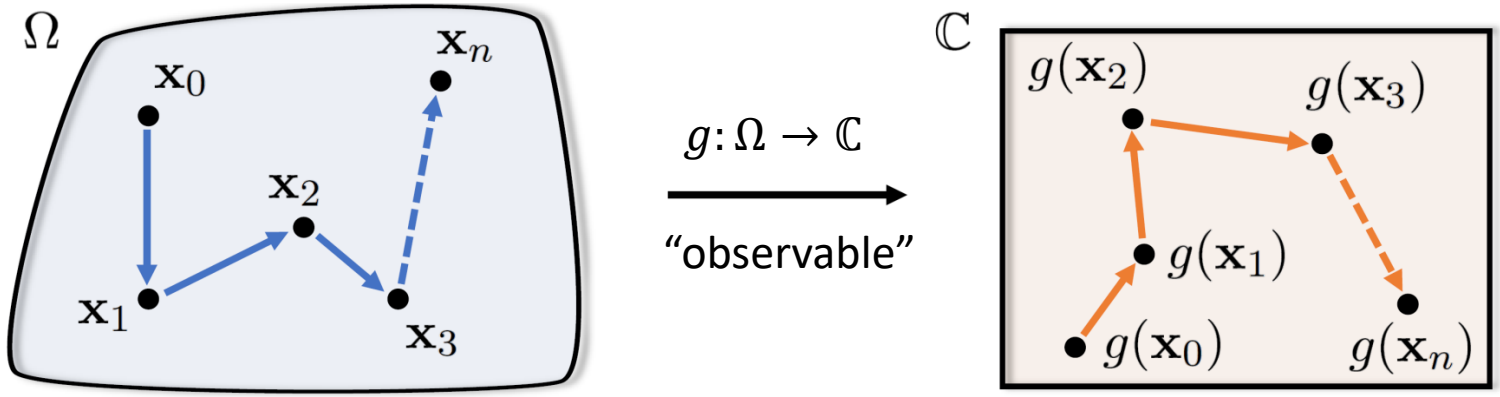
Koopman Operator $\mathcal{K}$: A global linearization



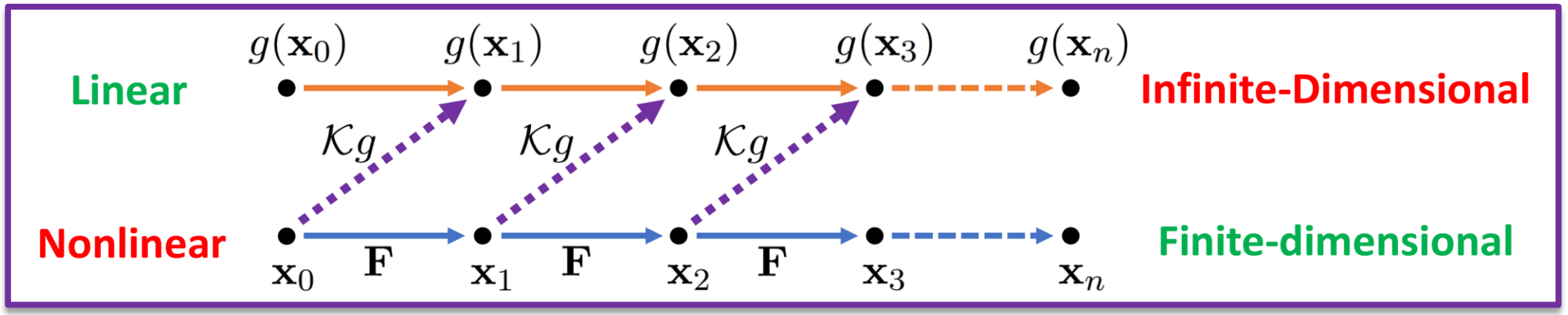
- $\mathcal{K}$ acts on functions $g: \Omega \to \mathbb{C}$, $[\mathcal{K}g](x) = g(F(x))$.
- Function space: g $\in L^2(\Omega, \omega)$, positive measure ω, inner product $\langle \cdot, \cdot \rangle$.

- 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.

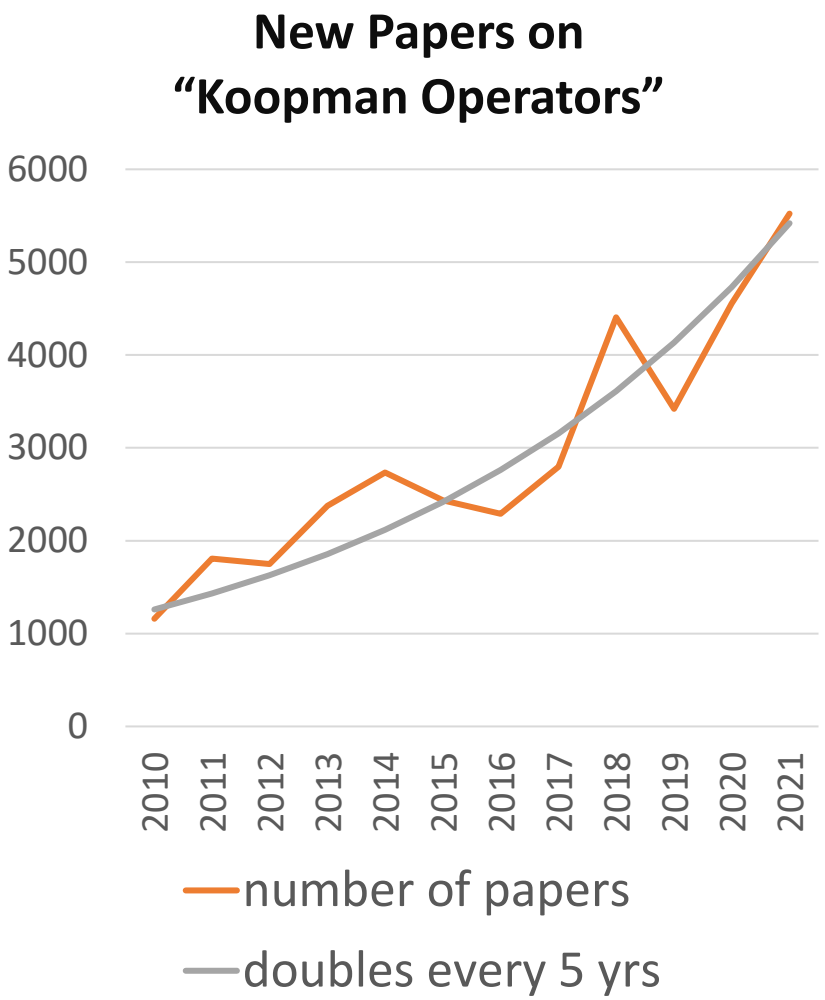
Koopman Operator $\mathcal{K}$: A global linearization

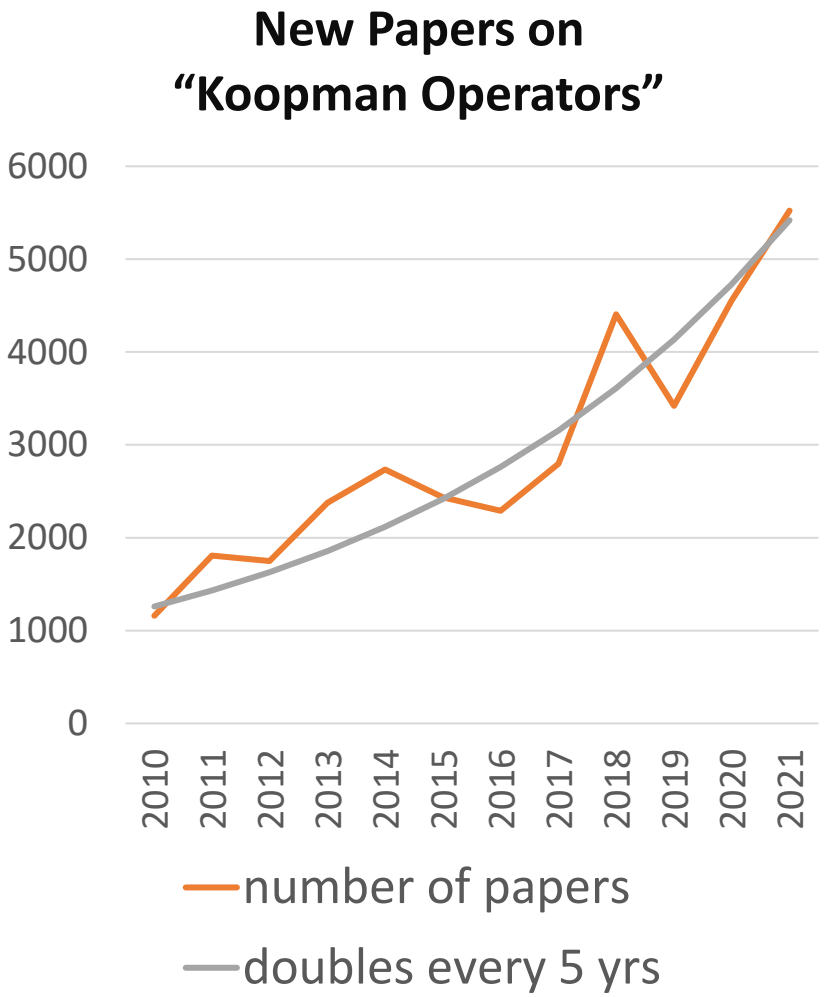


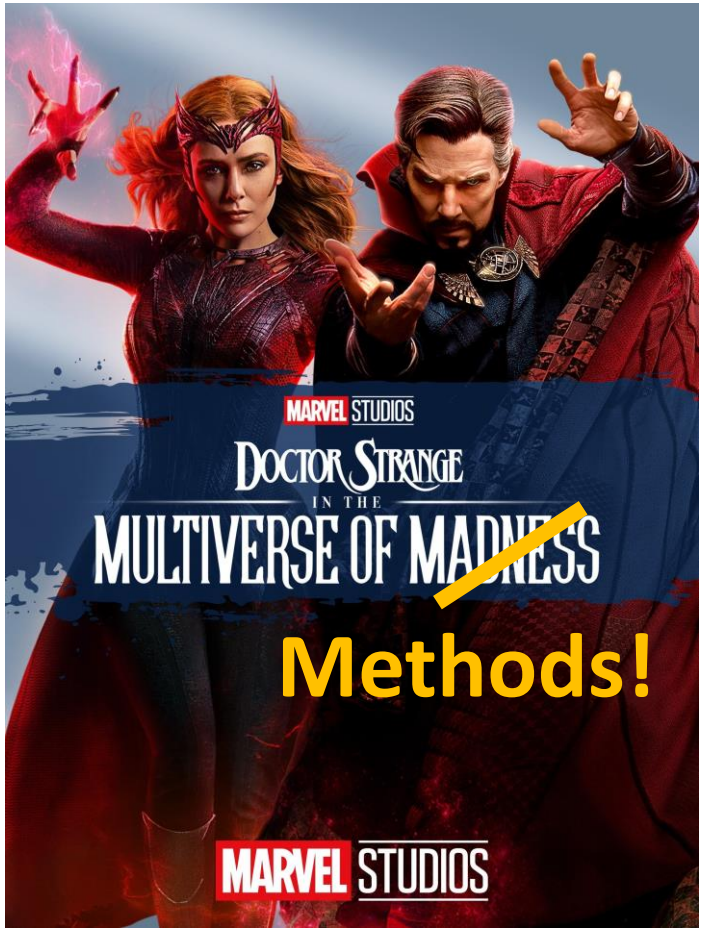
- $\mathcal{K}$ acts on functions $g: \Omega \to \mathbb{C}$, $[\mathcal{K}g](x) = g(F(x))$.
- Function space: g $\in L^2(\Omega, \omega)$, positive measure ω, inner product $\langle \cdot, \cdot \rangle$.



