

# Rigorous Limits of Learning in Dynamical Systems

Matthew Colbrook  
University of Cambridge

12/11/2024

*“To classify is to bring order into chaos.”* - **George Pólya**

C., Mezić, Stepanenko *“Limits and Powers of Koopman Learning,”* arxiv preprint, 2024.

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

# Data-driven dynamical systems

- Compact metric space  $(\mathcal{X}, d)$  – the state space

- $x \in \mathcal{X}$  – the state

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

Dynamics (geometry)  
19<sup>th</sup> century

- Borel measure  $\omega$  on  $\mathcal{X}$

- Function space  $L^2 = L^2(\mathcal{X}, \omega)$  (elements  $g$  called “observables”)

- Koopman operator  $\mathcal{K}_F: L^2 \rightarrow L^2$ ;  $[\mathcal{K}_F g](x) = g(F(x))$

- **Available** snapshot data:  $\left\{ \left( x^{(m)}, y^{(m)} = F(x^{(m)}) \right) : m = 1, \dots, M \right\}$

**NB:** Pointwise definition of  $\mathcal{K}_F$  needs  $F\#\omega \ll \omega$  – this will hold throughout.

**NB:**  $\mathcal{K}_F$  bounded equivalent to  $dF\#\omega/d\omega \in L^\infty$  – this will hold throughout (can be dropped).

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20<sup>th</sup> century

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19<sup>th</sup> century
- Analysis  
20<sup>th</sup> century
- Data  
21<sup>st</sup> century

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# Why you should care about Koopman

Fundamental in ergodic theory

Graduate Texts  
in Mathematics

Peter Walters

An Introduction  
to Ergodic Theory



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

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

E.g., key to ergodic theorems of Birkhoff and von Neumann.

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

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Can provide a *diagonalization* of a nonlinear system.

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continuous  
spectrum

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

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

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

**Spectral properties encode:** geometric features, invariant measures, transient behavior, long-time behavior, coherent structures, quasiperiodicity, etc.

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# Why you should care about Koopman

Fundamental in ergodic theory

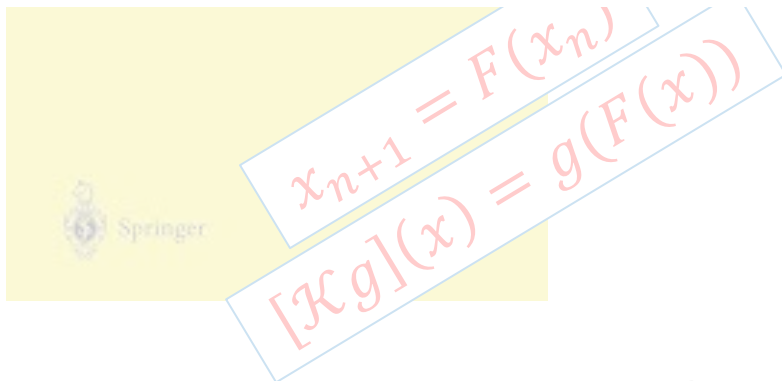
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$$g(x) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \overset{\text{eigenfunction of } \mathcal{K}}{\varphi_{\lambda_j}(x)} + \int_{-\pi}^{\pi} \overset{\text{continuous spectrum}}{\phi_{\theta,g}(x)} d\theta$$

