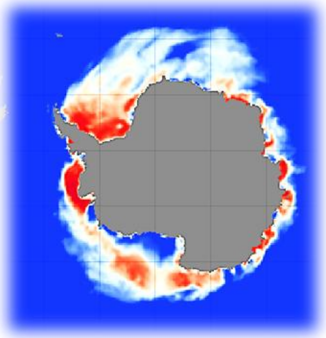

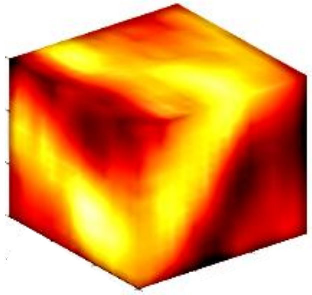

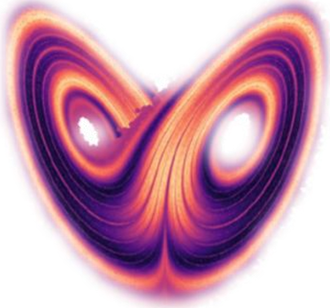

Data-Driven Spectra in Dynamical Systems

Matthew Colbrook

9th Dec 2025

UNIVERSITY OF CAMBRIDGE

"To <u>classify</u> is to bring order into chaos." - **George Pólya**

Cast of great collaborators!

Alex Townsend
(Cornell)

Igor Mezić
(UC Santa Barbara)

Alexei Stepanenko
(Cam. -> Industry)

Nicolas Boullé
(Imperial)

Gustav Conradie
(PhD student at Cambridge)

- C., Townsend. *"Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems."* **Communications on Pure and Applied Mathematics,** 2024.
- C., Mezić, Stepanenko*, "Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning."* (under revision at **Nature Communications**).
- Boullé, C., Conradie, *"Convergent Methods for Koopman Operators on Reproducing Kernel Hilbert Spaces."* (***SpecRKHS*** - **hot off the press: https://arxiv.org/abs/2506.15782**)

What is a Koopman operator?

- $\mathcal{X}$ – *the state space*
- $\mathcal{X} \ni x$ – *the state*

cts $F: \mathcal{X} \to \mathcal{X}$ – *the dynamics:* $x_{n+1} = F(x_n)$

Henri Poincaré
(Sorbonne)

• Poincaré, *''Les méthodes nouvelles de la mécanique céleste,''* **Vol. 2. Gauthier-Villars et fils, imprimeurs-libraires**, 1893.

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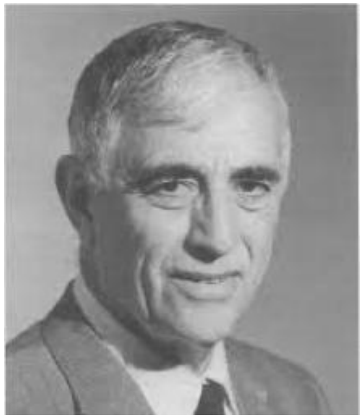
- Functions $g: \mathcal{X} \to \mathbb{C}$ a.k.a "observables"
- Koopman operator $\mathcal{K}_F$: $[\mathcal{K}_F g](x) = g(F(x))$

LINEAR!

Observe g one time step forward

Bernard Koopman
(Columbia)



John von Neumann
(IAS)

- 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.

What is a Koopman operator?

- $\mathcal{X}$ – *the state space*
- $\mathcal{X} \ni x$ – *the state*
- ***Unknown*** cts $F: \mathcal{X} \to \mathcal{X}$ – *the dynamics:* $x_{n+1} = F(x_n)$
- Functions $g: \mathcal{X} \to \mathbb{C}$ a.k.a "observables"
- Koopman operator $\mathcal{K}_F$: $[\mathcal{K}_F g](x) = g(F(x))$ LINEAR!
- ***Available*** snapshot data: $\left\{\left(x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right): m = 1, \dots, M\right\}$

Can we compute spectral properties from trajectory data?

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

Why?

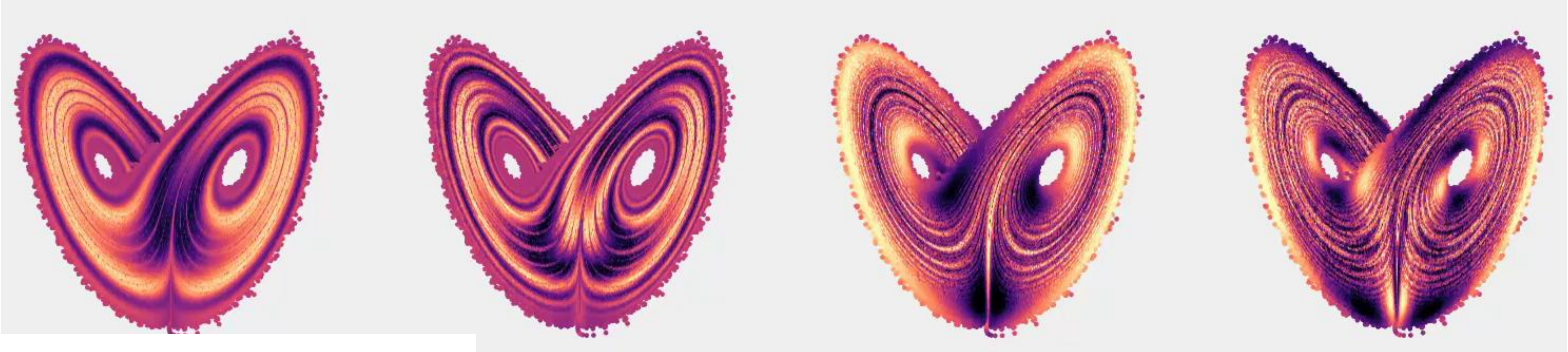
If $\|\mathcal{K}g - \lambda g\| \leq \varepsilon$, then $g(x_n) = [\mathcal{K}^n g](x_0) = \lambda^n g(x_0) + \mathcal{O}(n\varepsilon)$

Trades: Nonlinear, finite-dimensional $\Longrightarrow$ Linear, infinite-dimensional.

Why?

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

If $||\mathcal{K}g - \lambda g|| \leq \varepsilon$, then $g(x_n) = [\mathcal{K}^n g](x_0) = \lambda^n g(x_0) + \mathcal{O}(n\varepsilon)$



Coherent features!

Lorenz attractor

Trades: Nonlinear, finite-dimensional $\Longrightarrow$ Linear, infinite-dimensional.

Why?

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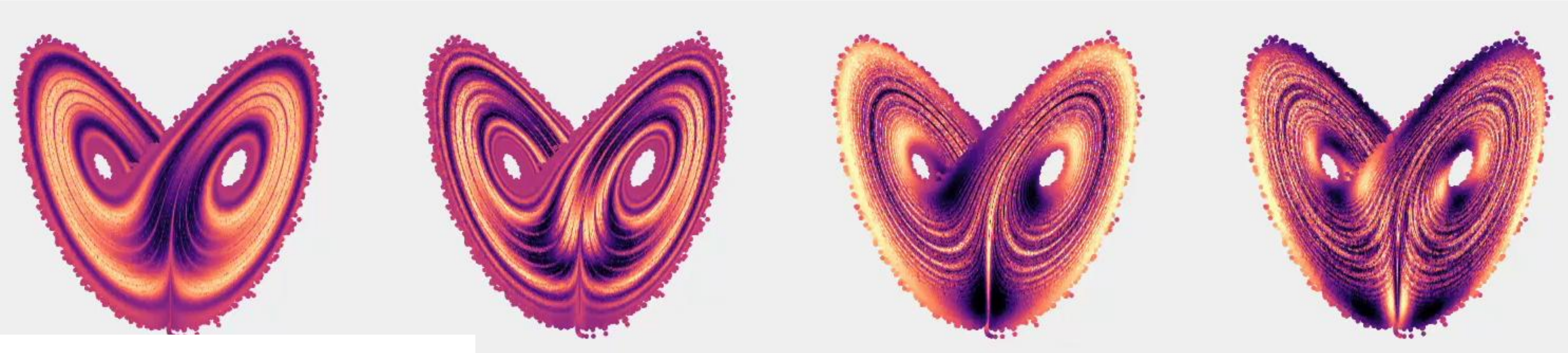
If $\|\mathcal{K}g - \lambda g\| \leq \varepsilon$, then $g(x_n) = [\mathcal{K}^n g](x_0) = \lambda^n g(x_0) + \mathcal{O}(n\varepsilon)$



Coherent features!

$$\mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}) = \{z \in \mathbb{C} : \exists g, \|g\| = 1, \|\mathcal{K}g - zg\| \leq \varepsilon\}$$

Trades: Nonlinear, finite-dimensional $\Longrightarrow$ Linear, infinite-dimensional.

Koopman Mode Decomposition

- Find (g_j, λ_j) with $\|\mathcal{K} g_j - \lambda_j g_j\| \leq \varepsilon$

Verified Eigenfunctions

- Expand state:

$$x \approx \sum_j c_j g_j(x)$$

coefficients, called "Koopman modes"