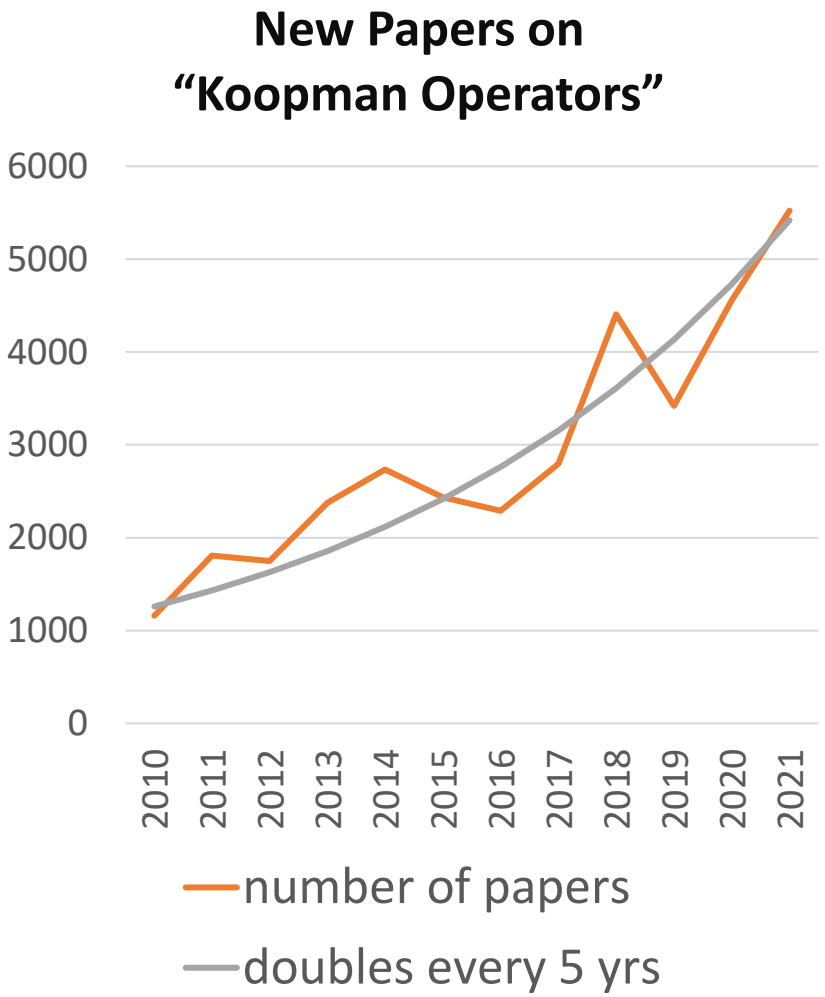
- Koopman, "*Hamiltonian systems and transformation in Hilbert space,*" **Proc. Natl. Acad. Sci. USA**, 1931.
- Koopman, v. Neumann, "*Dynamical systems of continuous spectra,*" **Proc. Natl. Acad. Sci. USA**, 1932.

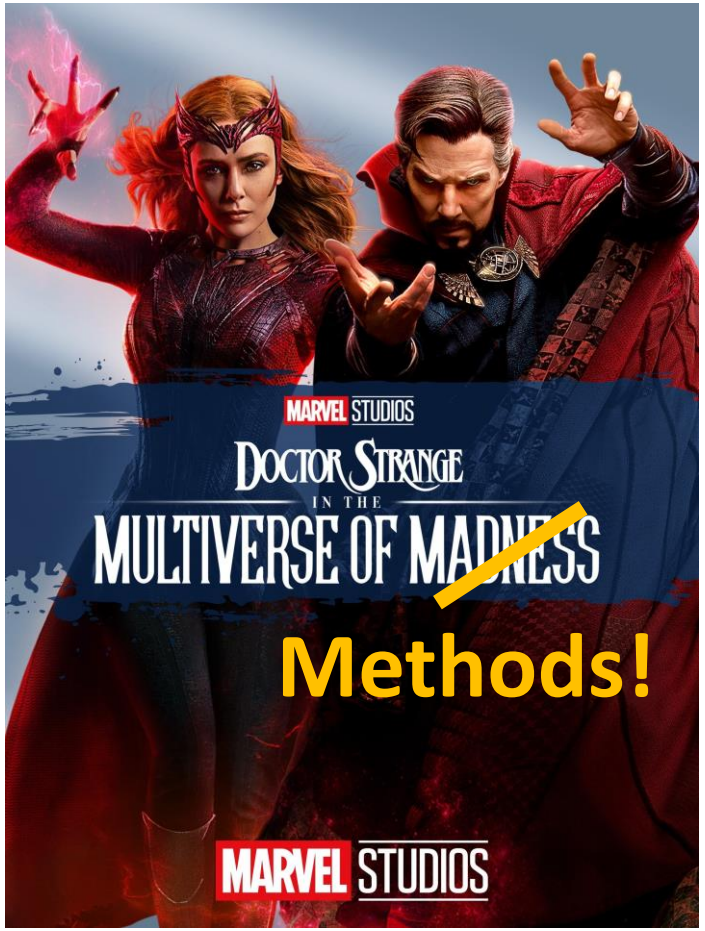

New Papers on
“Koopman Operators”
6000
5000
4000
3000
2000
1000
0
2010
2011
2012
2013
2014
2015
2016
2017
2018
2019
2020
2021
number of papers
doubles every 5 yrs



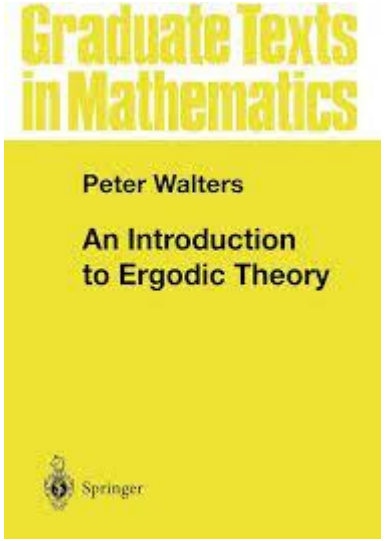


- C., "*The Multiverse of Dynamic Mode Decomposition Algorithms,*" **Handbook of Numerical Analysis**, 2024.





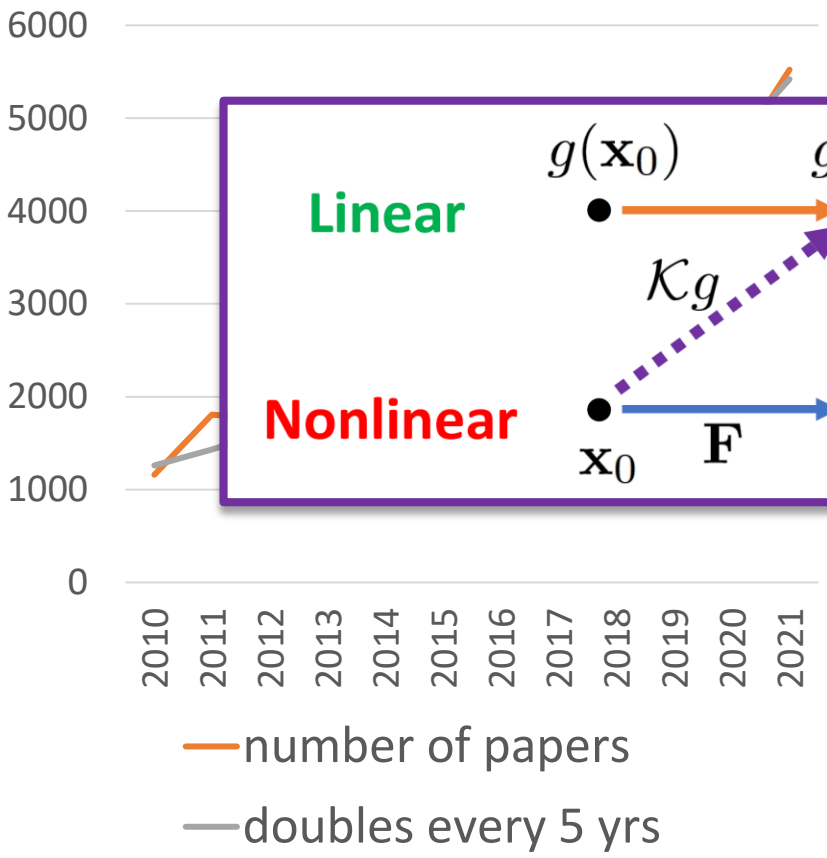
Koopman operators are classical in ergodic theory.



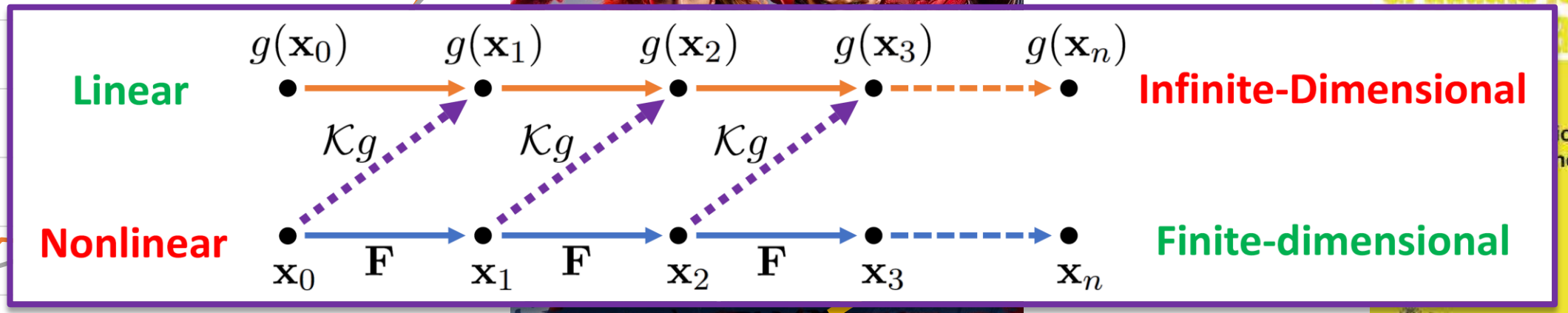
Why all this sudden interest?