**+ HUGE recent interest in their spectral properties...**



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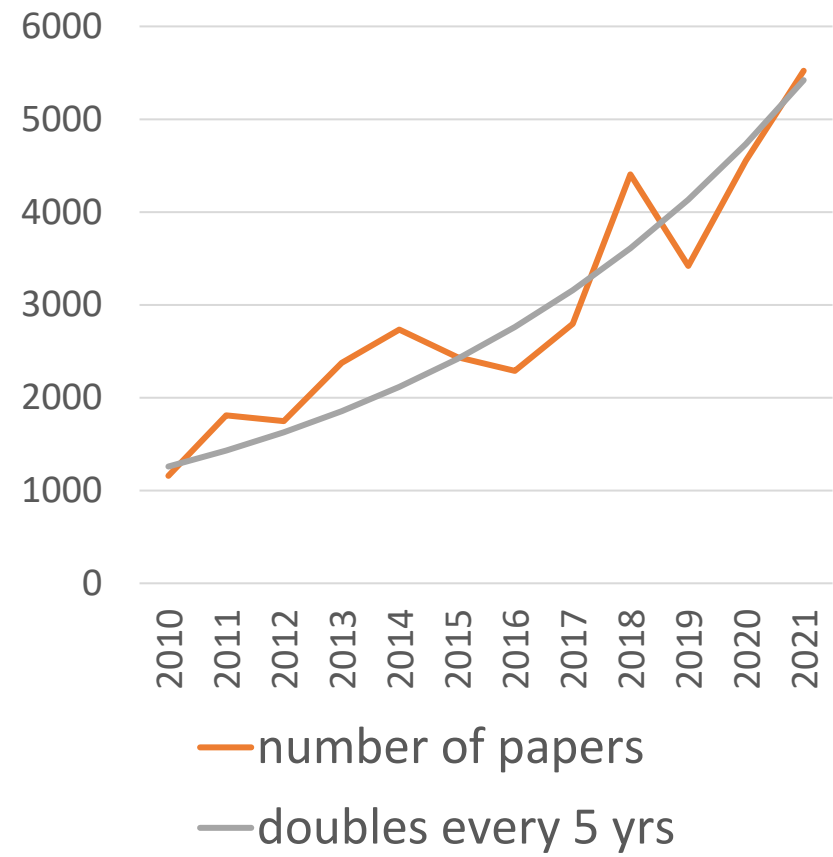
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### New Papers on "Koopman Operators"

# Central in data-driven era

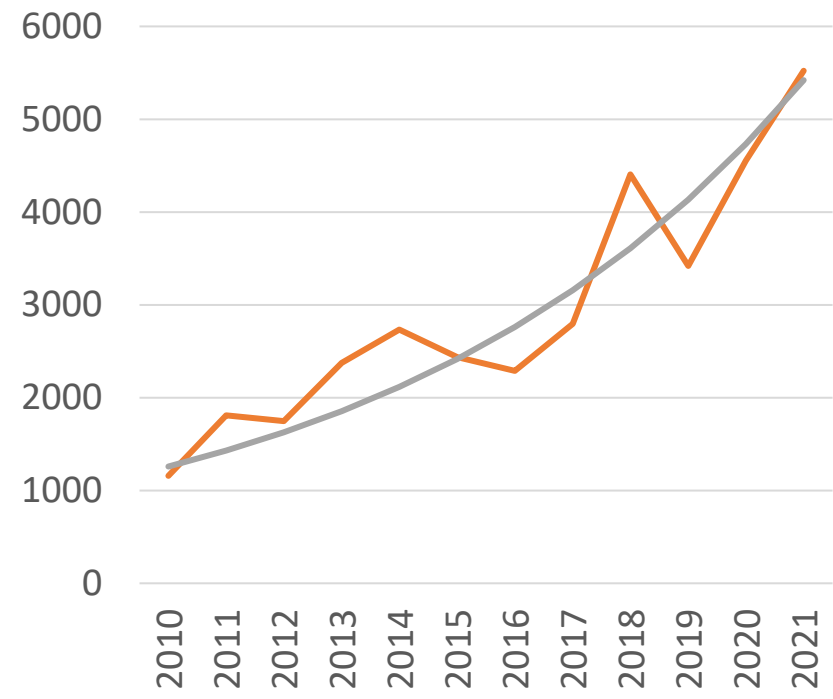


**Loads of applications!!!**



# New Papers on “Koopman Operators”

# Central in data-driven era



— number of papers  
 — doubles every 5 yrs

Loads of applications!!!

**2012**  
 CHAOS 22, 047510 (2012)

**Applied Koopmanism<sup>9)</sup>**  
 Marko Budišić, Ryan Mohr, and Igor Mezić  
 Department of Mechanical Engineering, University of California, Santa Barbara, California 93106-5070, USA  
 (Received 11 June 2012; accepted 30 November 2012; published online 11 December 2012)

A majority of methods from dynamical system analysis, especially those in applied settings, rely on Poincaré’s geometric picture that focuses on “dynamics of states.” While this picture has fueled our field for a century, it has shown difficulties in handling high-dimensional, ill-described, and

approach of ergodic theory through

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## Modern Koopman Theory for Dynamical Systems\*

**2022**

Steven L. Brunton<sup>†</sup>  
 Marko Budišić<sup>†</sup>  
 Erika Kaiser<sup>†</sup>  
 J. Nathan Kutz<sup>‡</sup>

**Abstract.** The field of dynamical systems is being transformed by the mathematical tools and algorithms emerging from modern computing and data-driven approaches. Asymptotic reductions are giving way to data-driven operator-theoretic or probabilistic frameworks. As a dominant perspective over the past decade, centered in terms of an infinite-dimensional linear operator measurement functions of the system. This linear perspective has tremendous potential to enable the prediction of systems with standard textbook methods developing finite-dimensional coordinate systems and model reduction. An approximately linear remains a central open challenge due primarily to three key factors: (1) there exist classical geometric approaches for dynamical systems; (2) measurements, making it ideal for leveraging big data; and (3) simple, yet powerful numerical algorithms (DMD), have been developed and extended in real-world applications. In this review, we provide a comprehensive overview of recent theoretical and applied developments in these methods with a diverse range of applications, describing recent theoretical and applied challenges in the rapidly growing field of machine learning and significantly transform the theory.