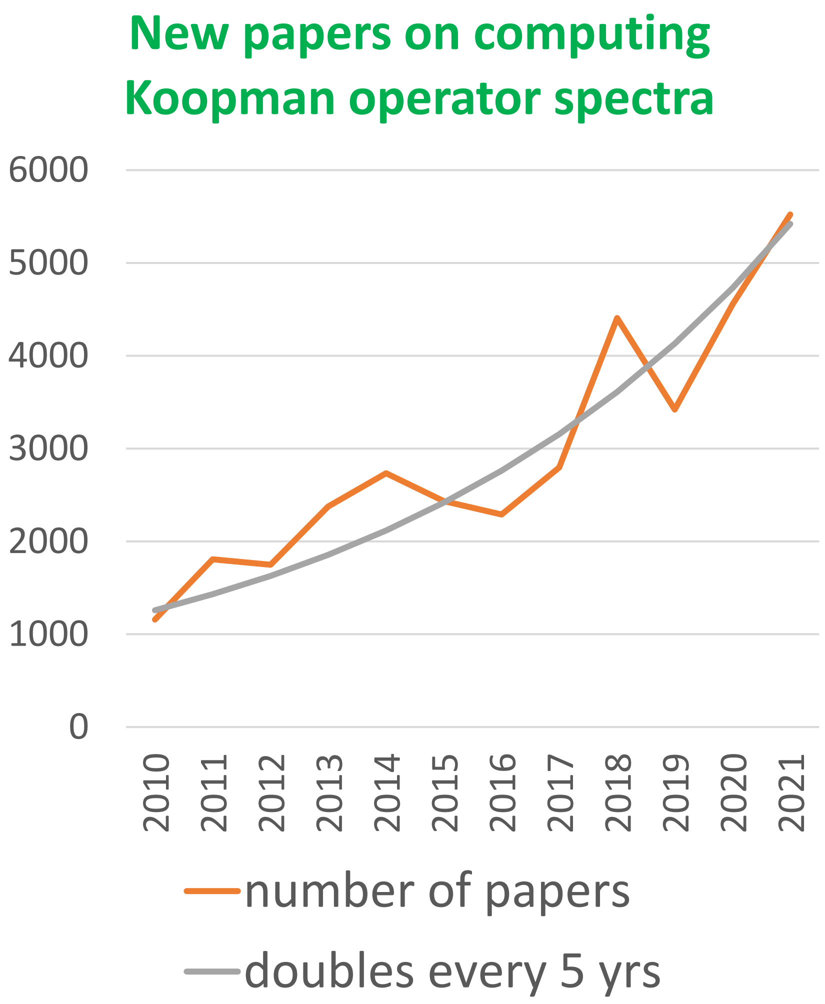
$$g(x_n) = [\mathcal{K}^n g](x_0)$$

- Forecasts:

$$x_n = \sum_j \lambda_j^n c_j g_j(x) + \mathcal{O}(n\varepsilon)$$

Intuition: A nonlinear separation of variables through a linear operator!

Koopmania*: A revolution in the big data era?



Very **little on convergence guarantees. *WHY?***

1. Koopman operators have been largely used in applied domains + distinct from NLA.

2. Infinite-dimensional spec. comp. notoriously hard …

Only recently have the tools been developed

GOAL: Compute spectral properties and figure out how hard this is.

The Standard (naïve?) Pipeline

DATA + DISCRETIZE $\mathcal{K}$

The Standard (naïve?) Pipeline

DATA + DISCRETIZE $\mathcal{K}$

FINITE-DIMENSIONAL NUMERICAL LINEAR ALGEBRA

The Standard (naïve?) Pipeline

DATA + DISCRETIZE $\mathcal{K}$

FINITE-DIMENSIONAL NUMERICAL LINEAR ALGEBRA

EIGENVALUES etc.

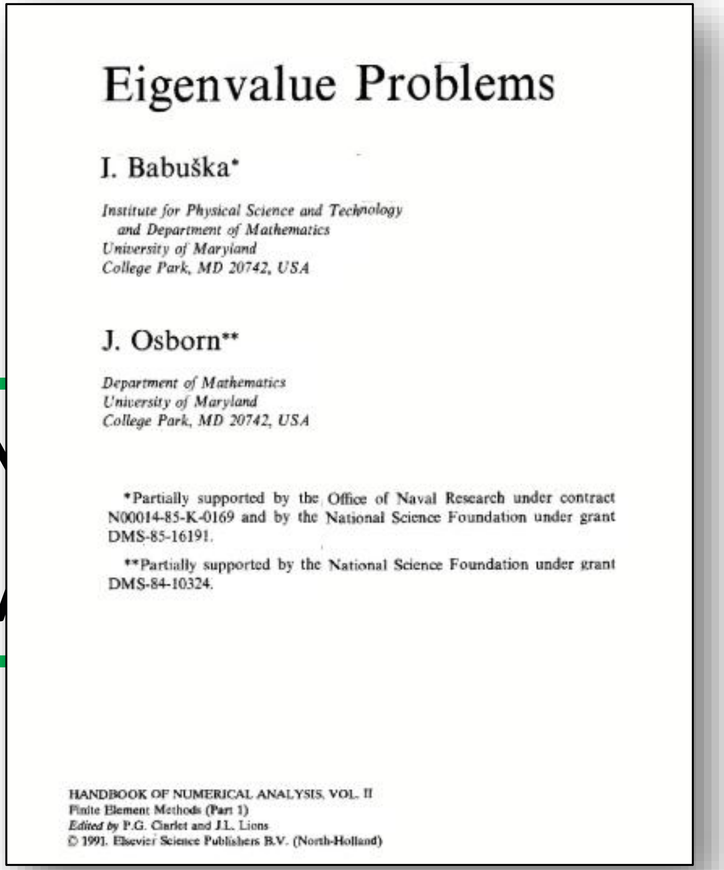
The Standard (naïve?) Pipeline

DATA + DISCRETIZE $\mathcal{K}$

FINITE-DIMEN
NUMERICAL LINE

EIGENVALUES etc.

Works great if you have a self-adjoint operator that is compact or has compact resolvent!


Eigenvalue Problems

J. Babuška*

Institute for Physical Science and Technology
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J. Osborn**

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College Park, MD 20742, USA

*Partially supported by the Office of Naval Research under contract N00014-85-K-0169 and by the National Science Foundation under grant DMS-85-16191.

**Partially supported by the National Science Foundation under grant DMS-84-10324.

HANDBOOK OF NUMERICAL ANALYSIS, VOL. II
Finite Element Methods (Part 1)
Edited by P.G. Ciarlet and J.L. Lions
© 1991, Elsevier Science Publishers B.V. (North-Holland)

The Standard (naïve?) Pipeline

DATA + DISCRETIZE $\mathcal{K}$

FINITE-DIMENSIONAL NUMERICAL LINEAR ALGEBRA

For Koopman?

EIGENVALUES etc.

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

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

Two-way infinite

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

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

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

Explicit example: Matrix approximation of $\mathcal{K}$ (EDMD)

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

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

quadrature points

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

quadrature weights

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

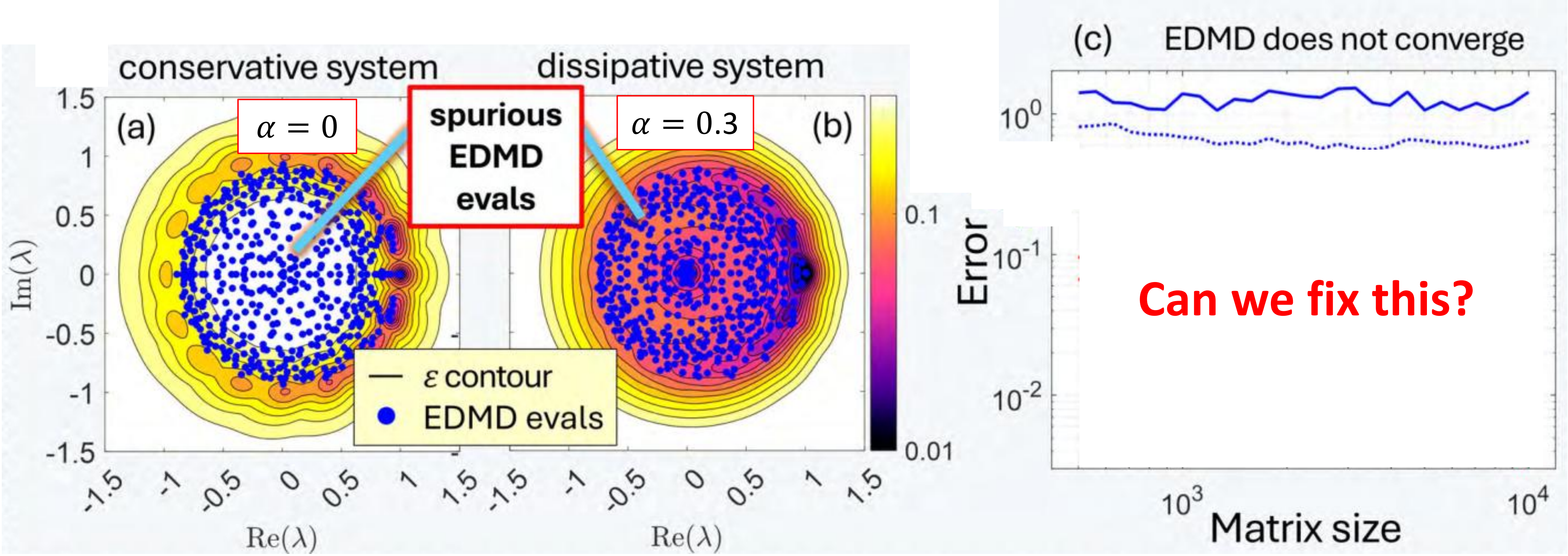
Galerkin Approximation

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

- 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.

EDMD doesn't converge!

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



The fix: Residual DMD (ResDMD)

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

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

- C., Townsend, "*Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*," **Commun. Pure Appl. Math.**, 2023.
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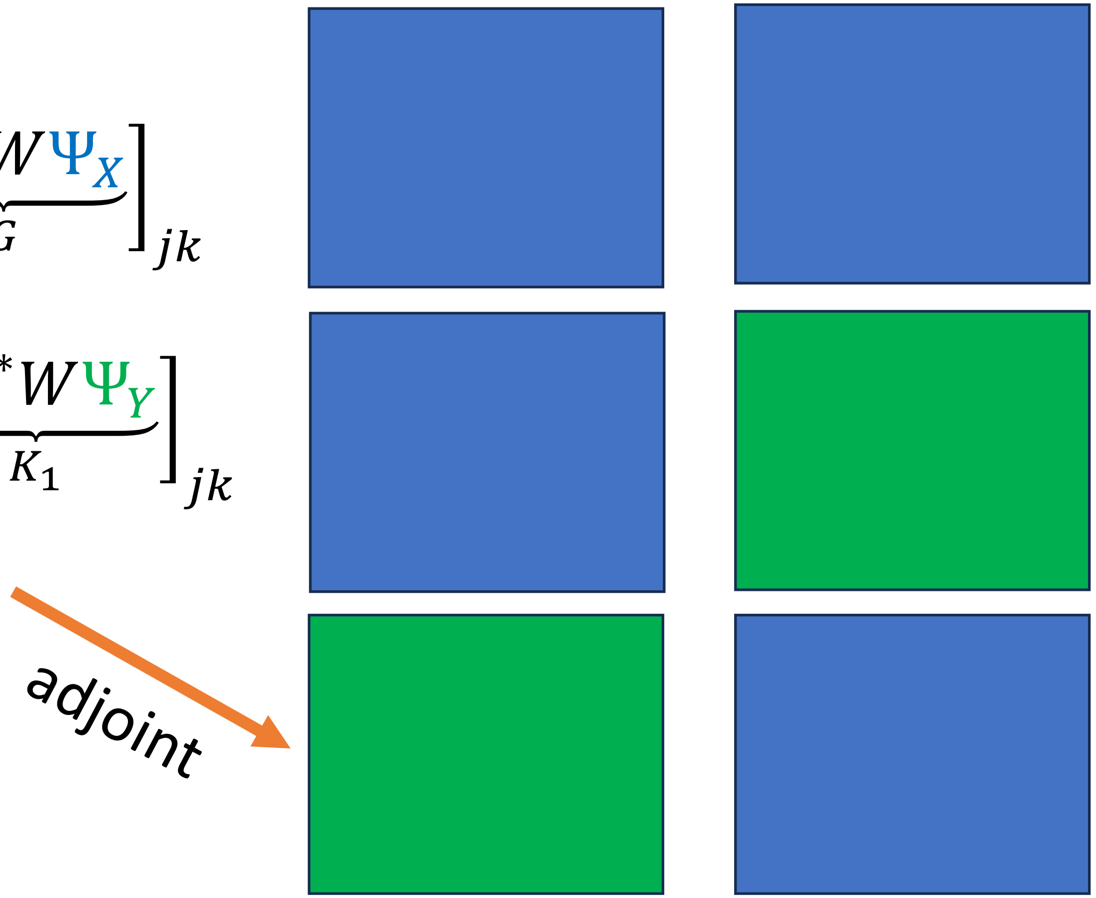