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

New Papers on "Koopman Operators"



Koopman operators are classical in ergodic theory.



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 $g(x) = w^{\mathrm{T}}x$,

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

Eigenfunction

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

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

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

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

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

$$g(x_n) = [\mathcal{K}^n g](x_0)$$

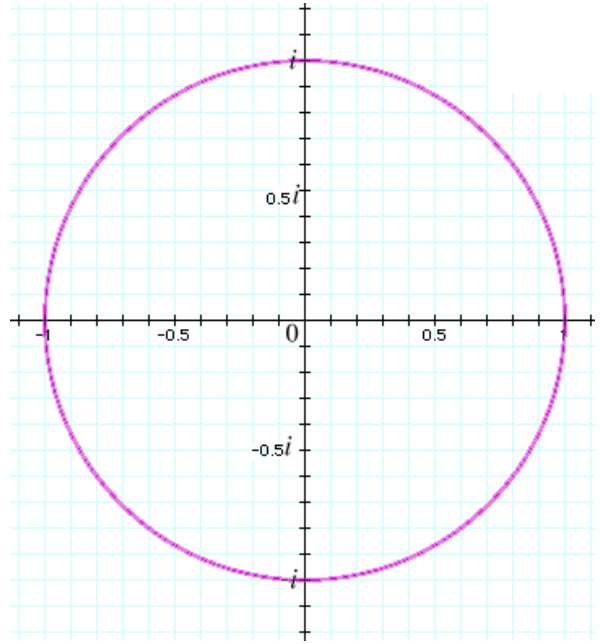
Assume: System is **measure-preserving** (F preserves ω)

$$\Leftrightarrow \|\mathcal{K}g\| = \|g\| \text{ (isometry)}$$

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

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

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



Spectral measure
(see later) on boundary

Our setting – unitary evolution

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

$$g(x_n) = [\mathcal{K}^n g](x_0)$$

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

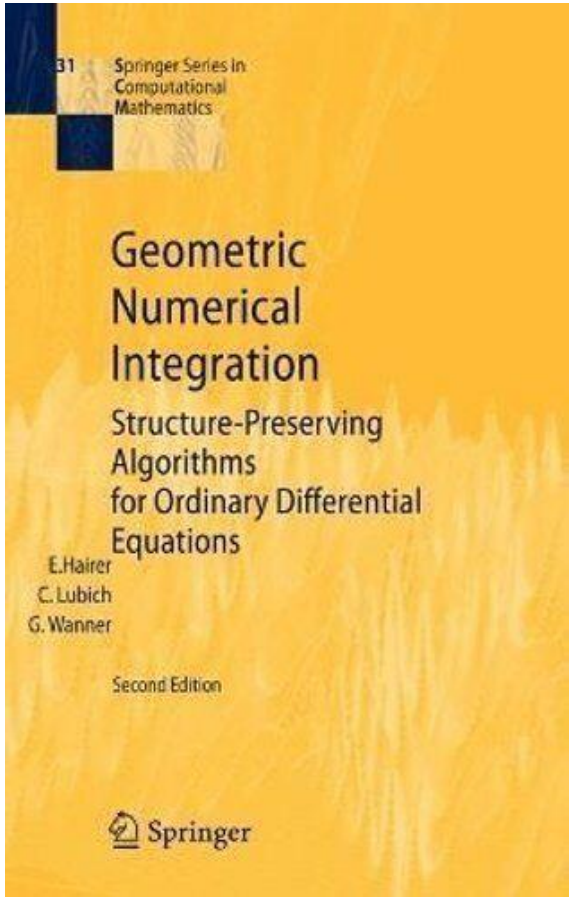
$$\Leftrightarrow \|\mathcal{K}g\| = \|g\| \text{ (isometry)}$$

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

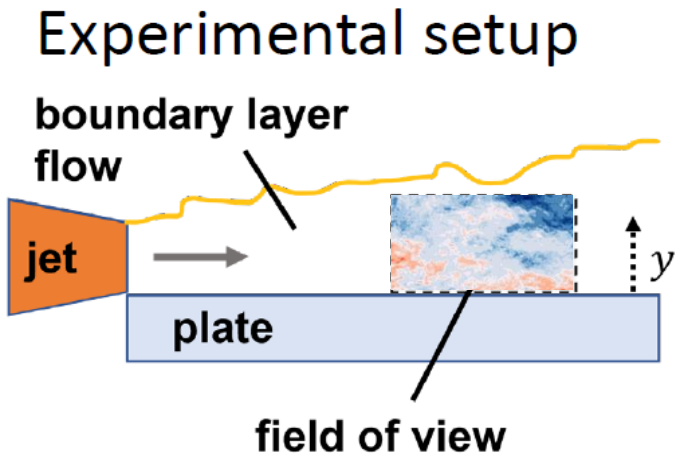
$$\Rightarrow \mathrm{Spec}(\mathcal{K}) \subseteq \{z : |z| \leq 1\}$$

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

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



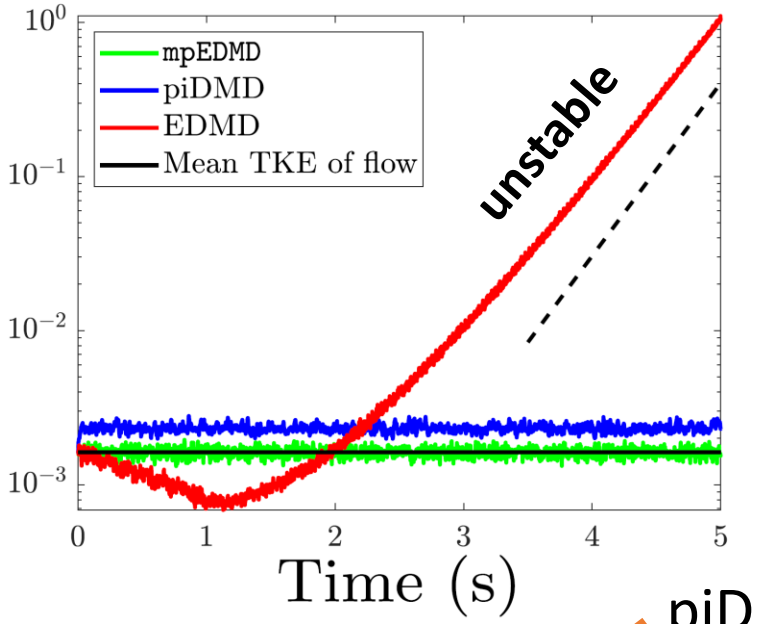
Motivating example



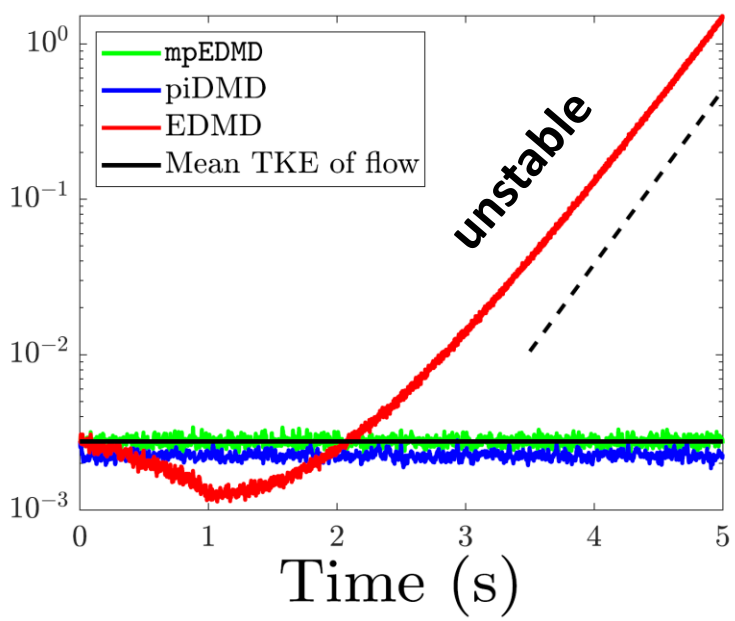
- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension (d) $\approx 100{,}000$ (velocity at measurement points)

*PIV data provided by Máté Szőke (Virginia Tech)

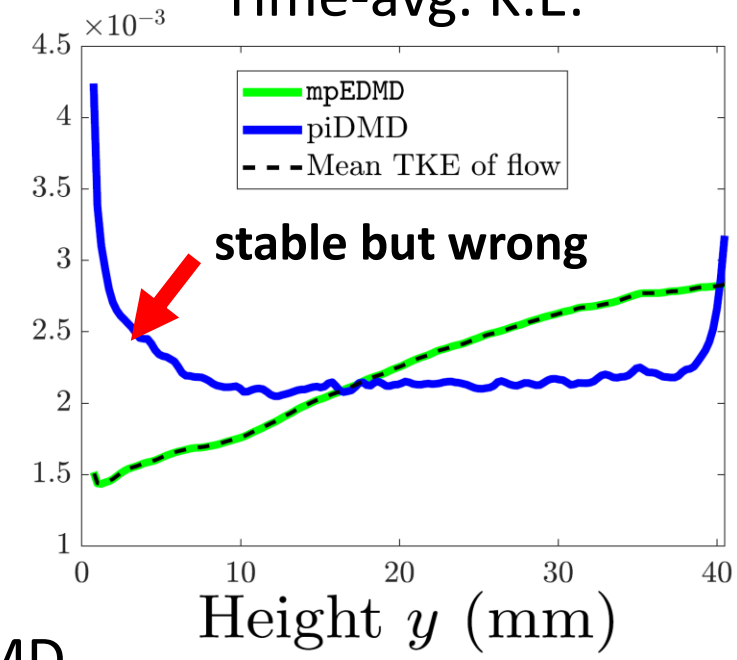
Turbulent K.E. y=5mm



Turbulent K.E. y=35mm



Time-avg. K.E.