**Key words.** dynamical systems, Koopman operator, data-driven theory, operator theory, dynamic mode decomposition

**AMS subject classifications.** 34A34, 37A30, 37C10, 37M10, 37M25

## The multiverse of dynamic mode decomposition algorithms

**2024**

Matthew J. Colbrook  
 Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge, United Kingdom  
 e-mail address: m.colbrook@damtp.cam.ac.uk

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| 2.2.288 The least-squares                                      |            |  |

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

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

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

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

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

# New Papers on "Koopman Operators"

# Central in data-driven era



2012

### Applied Koopmanism<sup>9)</sup>

Marko Budišić, Ryan Mohr, and Igor Mezić  
 Department of Mechanical Engineering, University of California, Santa Barbara, CA 93106, USA  
 (Received 11 June 2012; accepted 30 November 2012; published online 11 December 2012)

A majority of methods from dynamical system analysis, especially Poincaré's geometric picture that focuses on "dynamics of stable manifolds," has shown difficulties in handling high-dimensional uncertain systems, which are more and more common in engineering "big data" measurements. This overview article presents an alternative picture, based on the "dynamics of observables" picture. This picture (DMD), have been developed and extended in real-world applications. In this review, we provide a survey of operator theory, describing recent theoretical and engineering these methods with a diverse range of applications and challenges in the rapidly growing field of machine learning and significantly transform the theoretical and computational landscape of dynamical systems.

CHAOS 22, 047510 (2012)



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### Modern Koopman Theory for

**Issue:** Many practitioners view it as a magic bullet, but standard algorithms typically fail to converge! (Inf-dim spectral problems.)

**Question:** When can we reliably learn Koopman spectral properties from system data, and when is it impossible?

—number of papers  
 —doubles every 5 yrs

## Loads of applications!!!

**Key words.** dynamical systems, Koopman operator, data-driven theory, operator theory, dynamic mode decomposition

**AMS subject classifications.** 34A34, 37A30, 37C10, 37M10, 37M20, 37M25, 37M26, 37M27, 37M28, 37M30, 37M31, 37M32, 37M33, 37M34, 37M35, 37M36, 37M37, 37M38, 37M39, 37M40, 37M41, 37M42, 37M43, 37M44, 37M45, 37M46, 37M47, 37M48, 37M49, 37M50, 37M51, 37M52, 37M53, 37M54, 37M55, 37M56, 37M57, 37M58, 37M59, 37M60, 37M61, 37M62, 37M63, 37M64, 37M65, 37M66, 37M67, 37M68, 37M69, 37M70, 37M71, 37M72, 37M73, 37M74, 37M75, 37M76, 37M77, 37M78, 37M79, 37M80, 37M81, 37M82, 37M83, 37M84, 37M85, 37M86, 37M87, 37M88, 37M89, 37M90, 37M91, 37M92, 37M93, 37M94, 37M95, 37M96, 37M97, 37M98, 37M99, 37M00

Cambridge, United Kingdom  
e-mail address: m.colbrook@damp.cam.ac.uk

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# Outline

**Question:** *When can we reliably learn Koopman spectral properties from system data, and when is it impossible?*

- Constructing adversaries – *impossibility theorem*      **(a general strategy)**
- Towers of algorithms – *possibility theorem*      **(problem-specific algorithm)**
- The Solvability Complexity Index Hierarchy – *classifications* **(general tool)**
- Where does this leave us?

# Theorem A (impossibility)

Implies  $\mathcal{K}$  is unitary



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

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

**Theorem A:** There **does not exist** any sequence of deterministic algorithms  $\{\Gamma_n\}$  using  $\mathcal{T}_F$  such that  $\lim_{n \rightarrow \infty} \Gamma_n(F) = \text{Sp}(\mathcal{K}_F) \quad \forall F \in \Omega_{\mathbb{D}}.$

**NB:** Similarly, no random algorithms converging with probability  $> 1/2$ .

# Proof idea: Constructing an adversary

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

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

*Conjugacy of data ( $x_j \rightarrow y_j$ ) with  $F_0$*

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

# Proof idea: Constructing an adversary

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

Build an **adversarial**  $F$  ...