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Residuals: $g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j,\ \|\mathcal{K}g - \lambda g\|^2 = \langle \mathcal{K}g - \lambda g, \mathcal{K}g - \lambda g \rangle$

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

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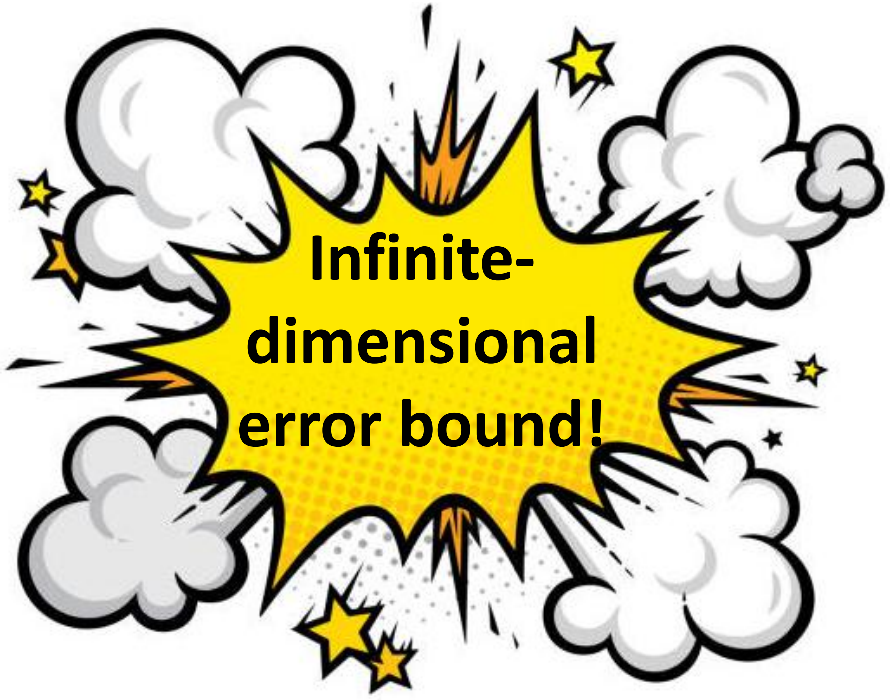

Residuals: $g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j$, $\|\mathcal{K}g - \lambda g\|^2 = \lim_{M\to\infty} \mathbf{g}^* [K_2 - \lambda K_1{}^* - \bar{\lambda} K_1 + |\lambda|^2 G] \mathbf{g}$

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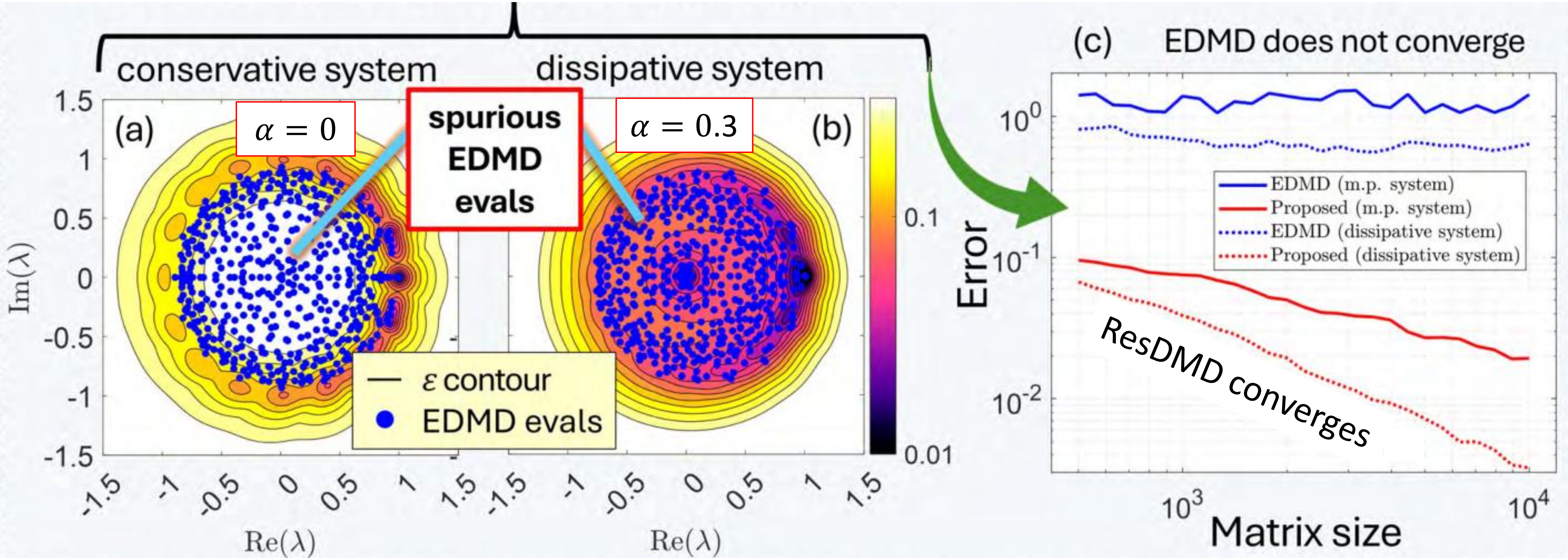
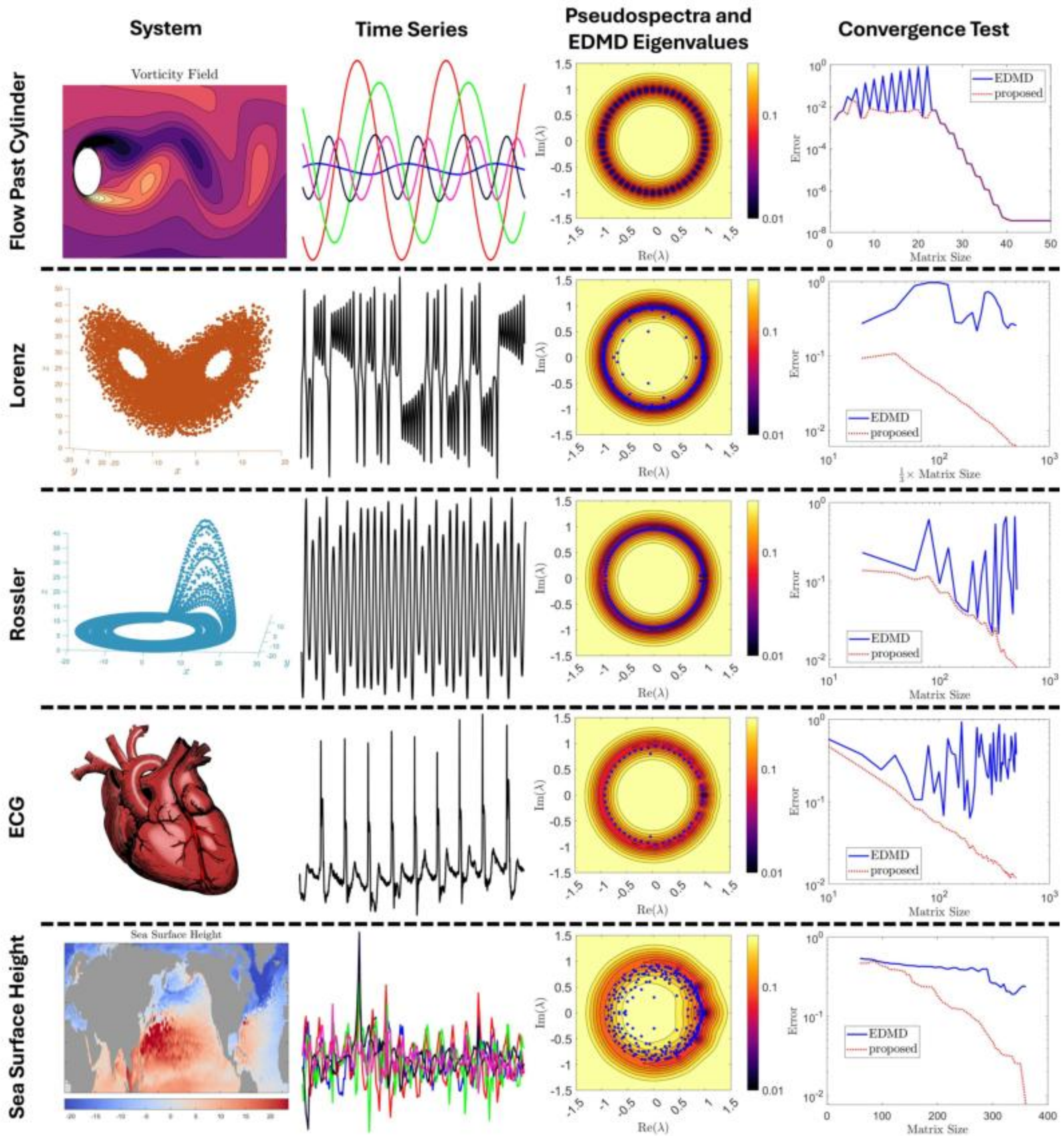
ResDMD does converge!