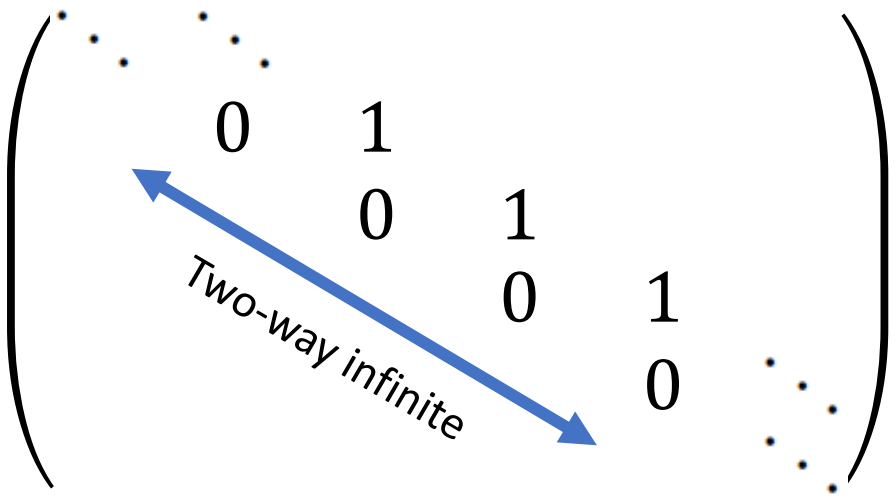
piDMD

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.

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

$e_j \to e_{j-1}$



truncate /discretize

Jordan block!

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

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

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

Caution

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

The most important slide

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

polar decomposition

Circulant matrix

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

- 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)

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

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

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

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

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

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

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

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

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

A simple alteration

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

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

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

A simple alteration

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

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

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

quadrature

orthogonal Procrustes problem

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

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 $\mathbf{\Psi}_X$ 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:

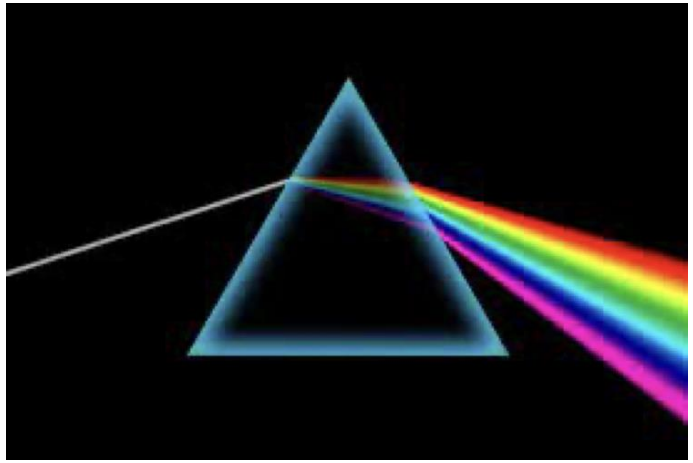
- As $M \to \infty$, EDMD: $\mathcal{P}_{V_N}\mathcal{K}\mathcal{P}_{V_N}^*$, mpEDMD: unitary part of polar decomp. of $\mathcal{P}_{V_N}\mathcal{K}\mathcal{P}_{V_N}^*$.
- Orthogonal Procrustes = constrained total least squares $\Longrightarrow$ better stability to noise!

Convergence theory

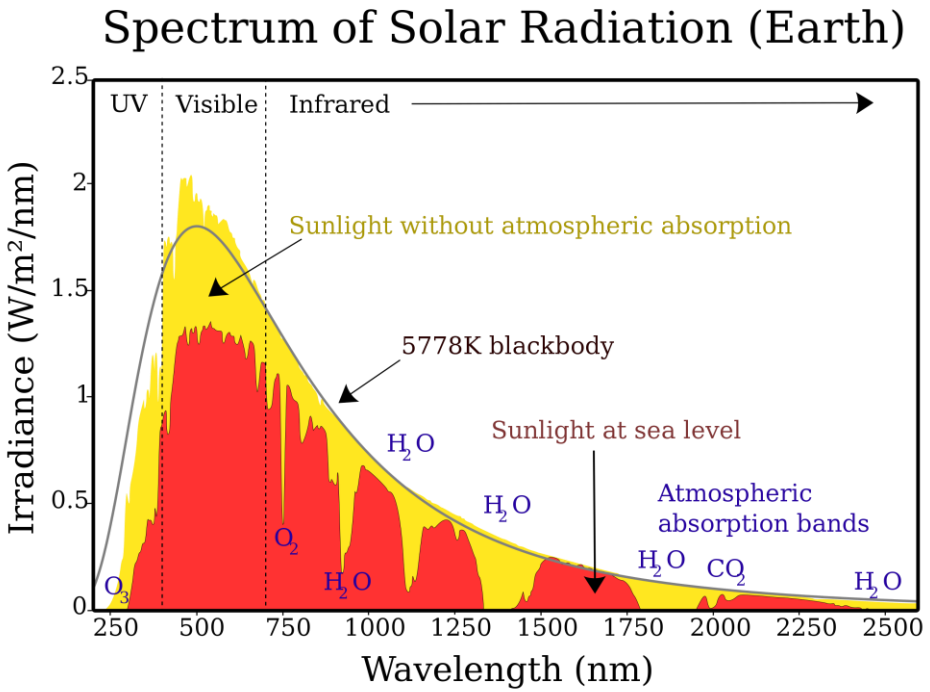
Key ingredient: **unitary** discretization.

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 $\mathcal{L}\colon \mathcal{D}(\mathcal{L}) \to \mathcal{H}$. 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

moments

μ_g probability measures on $\mathbb{T}$

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

$\lambda = \exp(i\theta)$ 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 $\varphi\colon \mathbb{T} \to \mathbb{C}$, $g \in L^2(\Omega, \omega)$ 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 $\mathbb{K}$

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

Key ingredients:

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

Convergence of scalar-valued measures

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

Captures weak convergence of measures

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

Theorem: Suppose quad. rule converges, $\lim_{N\to\infty} \operatorname{dist}(h, V_N) = 0$ 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 $\lim_{N\to\infty} \|g - \Psi \boldsymbol{g}_N\| = 0$,

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

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

Matching autocorrelations!

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

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

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 $\mathbb{K}$

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

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!

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

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

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

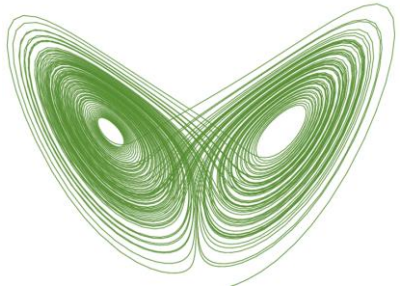
Two methods:

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

- 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

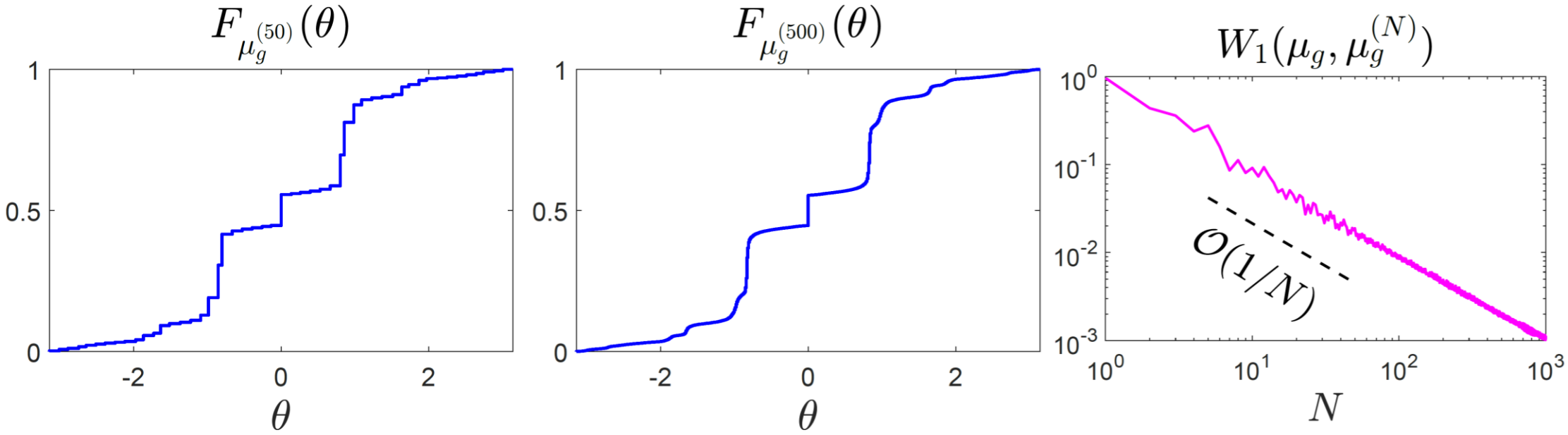
Lorenz system



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

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

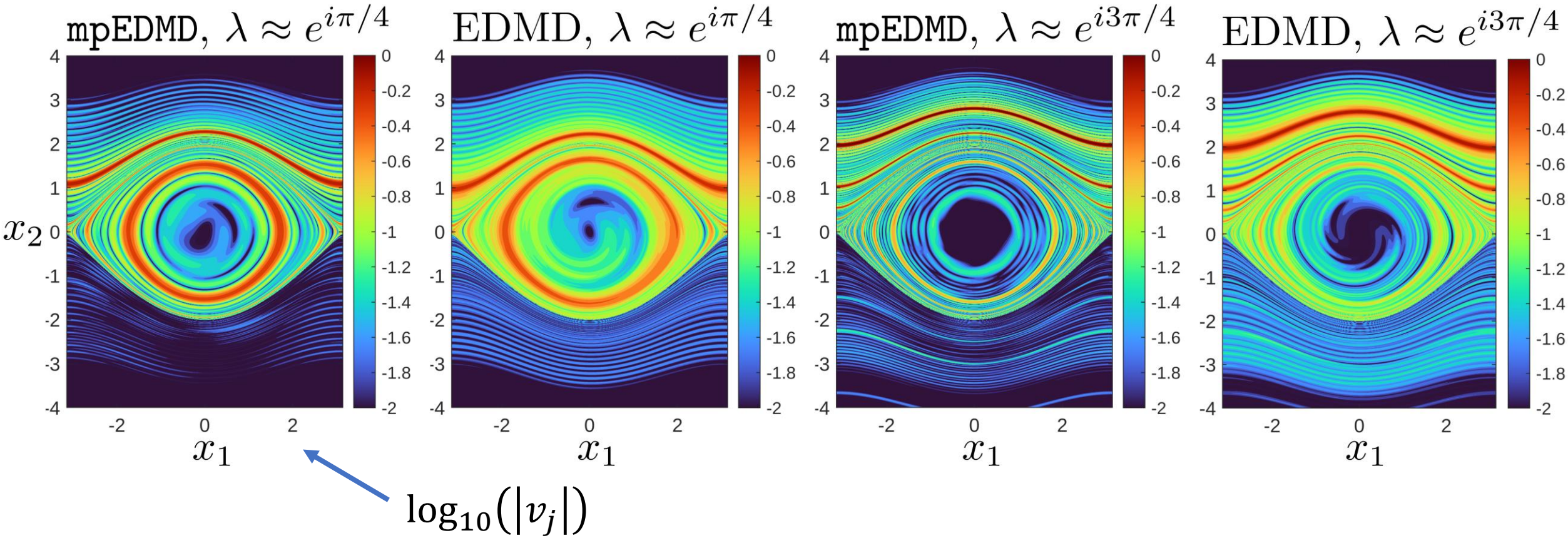
Cdf: $F_\mu(\theta) = \mu(\{\exp(it) : \pi \le t \le \theta\})$