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

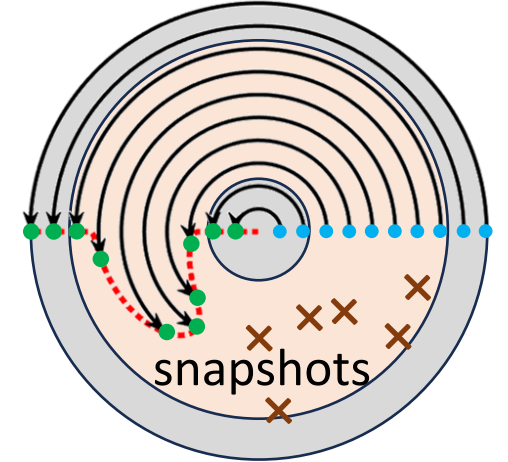
# Proof idea: Constructing an adversary

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

Build an **adversarial**  $F$ ...

$$\widetilde{F}_1(r, \theta) = (r, \theta + \pi + \phi(r)), \text{supp}(\phi) \subset [1/4, 3/4]$$

$$\text{Sp}(\mathcal{K}_{\widetilde{F}_1}) = \mathbb{T} \text{ (unit circle).}$$



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



# Proof idea: Constructing an adversary

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

Build an **adversarial**  $F$  ...

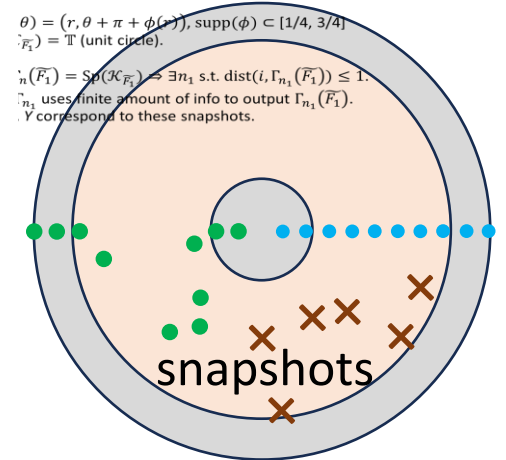
$$\widetilde{F}_1(r, \theta) = (r, \theta + \pi + \phi(r)), \text{supp}(\phi) \subset [1/4, 3/4]$$

$$\text{Sp}(\mathcal{K}_{\widetilde{F}_1}) = \mathbb{T} \text{ (unit circle)}.$$

$$\lim_{n \rightarrow \infty} \Gamma_n(\widetilde{F}_1) = \text{Sp}(\mathcal{K}_{\widetilde{F}_1}) \Rightarrow \exists n_1 \text{ s.t. } \text{dist}(i, \Gamma_{n_1}(\widetilde{F}_1)) \leq 1.$$

**BUT**  $\Gamma_{n_1}$  uses finite amount of info to output  $\Gamma_{n_1}(\widetilde{F}_1)$ .

Let  $X, Y$  correspond to these snapshots.



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

# Proof idea: Constructing an adversary

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

Build an **adversarial**  $F$ ...

$$\widetilde{F}_1(r, \theta) = (r, \theta + \pi + \phi(r)), \text{supp}(\phi) \subset [1/4, 3/4]$$

$$\text{Sp}(\mathcal{K}_{\widetilde{F}_1}) = \mathbb{T} \text{ (unit circle).}$$

$$\lim_{n \rightarrow \infty} \Gamma_n(\widetilde{F}_1) = \text{Sp}(\mathcal{K}_{\widetilde{F}_1}) \Rightarrow \exists n_1 \text{ s.t. } \text{dist}(i, \Gamma_{n_1}(\widetilde{F}_1)) \leq 1.$$