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

Compute $\mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K})$, local adaptive control on $\varepsilon \downarrow 0$




System
Time Series
Pseudospectra and EDMD Eigenvalues
Convergence Test
Flow Past Cylinder
Vorticity Field
Lorenz
Rossler
ECG
Sea Surface Height
Re(λ)
Im(λ)
Error
Matrix Size
EDMD
proposed

Can maths help guide the way?

Consider space of observables with finite energy: $L^2(\mathcal{X}, \omega)$

Theorem: There **exists** algorithms $\Gamma_{N,M}$ using snapshots such that

$$\lim_{N\to\infty}\lim_{M\to\infty}\Gamma_{N,M}(F) = \mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}_F)$$

for all systems.

N = size of basis, **M = amount of data (quadrature)**

$$\mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}) = \{z \in \mathbb{C} : \exists g, \|g\| = 1, \|\mathcal{K}g - zg\| \leq \varepsilon\}$$

- C., Mezić, Stepanenko, "Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning," **preprint**, 2025.

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N = **size of basis,** M = **amount of data (quadrature)**

Double limit $\lim_{N\to\infty}\lim_{M\to\infty}$ **Can we do better?**

- C., Mezić, Stepanenko, "Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning," **preprint**, 2025.

Adversaries: Double limit is necessary!

Implies $\mathcal{K}$ is unitary

Class of systems: $\Omega_{\mathbb{D}} = \{F: \overline{\mathbb{D}} \to \overline{\mathbb{D}} \mid F \text{ cts, measure preserving, invertible}\}.$

Data an algorithm can use: $\mathcal{T}_F = \{(x, y_m) \mid x \in \overline{\mathbb{D}}, \|F(x) - y_m\| \leq 2^{-m}\}.$

Theorem: There **does not exist** any sequence of deterministic algorithms $\{\Gamma_n\}$ using $\mathcal{T}_F$ such that $\lim_{n\to\infty} \Gamma_n(F) = \mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}_F)\ \forall F \in \Omega_{\mathbb{D}}$.

NB:

- n can index anything.
- Universal - any type of algorithm or computational model.
- Similarly, no random algorithms converging with probability $> 1/2$.

- C., Mezić, Stepanenko, "Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning," **preprint**, 2025.

Proof idea: Constructing an adversary

F_0: rotation by π, $\mathrm{Sp}(\mathcal{K}_{F_0}) = \{\pm 1\}$

Phase transition lemma: Let $X = \{x_1, \dots, x_N\}, Y = \{y_1, \dots, y_N\}$ be distinct points in annulus $\mathcal{A} = \{x \in \mathbb{D} | 0 < R < \|x\| < r < 1\}$ with $X \cap Y = \emptyset$. There exists a measure-preserving homeomorphism H such that H acts as the identity on $\mathbb{D} \backslash \mathcal{A}$ and $H(y_j) = F_0(H(x_j)), j = 1, \dots, N$.

Conjugacy of <u>data</u> ($x_j \to y_j$) with F_0

Idea: Use lemma to trick any algorithm into oscillating between spectra.

- Brown and Halperin. "*On certain area-preserving maps.*" **Annals of Mathematics**, 1935.

Proof idea: Constructing an adversary

Suppose (for contradiction) $\{\Gamma_n\}$ uses $\mathcal{T}_F$, $\lim_{n\to\infty}\Gamma_n(F) = \mathrm{Sp}(\mathcal{K}_F)\ \ \forall F \in \Omega_{\mathbb{D}}$.

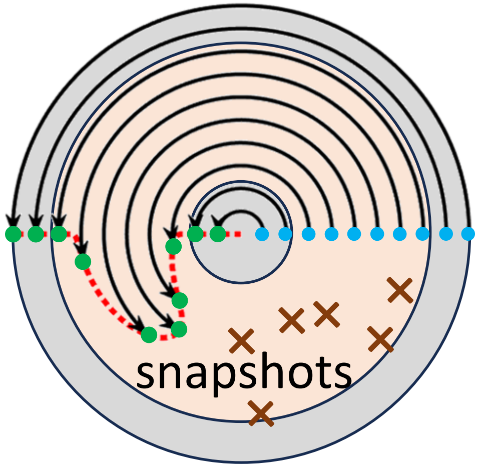
Build an adversarial F…

$\mathcal{T}_F = \{(x, y_m) \mid \|F(x) - y_m\| \leq 2^{-m}\}$

Proof idea: Constructing an adversary

Suppose (for contradiction) $\{\Gamma_n\}$ uses $\mathcal{J}_F$, $\lim_{n\to\infty}\Gamma_n(F) = \mathrm{Sp}(\mathcal{K}_F)\ \ \forall F \in \Omega_{\mathbb{D}}$.

Build an adversarial F…



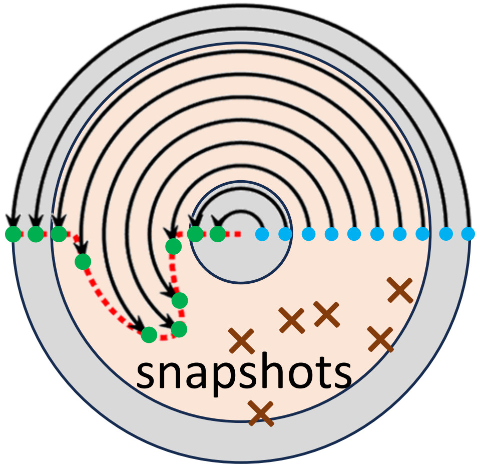
$\widetilde{F_1}(r,\theta) = \big(r, \theta + \pi + \phi(r)\big)$, $\mathrm{supp}(\phi) \subset [1/4, 3/4]$
$\mathrm{Sp}(\mathcal{K}_{\widetilde{F_1}}) = \mathbb{T}$ (unit circle).

$\mathcal{J}_F = \{(x, y_m) \mid \|F(x) - y_m\| \le 2^{-m}\}$

Proof idea: Constructing an adversary

Suppose (for contradiction) $\{\Gamma_n\}$ uses $\mathcal{T}_F$, $\lim_{n\to\infty} \Gamma_n(F) = \mathrm{Sp}(\mathcal{K}_F)\ \ \forall F \in \Omega_{\mathbb{D}}$.

Build an adversarial F...



$\widetilde{F_1}(r,\theta) = \big(r, \theta + \pi + \phi(r)\big)$, supp$(\phi) \subset [1/4, 3/4]$
$\mathrm{Sp}(\mathcal{K}_{\widetilde{F_1}}) = \mathbb{T}$ (unit circle).

$\lim_{n\to\infty} \Gamma_n(\widetilde{F_1}) = \mathrm{Sp}(\mathcal{K}_{\widetilde{F_1}}) \Rightarrow \exists n_1$ s.t. $\mathrm{dist}(i, \Gamma_{n_1}(\widetilde{F_1})) \le 1$.
BUT Γ_{n_1} uses finite amount of info to output $\Gamma_{n_1}(\widetilde{F_1})$.
Let X, Y correspond to these snapshots.

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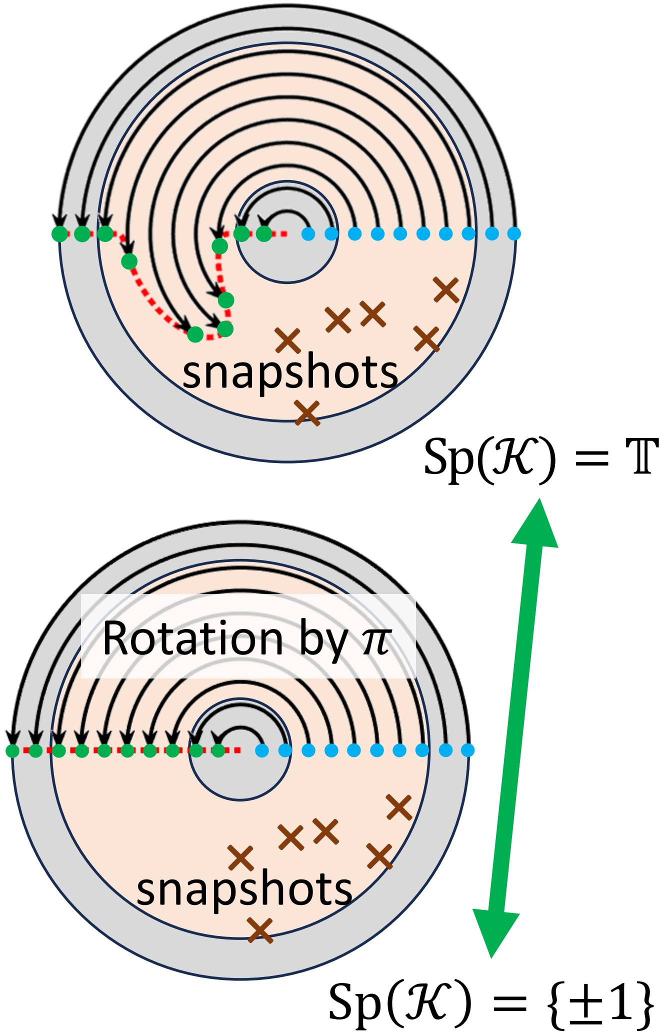
Let X, Y correspond to these snapshots.