Nonlinear pendulum

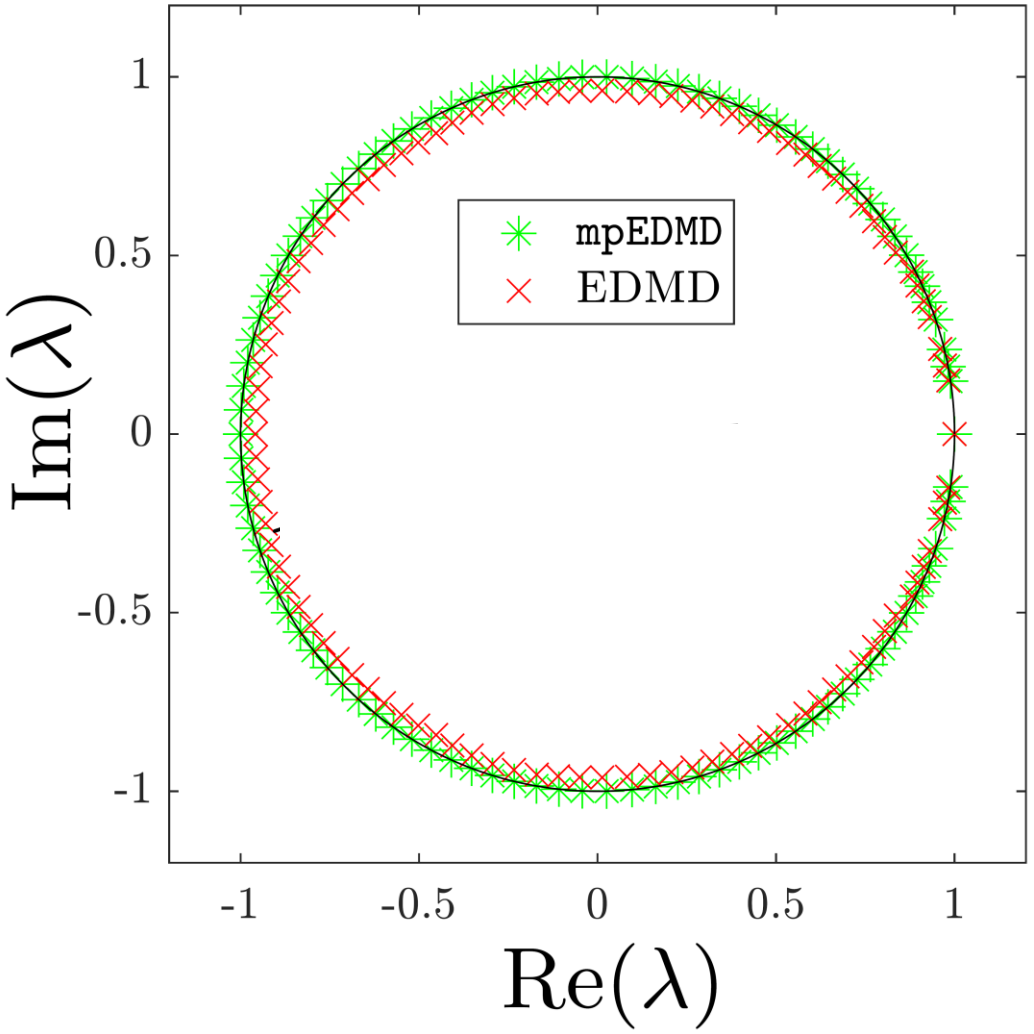
$$\dot{x}_1 = x_2, \qquad \dot{x}_2 = -\sin(x_1), \qquad \Omega = [-\pi, \pi]_{\text{per}} \times \mathbb{R}, \qquad \Delta_t = 0.5$$