Lemma: $F_1 = H_1^{-1} \circ F_0 \circ H_1$ on annulus $\mathcal{A}_1$.
Consistent data $\Rightarrow \Gamma_{n_1}(F_1) = \Gamma_{n_1}\big(\widetilde{F_1}\big)$, $\mathrm{dist}(i, \Gamma_{n_1}(F_1)) \leq 1$
BUT $\mathrm{Sp}(\mathcal{K}_{F_1}) = \mathrm{Sp}(\mathcal{K}_{F_0}) = \{\pm 1\}$



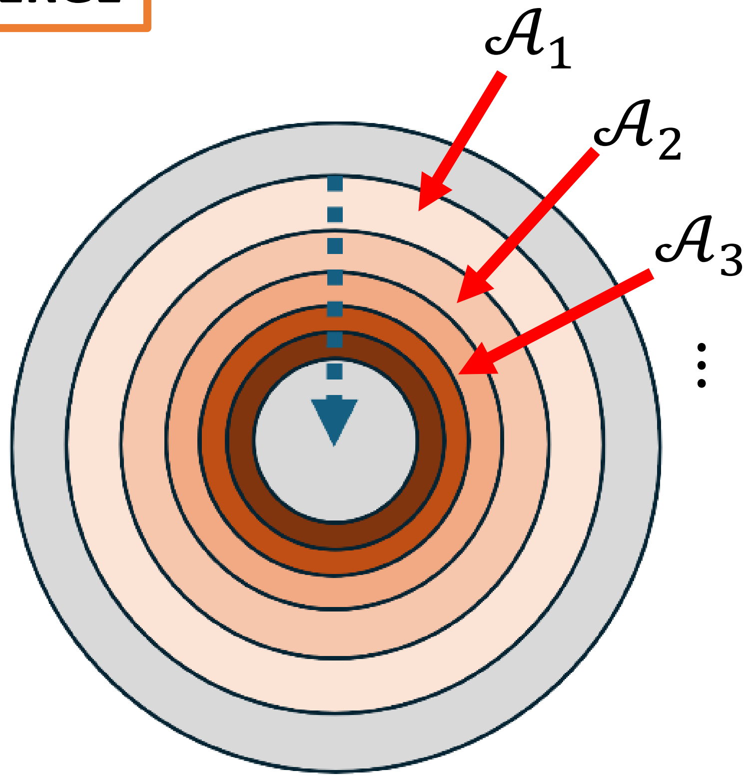
Proof idea: Constructing an adversary

Inductive step: Repeat on annuli, $F_k = H_k^{-1} \circ F_0 \circ H_k$ on $\mathcal{A}_k$. $F = \lim_{k\to\infty} F_k$

Consistent data $\Rightarrow \Gamma_{n_k}(F) = \Gamma_{n_k}(\widetilde{F_k})$, $\mathrm{dist}(i, \Gamma_{n_k}(F)) \leq 1$, $n_k \to \infty$

BUT $\mathrm{Sp}(\mathcal{K}_F) = \mathrm{Sp}(\mathcal{K}_{F_0}) = \{\pm 1\}$

CANNOT CONVERGE



Cascade of disks

Proof idea: Constructing an adversary

Inductive step: Repeat on annuli, $F_k = H_k^{-1} \circ F_0 \circ H_k$ on $\mathcal{A}_k$. $F = \lim_{k\to\infty} F_k$

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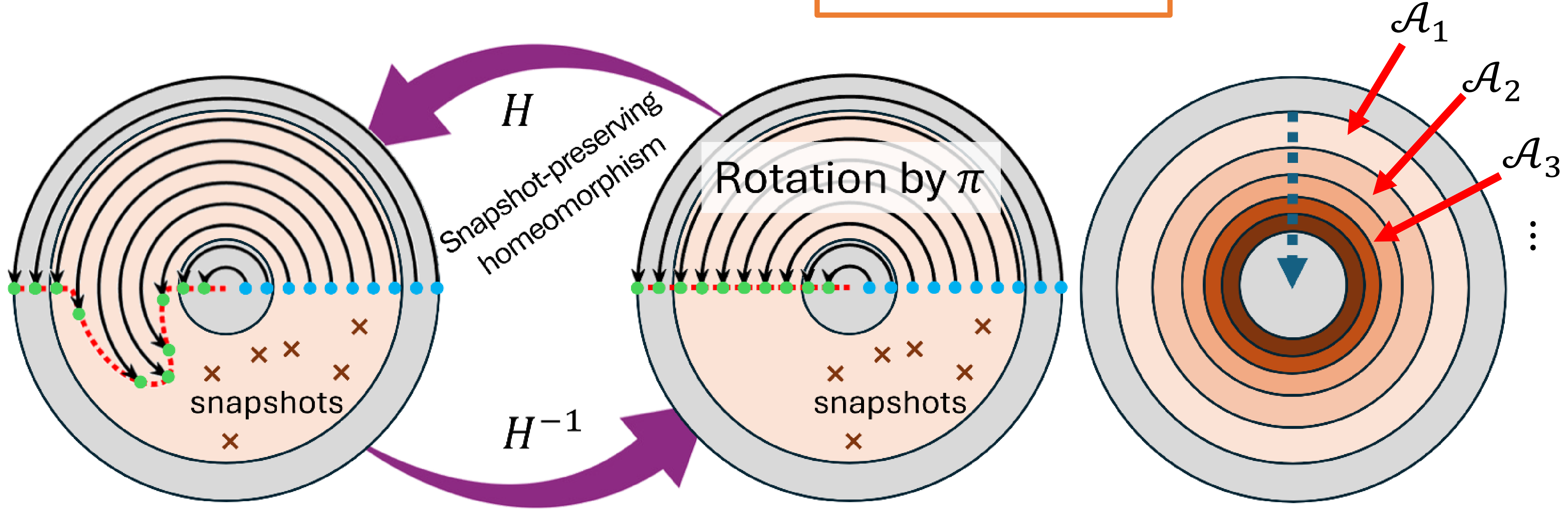
CANNOT CONVERGE



$\mathrm{Sp}(\mathcal{K}) = \{z : |z| = 1\}$ ⟷ $\mathrm{Sp}(\mathcal{K}) = \{\pm 1\}$ Cascade of disks

Classifications: *Solvability Complexity Index (SCI)*

SCI: Fewest number of limits needed to solve a computational problem.

- Δ_1: One limit, full error control. E.g., $d(\Gamma_n(F), \mathrm{Sp}(\mathcal{K}_F)) \leq 2^{-n}$.
- Δ_{m+1}: SCI $\leq m$.
- Σ_m: SCI $\leq m$, final limit from below.

$$\text{E.g., } \Sigma_1: \sup_{z\in\Gamma_n(F)} \mathrm{dist}(z, \mathrm{Sp}(\mathcal{K}_F)) \leq 2^{-n}.$$

- Π_m: SCI $\leq m$, final limit from above.

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- Hansen, “On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators.” **J. Am. Math. Soc.**, 2011.
- C., “*The foundations of infinite-dimensional spectral computations,*” **PhD diss.**, University of Cambridge, 2020.
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trust output

verification

covers spectrum

- Hansen, "On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators." **J. Am. Math. Soc.**, 2011.
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Lots of SCI upper bounds lurking in Koopman literature!

SCI: Fewest number of limits needed to solve a computational problem.

Algorithm	Comments/Assumptions	Spectral Problem's Corresponding SCI Upper Bound			
		KMD	*Spectrum*	*Spectral Measure (if m.p.)*	*Spectral Type (if m.p.)*
Extended DMD [47]	general L^2 spaces	SCI $\leq 2^*$	N/C	N/C	n/a
Residual DMD [44]	general L^2 spaces	SCI $\leq 2^*$	SCI $\leq 3^*$	SCI $\leq 2^*$	varies, see [84] e.g., a.c. density: SCI $\leq 2^*$
Measure-preserving EDMD [45]	m.p. systems	SCI ≤ 1	N/C	SCI $\leq 2^*$ (general) SCI ≤ 1 (delay-embedding)	n/a
Hankel DMD [85]	m.p. ergodic systems	SCI $\leq 2^*$	N/C	N/C	n/a
Periodic approximations [86]	m.p. + ω a.c.	SCI ≤ 2	N/C	SCI ≤ 2 (see [87])	a.c. density: SCI ≤ 3
Christoffel–Darboux kernel [40]	m.p. ergodic systems	SCI ≤ 3	n/a	SCI ≤ 2	e.g., a.c. density: SCI ≤ 2
Generator EDMD [88]	cts.-time, samples ∇F (otherwise additional limit)	SCI ≤ 2	N/C	SCI ≤ 2 (see [89])	n/a
Compactification [42]	cts.-time, m.p. ergodic systems	SCI ≤ 4	N/C	SCI ≤ 4	n/a
Resolvent compactification [43]	cts.-time, m.p. ergodic systems	SCI ≤ 5	N/C	SCI ≤ 5	n/a
Diffusion maps [90] (see also [10])	cts.-time, m.p. ergodic systems	SCI ≤ 3	n/a	n/a	n/a

Are these sharp?

Previous techniques prove upper bounds on SCI.

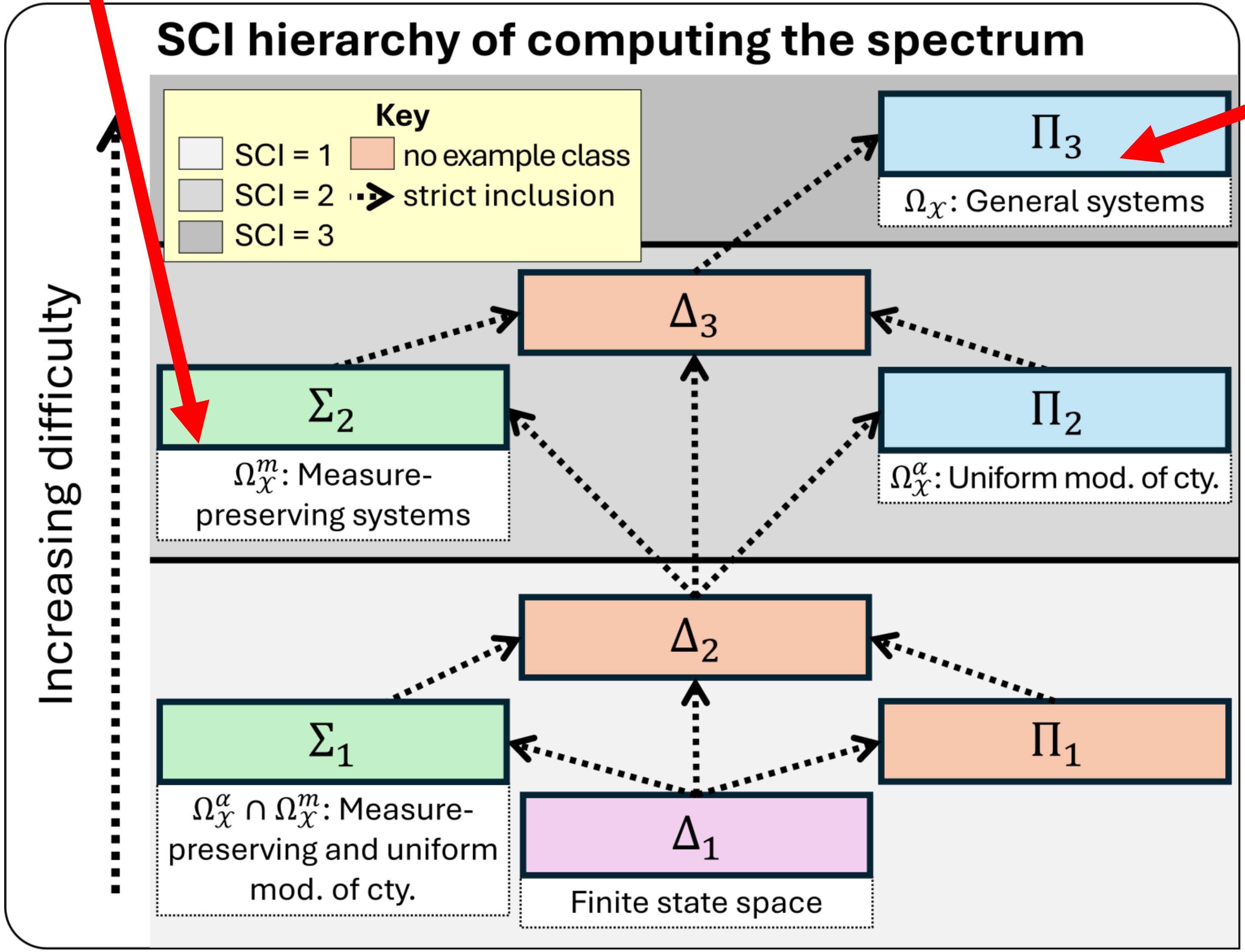
"N/C": method need not converge. "n/a": algorithm not applicable to problem.