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

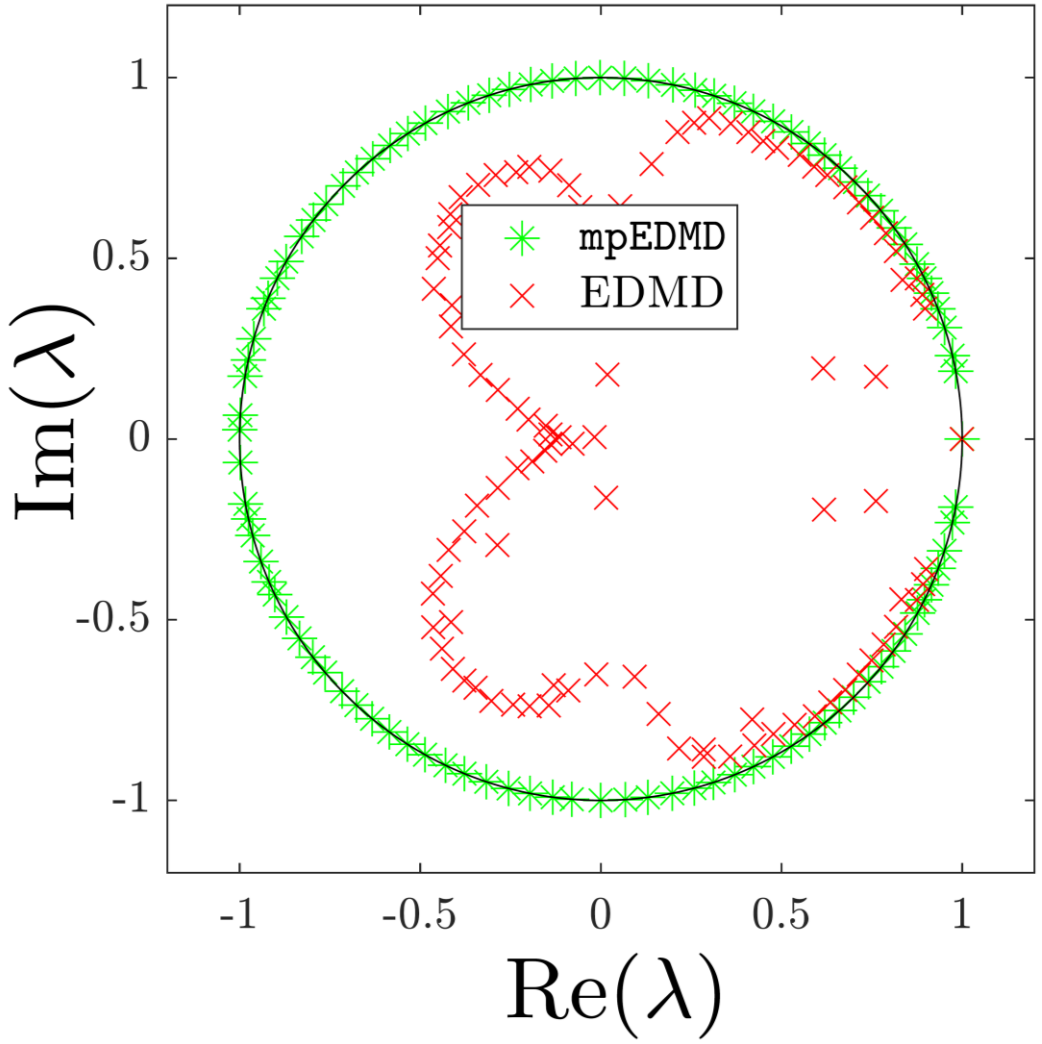


Nonlinear pendulum

Noise free

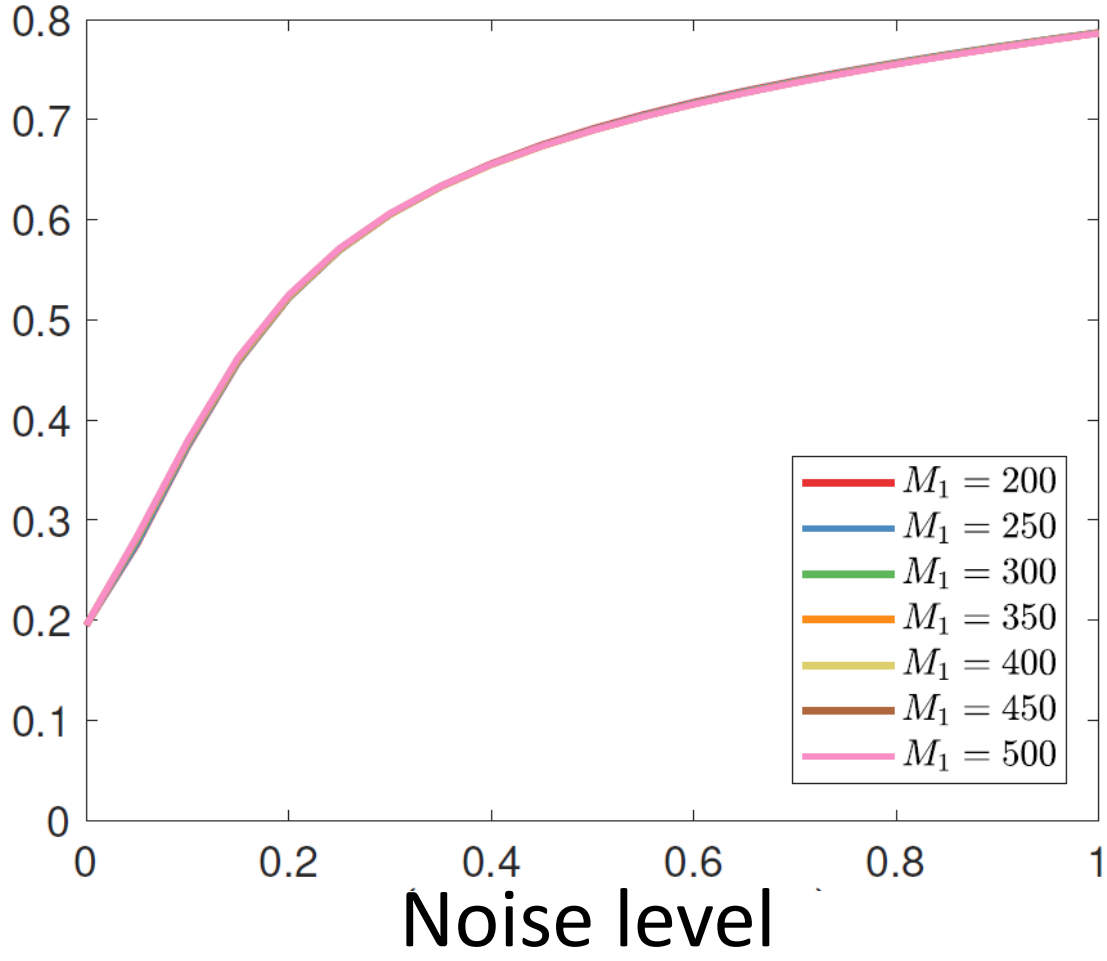


10% Gauss. noise for Ψ_X, Ψ_Y



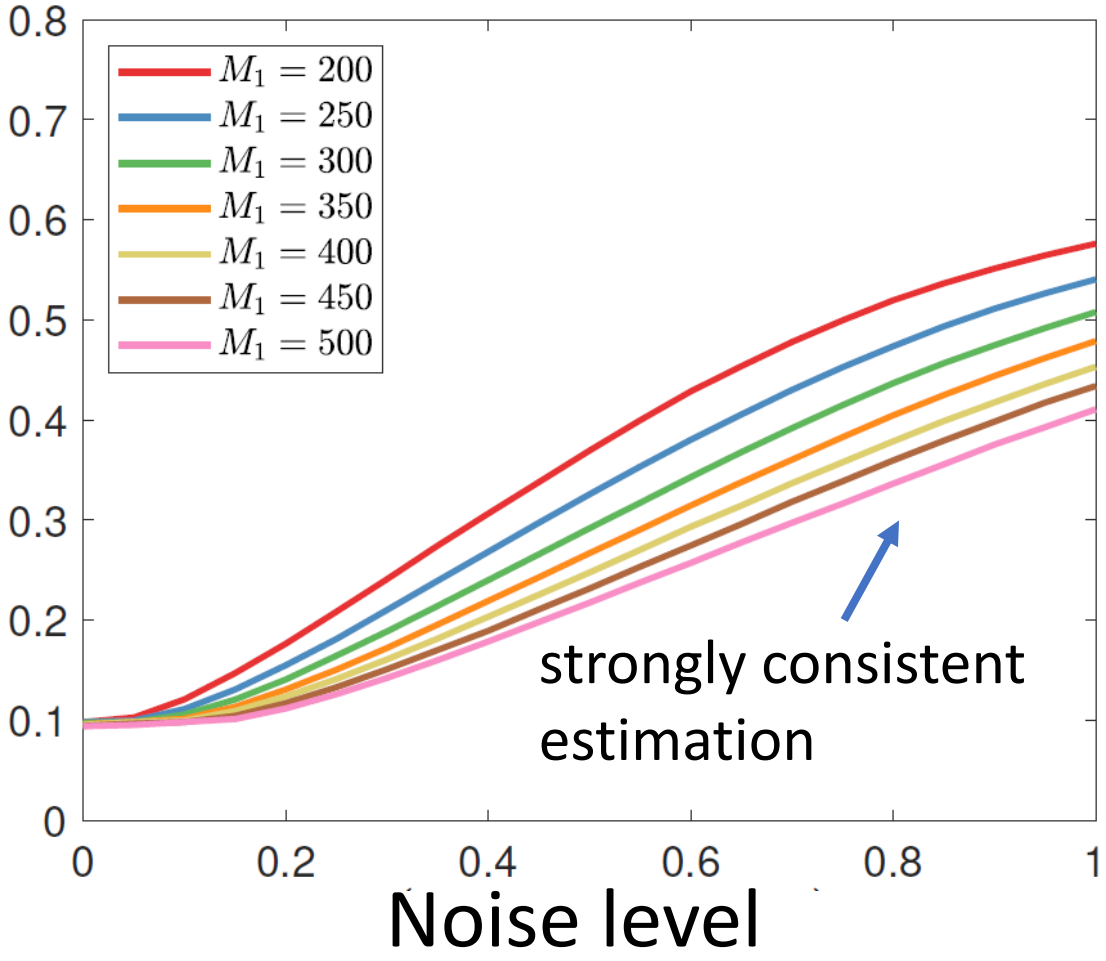
Robustness to noise: Gauss. noise for Ψ_X, Ψ_Y

Mean residual (EDMD)



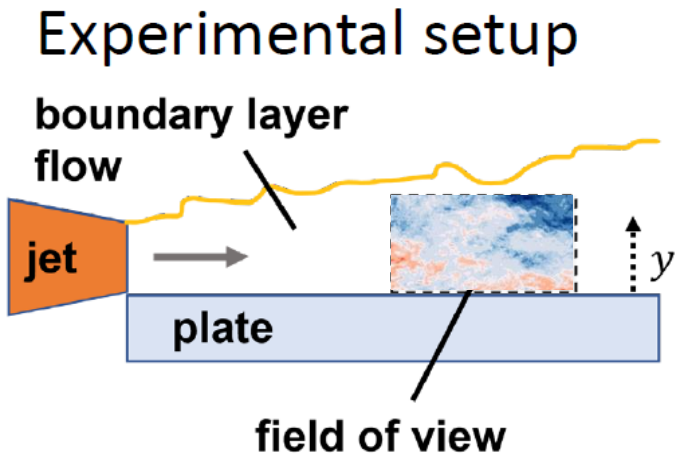
Noise level

Mean residual (mpEDMD)



Noise level

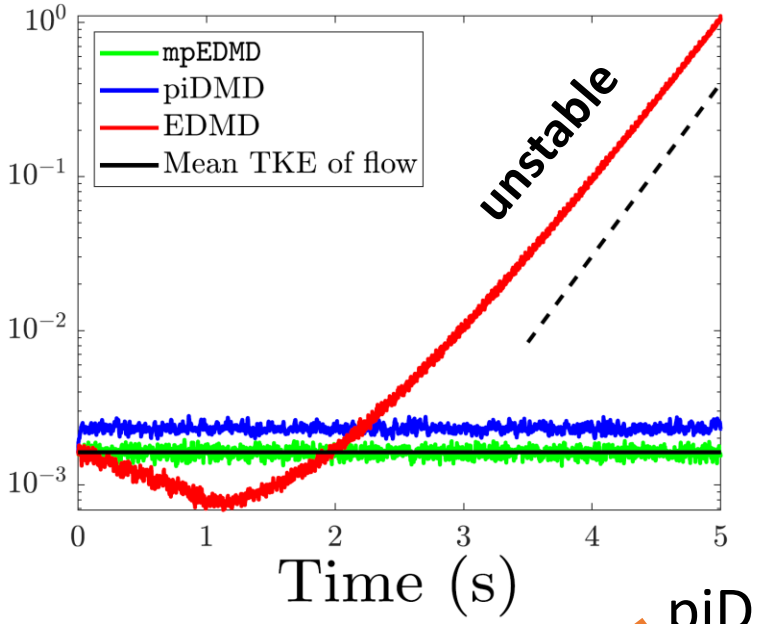
Motivating example



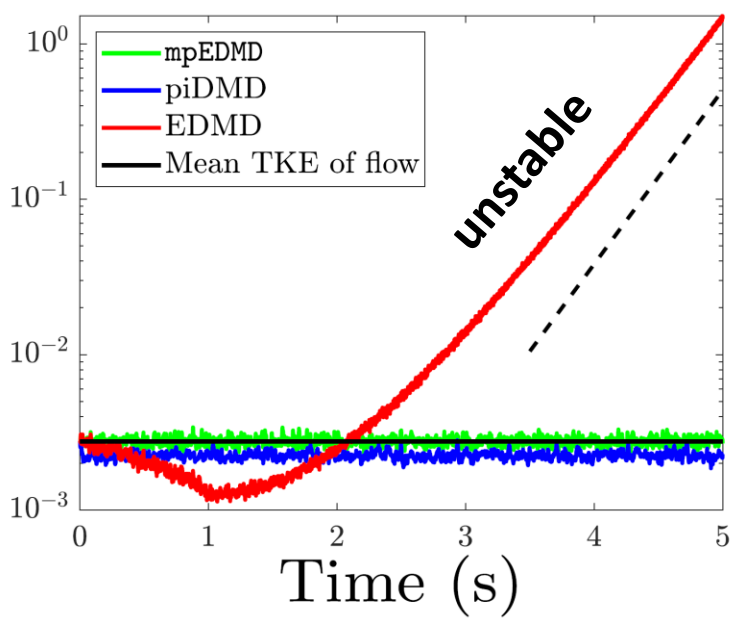
- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension (d) $\approx$ 100,000 (velocity at measurement points)

*PIV data provided by Máté Szőke (Virginia Tech)