Also in Ulam's method for Markov processes, SRB measure computation, control,…

Lower + upper bounds

Classification for Koopman

3 limits needed in general!



Different classes:

$\Omega_{\mathcal{X}} = \{F: \mathcal{X} \to \mathcal{X} \mid F \text{ cts}\}$

$\Omega_{\mathcal{X}}^m = \{F: \mathcal{X} \to \mathcal{X} \mid F \text{ cts, m. p.}\}$

$\Omega_{\mathcal{X}}^\alpha = \{F: \mathcal{X} \to \mathcal{X} \mid F \text{ mod. cty. } \alpha\}$

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

Optimal algorithms and classifications of dynamical systems.

- C., Mezić, Stepanenko, "Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning," **preprint**, 2025.

Peter Lax:

"The trick of the successful mathematician is to turn the question being asked into one he knows how to answer."

Johann Wolfgang von Goethe:

"Mathematicians are like Frenchmen: whatever you say to them they translate into their own language and forthwith it is something entirely different."

Let's perform this trick by changing the space…

Reproducing kernel Hilbert space (RKHS)

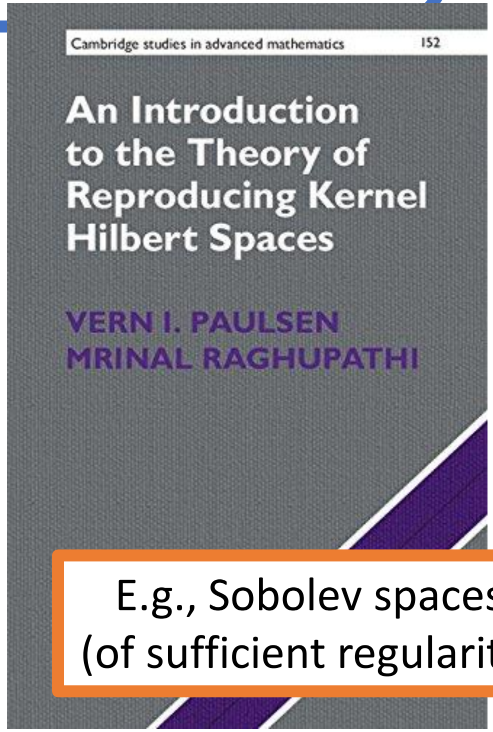
Hilbert space of functions on $\mathcal{X}$ s.t. $g \mapsto g(x)$ bounded $\forall x \in \mathcal{X}$.

Generated by a kernel $\mathfrak{K}: \mathcal{X} \times \mathcal{X} \to \mathbb{C}$

$$g(x) = \langle g, \mathfrak{K}_x \rangle, \qquad \mathfrak{K}(x, y) = \langle \mathfrak{K}_x, \mathfrak{K}_y \rangle = \mathfrak{K}_x(y)$$

Advantages over $L^2(\mathcal{X}, \omega)$:

- Forecasts: space bounds ⇒ pointwise bounds.
- High-dimensional systems practical through kernel trick.
- Fast methods for evaluating $\mathfrak{K}$.
- Different $\mathfrak{K}$ ⇒ different $\mathcal{K}$! Can be tailored to application. (This is where the community is currently heading.)
- Leads to fundamental "possibility" gains…



E.g., Sobolev spaces (of sufficient regularity)

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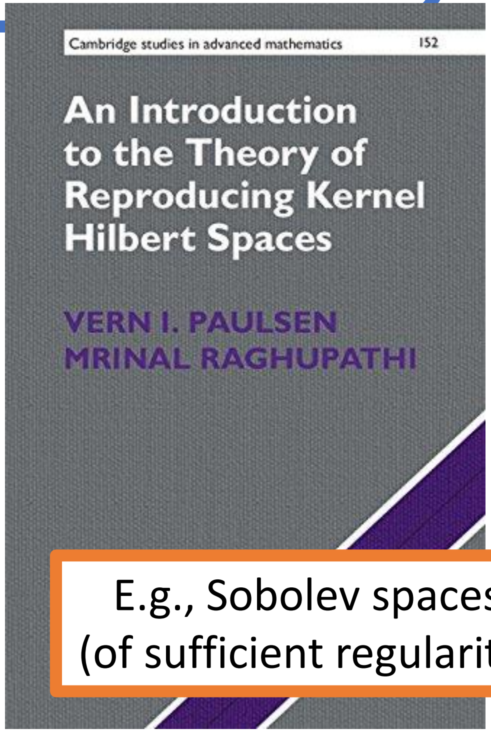


E.g., Sobolev spaces (of sufficient regularity)

SpecRKHS: Avoiding large data limit $M \to \infty$

Look at "Left eigenpairs" through $\mathcal{K}^*$: $\mathcal{K}^*\mathfrak{K}_x = \mathfrak{K}_{F(x)}$

Evolution of functionals. $g(x) = \langle g, \mathfrak{K}_x \rangle_{\mathcal{H}}$

No quadrature needed:

$$G_{jk} = \langle \mathfrak{K}_{x^{(k)}}, \mathfrak{K}_{x^{(j)}} \rangle = \mathfrak{K}(x^{(k)}, x^{(j)})$$

$$A_{jk} = \langle \mathcal{K}^*\mathfrak{K}_{x^{(k)}}, \mathfrak{K}_{x^{(j)}} \rangle = \left\langle \mathfrak{K}_{y^{(k)}}, \mathfrak{K}_{x^{(j)}} \right\rangle = \mathfrak{K}(y^{(k)}, x^{(j)})$$

$$R_{jk} = \langle \mathcal{K}^*\mathfrak{K}_{x^{(k)}}, \mathcal{K}^*\mathfrak{K}_{x^{(j)}} \rangle = \left\langle \mathfrak{K}_{y^{(k)}}, \mathfrak{K}_{y^{(j)}} \right\rangle = \mathfrak{K}(y^{(k)}, y^{(j)})$$

$$g = \sum_{m=1}^{M} \mathbf{g}_m \mathfrak{K}_{x^{(m)}}, \qquad \|\mathcal{K}^* g - \lambda g\|_{\mathcal{H}}^2 = \mathbf{g}^*(R - \lambda A^* - \bar{\lambda} A + G)\mathbf{g}$$

- Boullé, C., Conradie, *"Convergent Methods for Koopman Operators on Reproducing Kernel Hilbert Spaces,"* **preprint**, 2025.

SpecRKHS: Example algorithm

$$\text{res}^*(\lambda, \mathbf{g})^2 = \frac{\|\mathcal{K}^* g - \lambda g\|_{\mathcal{H}}^2}{\|g\|_{\mathcal{H}}^2} = \frac{\mathbf{g}^*\left[R - \lambda A^* - \bar{\lambda} A + G\right]\mathbf{g}}{\mathbf{g}^* G \mathbf{g}}$$

1. Compute $G, A, R \in \mathbb{C}^{N\times N}$ $(N = M)$
2. For z_k in grid, compute $\tau_k = \min_{g=\sum_{m=1}^{N} \mathbf{g}_m \mathfrak{K}_{x^{(m)}},} \text{res}^*(z_k, \mathbf{g})$, corresponding g_k (gen. SVD).
3. **Output:** $\{z_k : \tau_k < \varepsilon\}$, $\{g_k : \tau_k < \varepsilon\}$ (ε-pseudoeigenfunctions).

First convergent method for general $\mathcal{K}$

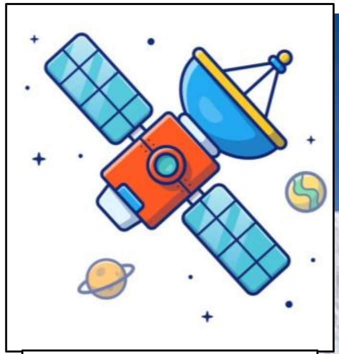
Theorem:

- **Error control:** $\{z_k : \tau_k < \varepsilon\} \subseteq \text{Sp}_{\text{ap},\varepsilon}(\mathcal{K}^*)$
- **Convergence:** Converges locally uniformly to $\text{Sp}_{\text{ap},\varepsilon}(\mathcal{K}^*)$ (as $N \to \infty$)

$$\text{Sp}_{\text{ap},\varepsilon}(\mathcal{K}^*) = \{z \in \mathbb{C} : \exists g, \|g\|_{\mathcal{H}} = 1, \|\mathcal{K}^* g - z g\|_{\mathcal{H}} \leq \varepsilon\}$$

- Boullé, C., Conradie, *"Convergent Methods for Koopman Operators on Reproducing Kernel Hilbert Spaces,"* **preprint**, 2025.

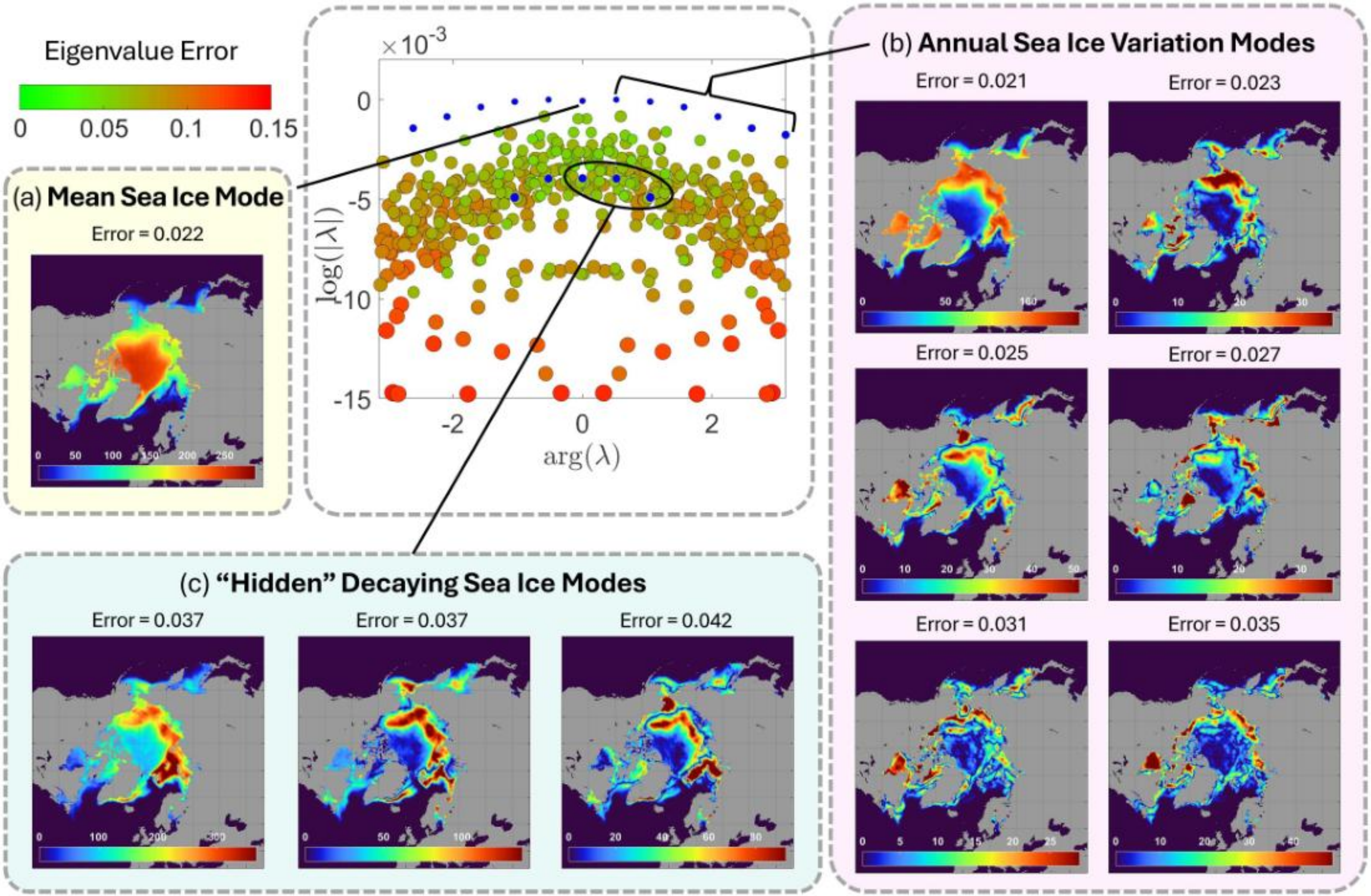
Practical gains: Sea ice forecasting



Satellite data

Motivation: Arctic amplification, polar bears, local communities, effect on extreme weather in Northern hemisphere,…

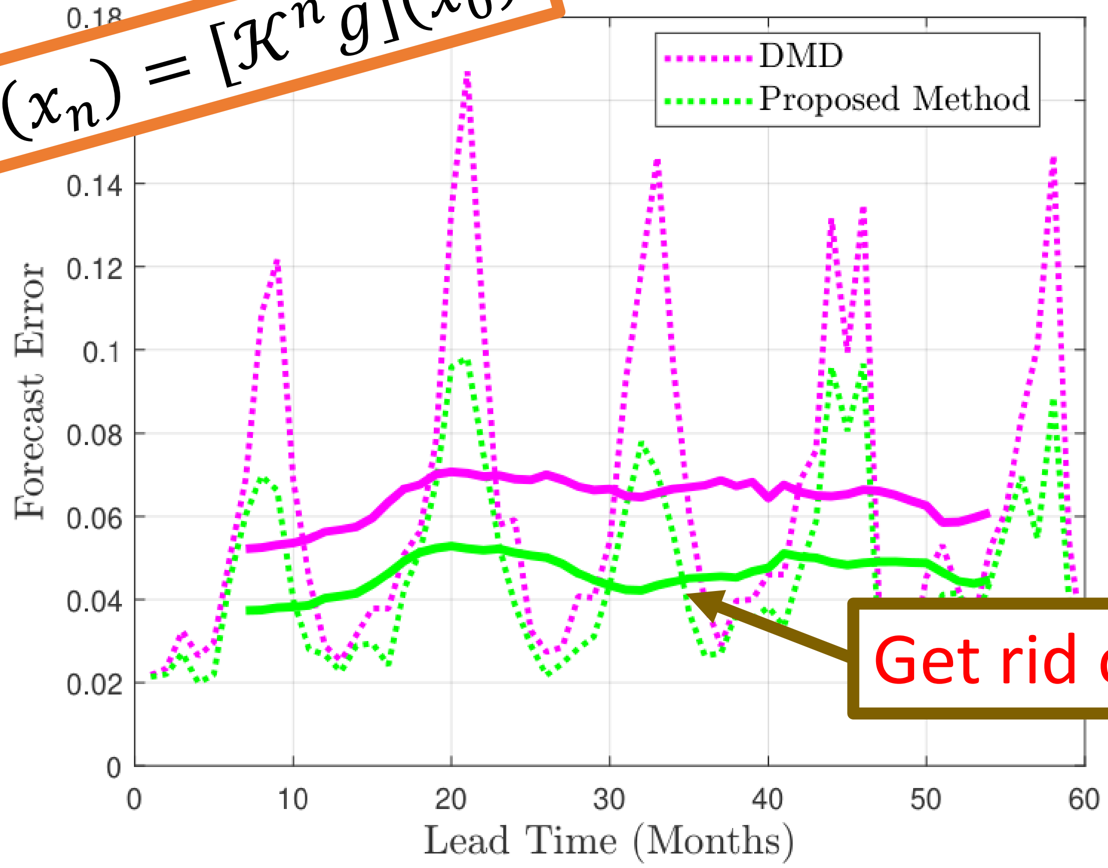
Problems: 1. Very hard to locate geographical significant regions.
2. Very hard to predict more than two months in advance.



- C., Mezić, Stepanenko, "Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning," **preprint**, 2025.

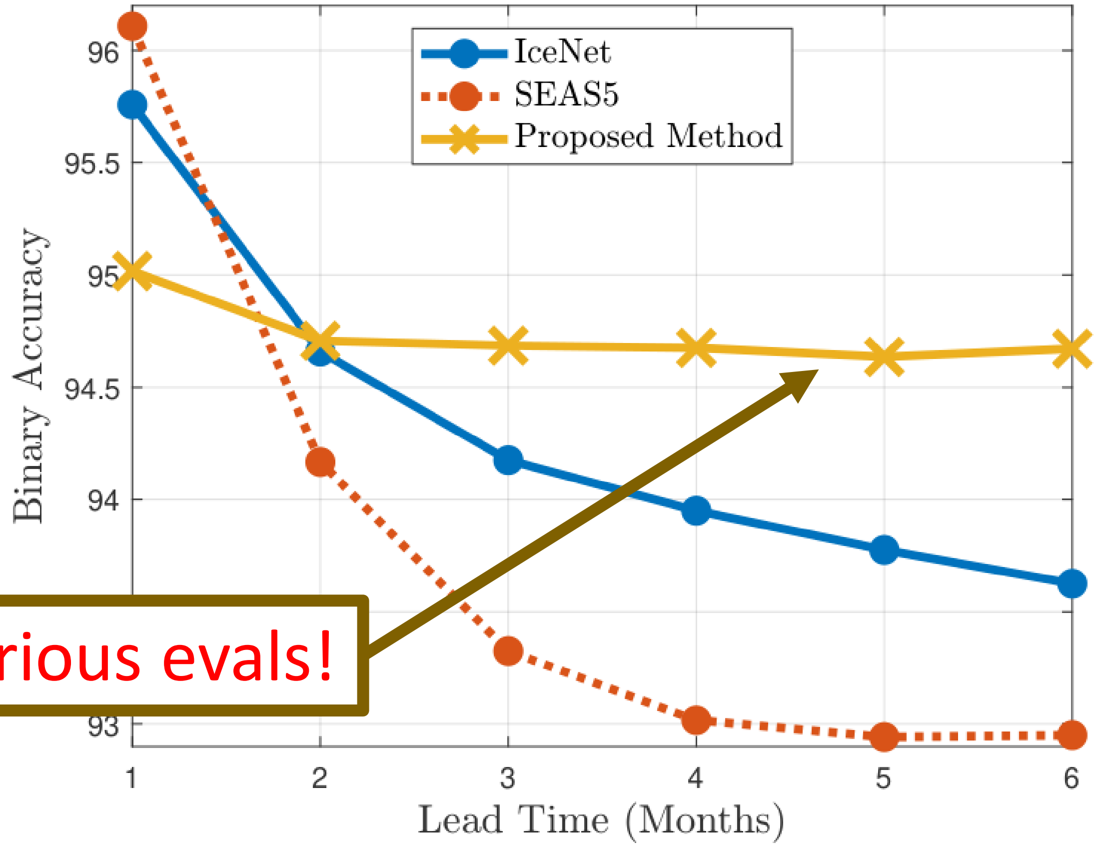
Avoid spurious evals ⇒ State-of-the-art forecasts

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



Relative mean squared error over 2016-2020. Model built from 2005-2015 data. (Solid lines moving 12-month mean.)

Get rid of spurious evals!