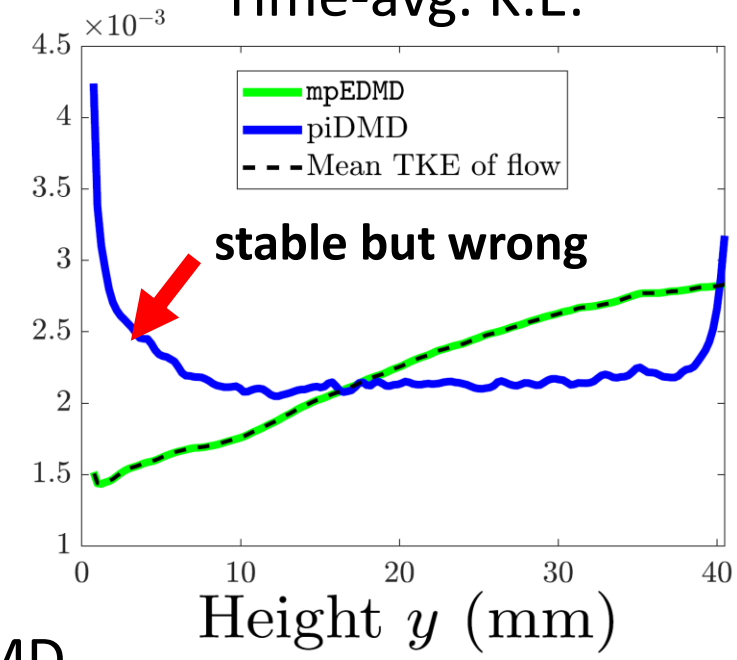
Turbulent K.E. y=5mm



Turbulent K.E. y=35mm



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

stable but wrong

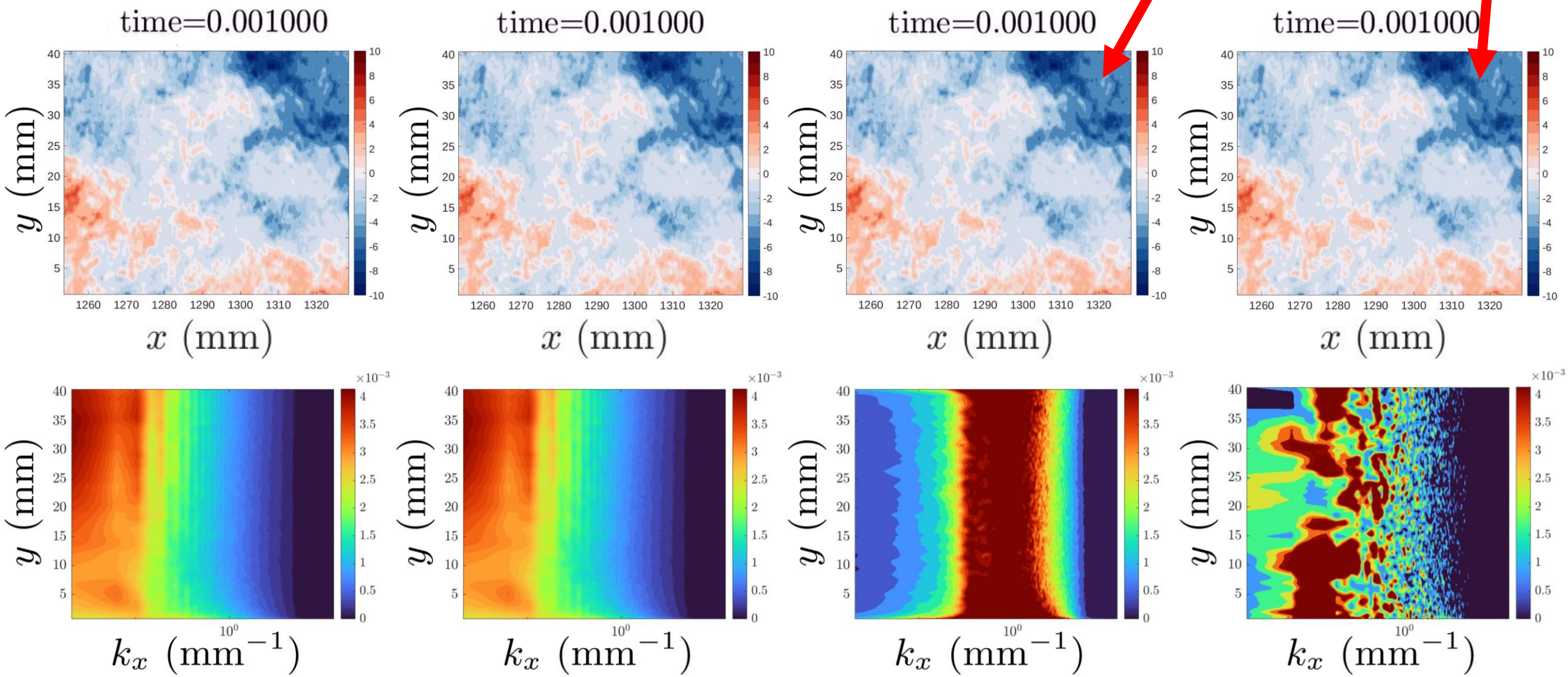
unstable

Flow

mpEDMD

piDMD

EDMD



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

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!

Newsjournal of the Society for Industrial and Applied Mathematics sinews.siam.org

siam news

Volume 56/ Issue 1
January/February 2023

Optimization and Learning with Zeroth-order Stochastic Oracles

By Stefan M. Wild

Mathematical optimization is a foundational technology for machine learning and the solution of design, decision, and control problems. In most optimization applications, the principal assumption is the availability of at least the

sequence is that material properties are only available via *in situ* and *in operando* characterization. In the context of optimization, this scenario is called a "zeroth-order oracle" — our knowledge about a particular system or property is data driven and limited by the black-box nature of measurement procurement. An additional challenge is

An optimization solver specifies a particular composition of solvents and bases, an operating temperature, and reaction times; this combination is then run through a continuous flow reactor. The material that exits the reactor is then automatically characterized

through an inline nuclear magnetic resonance detector that illuminates properties of the synthesized materials. These stochastic, zeroth-order oracle outputs return to the solver in a closed-loop setting that

See **Optimization** on page 3

derivatives are not available [5].

Given the pervasiveness of sensors and other experimental and observational data, these types of settings are arising in increasingly more science and engineering domains. For example, consider the ongoing search for novel materials for energy storage. In order to create viable new materials, we must move beyond pure theory and account for the actual processes that occur during materials synthesis. A necessary

variables and ξ is a random variable (e.g., a variable that is associated with the stochastic synthesis and measurement processes). The zeroth-order stochastic oracle is $f(\mathbf{x};\xi)$. We can specify values for the random variable only in certain problem settings; in others—such as the laboratory environment in Figure 1—doing so is impossible.

Figure 1 displays an instantiation of a data-driven optimization setting in a chemistry lab at Argonne National Laboratory's Materials Engineering Research Facility. The

Figure 1. *A continuous flow reactor at Argonne National Laboratory's Materials Engineering Research Facility uses the optimization solver ParMOO to perform autonomous discovery [2].*

Read more in SIAM News!

Nonprofit Org
U.S. Postage
PAID
Permit No 360
Bellmawr, NJ

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 $\boldsymbol{x}$ in a state space $\Omega \subset \mathbb{R}^d$ that is governed by an unknown and typically nonlinear function $\boldsymbol{F}: \Omega \to \Omega$:

$$\boldsymbol{x}_{n+1} = \boldsymbol{F}(\boldsymbol{x}_n), \quad n \geq 0. \qquad (1)$$

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 fixed points, periodic orbits, stable or unstable manifolds, and so forth. Although Poincaré's framework has revolutionized our understanding of dynamical systems, this approach has at least two challenges in many modern applications: (i) Obtaining a global understanding of the nonlinear dynamics and (ii) handling systems that are either too complex to analyze or offer incomplete information about the evolution (i.e., unknown, high-dimensional, and highly nonlinear $\boldsymbol{F}$).

Koopman operator theory, which originated with Bernard Koopman and John von Neumann [6, 7], provides a powerful alternative to the classical geometric view of dynamical systems because it addresses nonlinearity: the fundamental issue that underlies the aforementioned challenges.

We lift the nonlinear system (1) into an infinite-dimensional space of observable functions $g: \Omega \to \mathbb{C}$ via a Koopman operator $\mathcal{K}$:

$$\mathcal{K}g(\boldsymbol{x}_n) = g(\boldsymbol{x}_{n+1}).$$

The evolution dynamics thus become linear, allowing us to utilize generic solution techniques that are based on spectral decompositions. In recent decades, Koopman operators have captivated researchers because of emerging data-driven and numerical implementations that coincide with the rise of machine learning and high-performance computing [2].

One major goal of modern Koopman operator theory is to find a coordinate transformation with which a linear system may approximate even strongly nonlinear dynamics; this coordinate system relates to the spectrum of the Koopman operator. In 2005, Igor Mezić introduced the Koopman mode decomposition [8], which provided a theoretical basis for connecting the dynamic mode decomposition (DMD) with the Koopman operator [9, 10]. DMD quickly became the workhorse algorithm for computational approximations of the Koopman operator due to its simple and highly extensible formulation in terms of linear algebra, and the fact that it applies equally well to data-driven modeling when no governing equations are available. However, researchers soon realized that simply building linear models in terms of the primitive measured variables cannot sufficiently capture nonlinear dynamics beyond periodic and quasi-periodic phenomena. A major breakthrough occurred with the introduction of *extended* DMD (EDMD), which generalizes DMD to a broader class of basis functions in which to expand eigenfunctions of the Koopman operator [11].

See **Dynamical Systems** on page 4

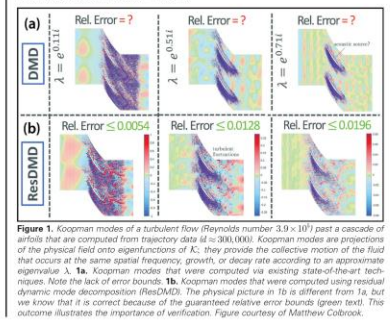


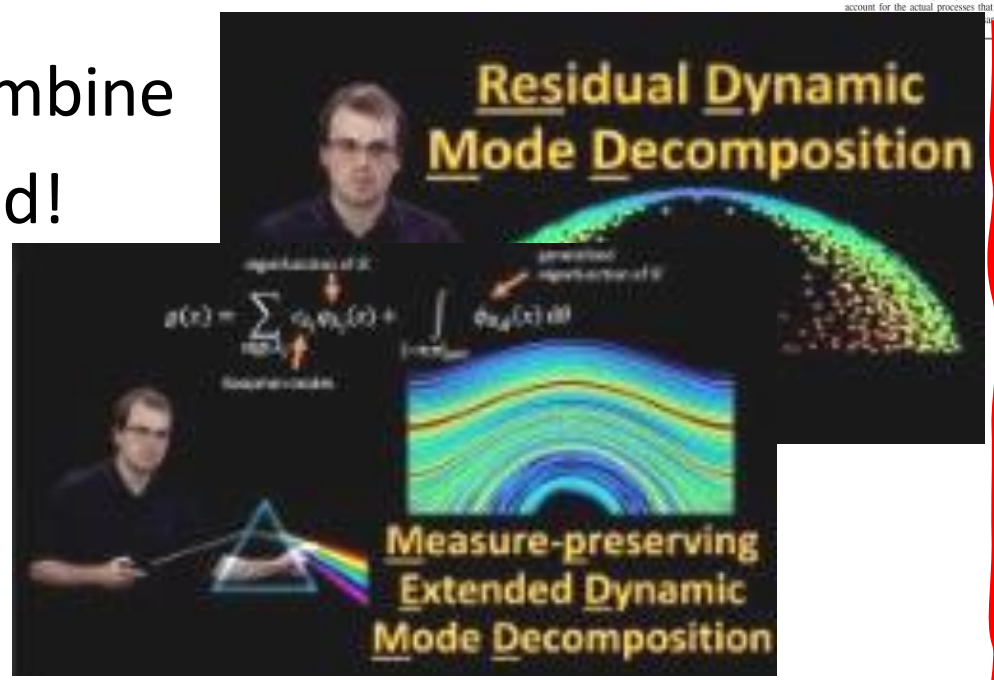
Figure 1. *Koopman modes of a turbulent flow (Reynolds number 3.9×10^3) past a cascade of airfoils that are computed from trajectory data (d = 300,000). Koopman modes are projections of the physical field onto eigenfunctions of $\mathcal{K}$; they provide the collective motion of the fluid that occurs at the same spatial frequency, growth, or decay rate according to an approximate eigenvalue λ. **1a.** Koopman modes that were computed via existing state-of-the-art techniques. Note the lack of error bounds. **1b.** Koopman modes that were computed using residual dynamic mode decomposition (ResDMD). The physical picture in 1b is different from 1a, but we know that it is correct because of the guaranteed relative error bounds (green text). This outcome illustrates the importance of verification. Figure courtesy of Matthew Colbrook.*

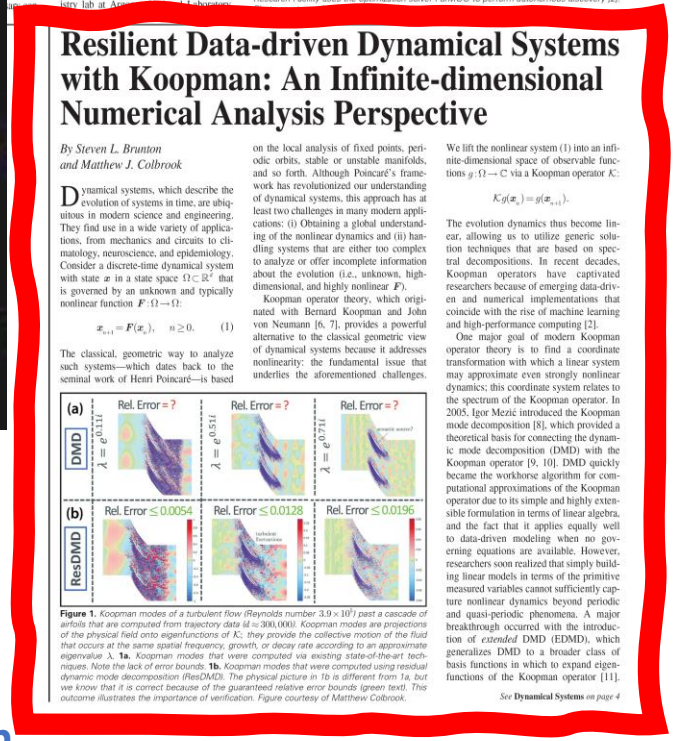
https://github.com/MColbrook/Measure-preserving-Extended-Dynamic-Mode-Decomposition

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!