Mean binary accuracy over test years 2012-2020. *(IceNet: Andersson et al, "Seasonal Arctic sea ice forecasting with probabilistic deep learning." Nature Communications, 2021.)*

- C., Mezić, Stepanenko, "Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning," **preprint**, 2025.

Optimal algorithms and classifications of systems

increasing difficulty →

Error control | **1 limit** | **2 limits** | **3 limits**

$$\Pi_1 \qquad \Pi_2 \qquad \Pi_3$$

$$\Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

$$\Sigma_1 \qquad \Sigma_2 \qquad \Sigma_3$$

Optimal algorithms and classifications of systems

$\varepsilon = 0$

increasing difficulty

Error control | **1 limit** | **2 limits** | **3 limits**

$L^2(\mathcal{X},\omega)$

$\Omega_{\mathcal{X}}^{\alpha} = \{F: \mathrm{mod.\,cty.}\,\alpha\}$
$d(F(x),F(y)) \leq \alpha(d(x,y))$

$\Omega_{\mathcal{X}}^{m} = \{F : F\ \mathrm{cts,\,m.\,p.}\}$

$\Omega_{\mathcal{X}} = \{F: F\ \mathrm{cts}\}$

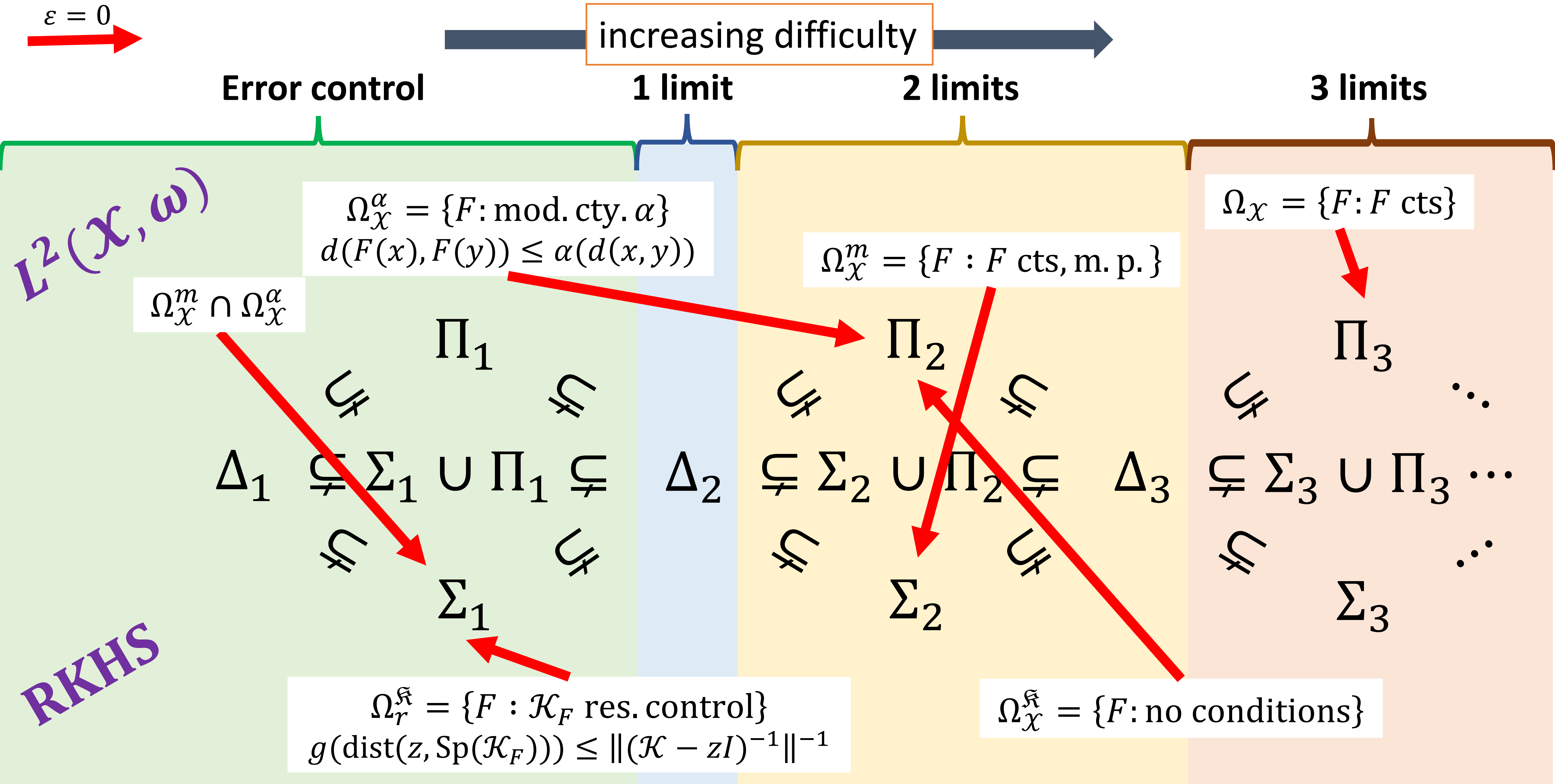
$\Omega_{\mathcal{X}}^{m} \cap \Omega_{\mathcal{X}}^{\alpha}$

$\Pi_1 \quad \Pi_2 \quad \Pi_3$

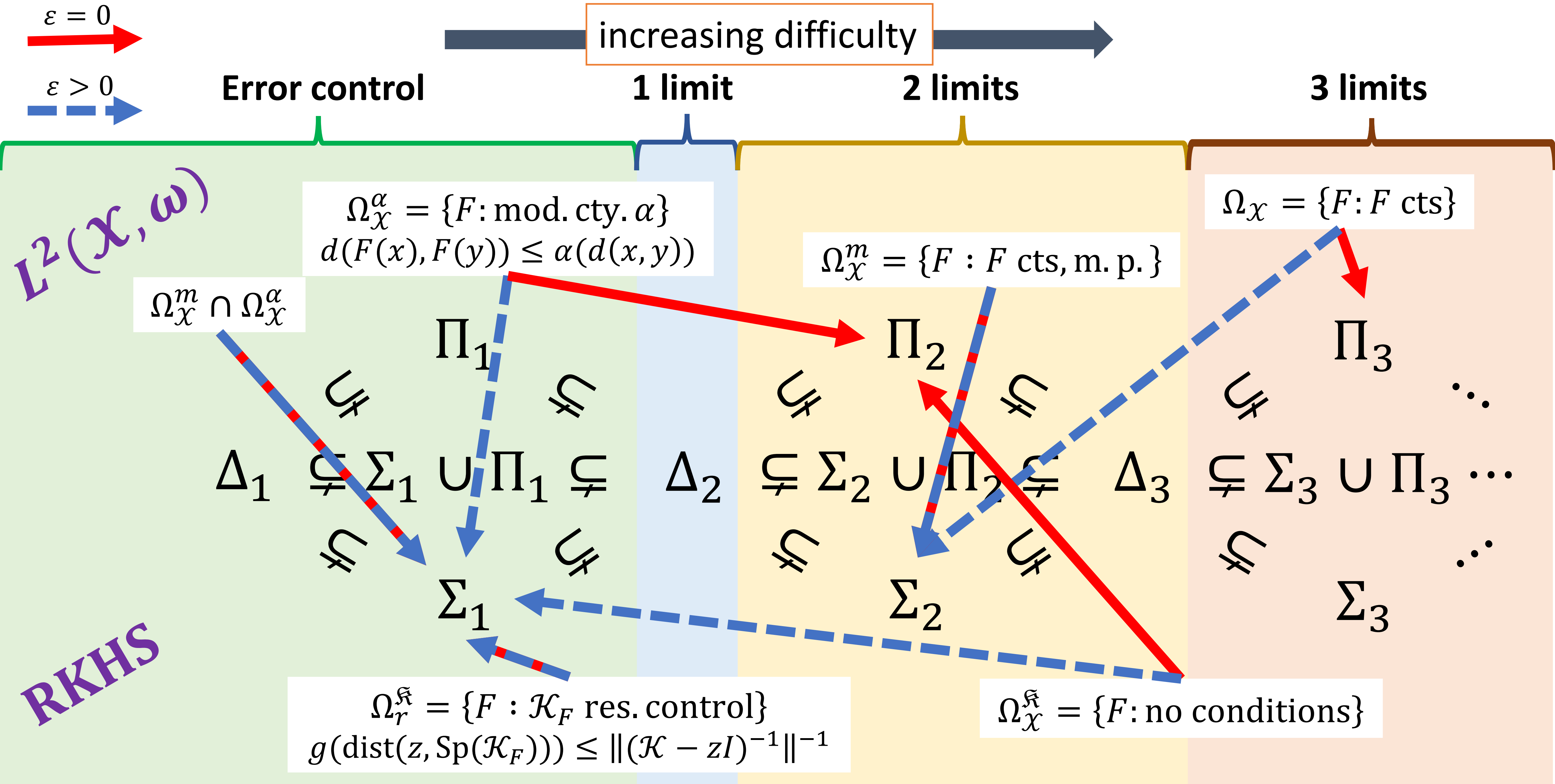
$$\Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

$\Sigma_1 \quad \Sigma_2 \quad \Sigma_3$

Optimal algorithms and classifications of systems



Optimal algorithms and classifications of systems



Pointers

1. Data-driven spectral problems for Koopman operators are hugely popular.
   BUT: Standard truncation methods often fail.

2. **General method with convergence for spectral properties** (spectra, pseudospectra, spectral measures etc.) of K. operators!

   E.g., Verification of approximate eigenfunctions leads to practical gains.

3. ***SCI hierarchy*** classifies computational problems:

   Lower bounds through method of *adversarial dynamics*.

   Upper bounds $\Longrightarrow$ new "inf.-dim." algorithms. *Rigorous, optimal, practical.*

$\longrightarrow$ We now have a near complete picture for Koopman on $L^2(\mathcal{X}, \omega)$ and RKHS!

NB: *Similar picture has emerged for spectral measures, dealing with continuous spectra (versus eigenvalues) and spectral type (different flavors of dynamics).*

Shameless plug…

Upcoming book with CUP:

INFINITE-DIMENSIONAL SPECTRAL COMPUTATIONS

Foundations, Algorithms, and Modern Applications

100s of: classifications, algorithms, examples (webpage: full code), figures, exercises (webpage: full solutions).

Out early 2026 (hopefully!)…

Contents

If something interests you, please speak to me after.

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