Short video summaries available on YouTube



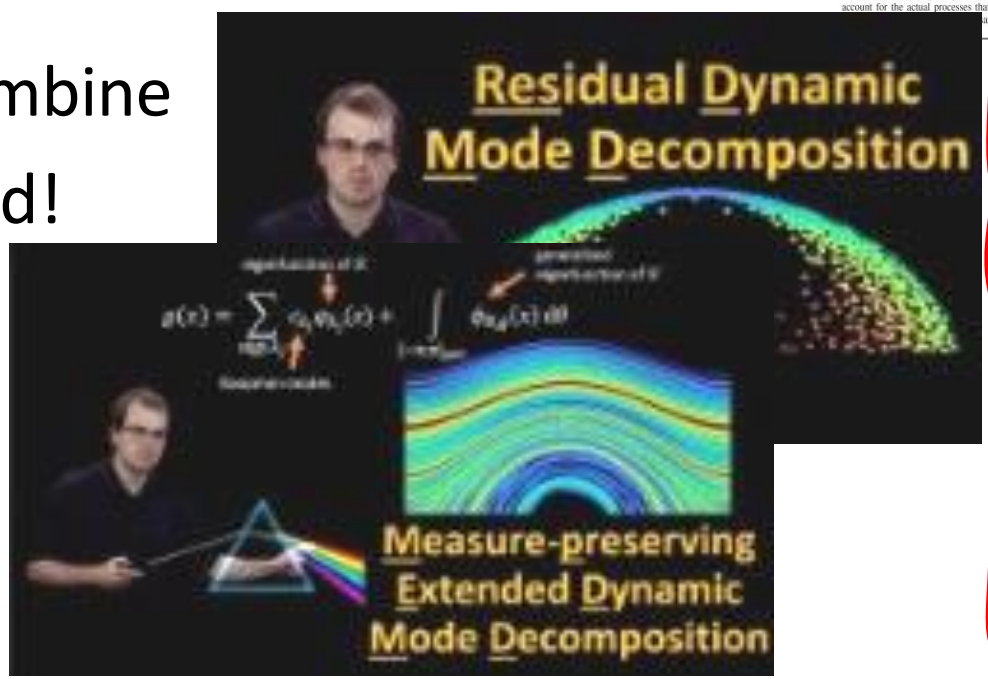


https://github.com/MColbrook/Measure-preserving-Extended-Dynamic-Mode-Decomposition

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!

Ongoing: Further structure preserving Koopman methods



Newsjournal of the Society for Industrial and Applied Mathematics sinews.siam.org

siam news

Volume 56/ Issue 1
January/February 2023

Optimization and Learning with Zeroth-order Stochastic Oracles

By Stefan M. Wild

Mathematical optimization is a foundational technology for machine learning and the solution of design, decision, and control problems. In most optimization applications, the principal assumption is the availability of at least the first-order derivatives of objective and constraint functions. This assumption is often nonrestrictive, since researchers can use techniques such as automatic differentiation and differentiable programming to obtain derivatives from the mathematical equations that underlie these functions. Derivative-free (or "zeroth-order") optimization addresses settings wherein such derivatives are not available [5].

Given the pervasiveness of sensors and other experimental and observational data, these types of settings are arising in increasingly more science and engineering domains. For example, consider the ongoing search for novel materials for energy storage. In order to create viable new materials, we must move beyond pure theory and account for the actual processes that occur

sequence is that material properties are only available via *in situ* and *in operando* characterization. In the context of optimization, this scenario is called a "zeroth-order oracle" — our knowledge about a particular system or property is data driven and limited by the black-box nature of measurement procurement. An additional challenge is that such measurements are subject to random variations, meaning that researchers are dealing with zeroth-order *stochastic* oracles.

We can compactly express this type of optimization problem as

$$\min_{x \in \mathbb{R}^n} \mathbb{E}_\xi \left[f(\mathbf{x}; \xi) \right],$$

where $\mathbf{x}$ denotes the vector of n decision variables and ξ is a random variable (e.g., a variable that is associated with the stochastic synthesis and measurement processes). The zeroth-order stochastic oracle is $f(\mathbf{x}; \xi)$. We can specify values for the random variable only in certain problem settings; in others—such as the laboratory environment in Figure 1—doing so is impossible.

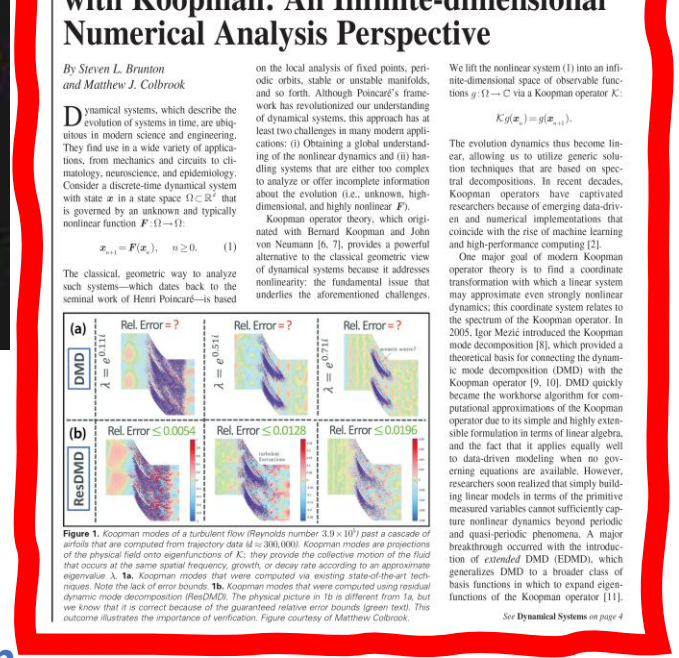
Figure 1 displays an instantiation of a data-driven optimization setting in a chemistry lab at Ar

An optimization solver specifies a particular composition of solvents and bases, an operating temperature, and reaction times; this combination is then run through a continuous flow reactor. The material that exits the reactor is then automatically characterized

See **Optimization** on page 3

through an inline nuclear magnetic resonance detector that illuminates properties of the synthesized materials. These stochastic, zeroth-order oracle outputs return to the solver in a closed-loop setting that

Figure 1. *A continuous flow reactor at Argonne National Laboratory's Materials Engineering Research Facility uses the optimization solver PariMOO to perform autonomous discovery [2].*



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 $\boldsymbol{x}$ in a state space $\Omega \subset \mathbb{R}^d$ that is governed by an unknown and typically nonlinear function $\boldsymbol{F}: \Omega \to \Omega$:

$$\boldsymbol{x}_{n+1} = \boldsymbol{F}(\boldsymbol{x}_n), \quad n \geq 0. \qquad (1)$$

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 fixed points, periodic orbits, stable or unstable manifolds, and so forth. Although Poincaré's framework has revolutionized our understanding of dynamical systems, this approach has at least two challenges in many modern applications: (i) Obtaining a global understanding of the nonlinear dynamics and (ii) handling systems that are either too complex to analyze or offer incomplete information about the evolution (i.e., unknown, high-dimensional, and highly nonlinear $\boldsymbol{F}$).

Koopman operator theory, which originated with Bernard Koopman and John von Neumann [6, 7], provides a powerful alternative to the classical geometric view of dynamical systems because it addresses nonlinearity: the fundamental issue that underlies the aforementioned challenges.

We lift the nonlinear system (1) into an infinite-dimensional space of observable functions $g: \Omega \to \mathbb{C}$ via a Koopman operator $\mathcal{K}$:

$$\mathcal{K}g(\boldsymbol{x}_n) = g(\boldsymbol{x}_{n+1}).$$

The evolution dynamics thus become linear, allowing us to utilize generic solution techniques that are based on spectral decompositions. In recent decades, Koopman operators have captivated researchers because of emerging data-driven and numerical implementations that coincide with the rise of machine learning and high-performance computing [2].

One major goal of modern Koopman operator theory is to find a coordinate transformation with which a linear system may approximate even strongly nonlinear dynamics; this coordinate system relates to the spectrum of the Koopman operator. In 2005, Igor Mezić introduced the Koopman mode decomposition [8], which provided a theoretical basis for connecting the dynamic mode decomposition (DMD) with the Koopman operator [9, 10]. DMD quickly became the workhorse algorithm for computational approximations of the Koopman operator due to its simple and highly extensible formulation in terms of linear algebra, and the fact that it applies equally well to data-driven modeling when no governing equations are available. However, researchers soon realized that simply building linear models in terms of the primitive measured variables cannot sufficiently capture nonlinear dynamics beyond periodic and quasi-periodic phenomena. A major breakthrough occurred with the introduction of *extended* DMD (EDMD), which generalizes DMD to a broader class of basis functions in which to expand eigenfunctions of the Koopman operator [11].

See **Dynamical Systems** on page 4

Figure 1. *Koopman modes of a turbulent flow (Reynolds number 3.9×10^3) past a cascade of airfoils that are computed from trajectory data (d = 300,000). Koopman modes are projections of the physical field onto eigenfunctions of $\mathcal{K}$; they provide the collective motion of the fluid that occurs at the same spatial frequency, growth, or decay rate according to an approximate eigenvalue λ.* **1a.** *Koopman modes that were computed via existing state-of-the-art techniques. Note the lack of error bounds.* **1b.** *Koopman modes that were computed using residual dynamic mode decomposition (ResDMD). The physical picture in 1b is different from 1a, but we know that it is correct because of the guaranteed relative error bounds (green text). This outcome illustrates the importance of verification. Figure courtesy of Matthew Colbrook.*

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

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."