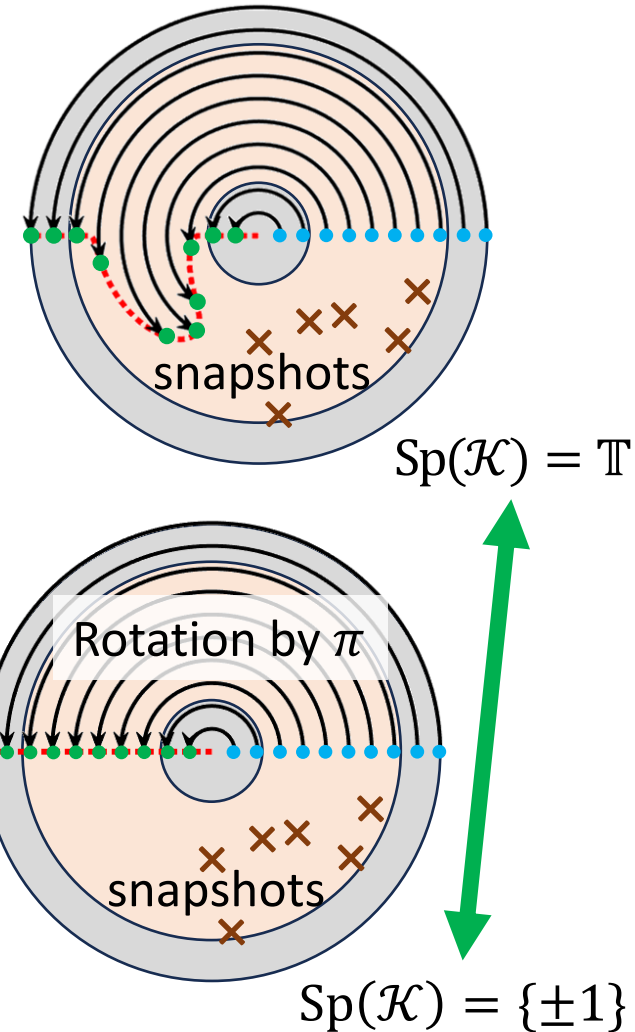
**BUT**  $\Gamma_{n_1}$  uses finite amount of info to output  $\Gamma_{n_1}(\widetilde{F}_1)$ .

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  $\Rightarrow \Gamma_{n_1}(F_1) = \Gamma_{n_1}(\widetilde{F}_1)$ ,  $\text{dist}(i, \Gamma_{n_1}(F_1)) \leq 1$

**BUT**  $\text{Sp}(\mathcal{K}_{F_1}) = \text{Sp}(\mathcal{K}_{F_0}) = \{\pm 1\}$



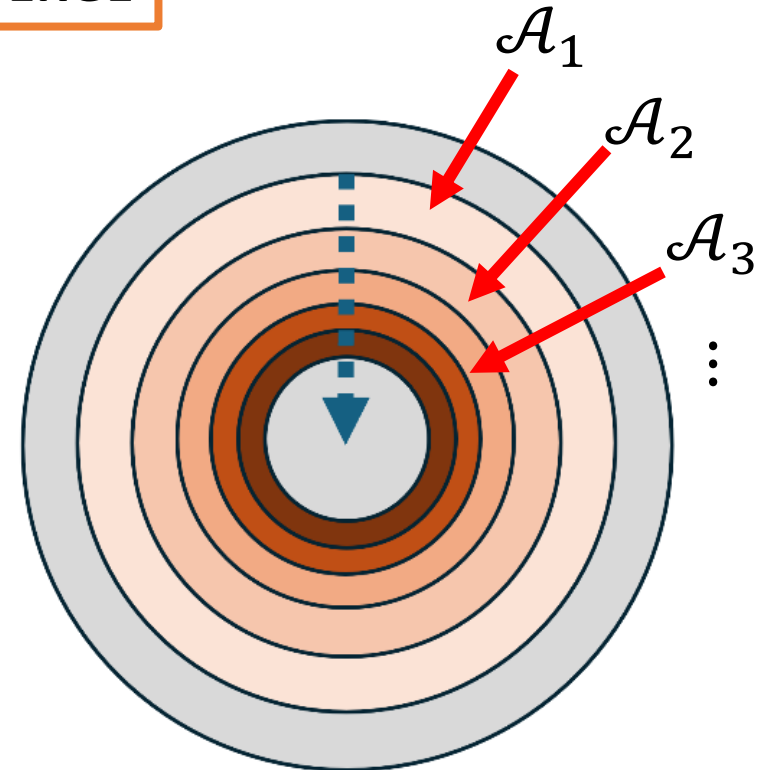
# Proof idea: Constructing an adversary

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

Consistent data  $\Rightarrow \Gamma_{n_k}(F) = \Gamma_{n_k}(\widetilde{F}_k)$ ,  $\text{dist}(i, \Gamma_{n_k}(F)) \leq 1$ ,  $n_k \rightarrow \infty$

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

**CANNOT CONVERGE**



Cascade of disks

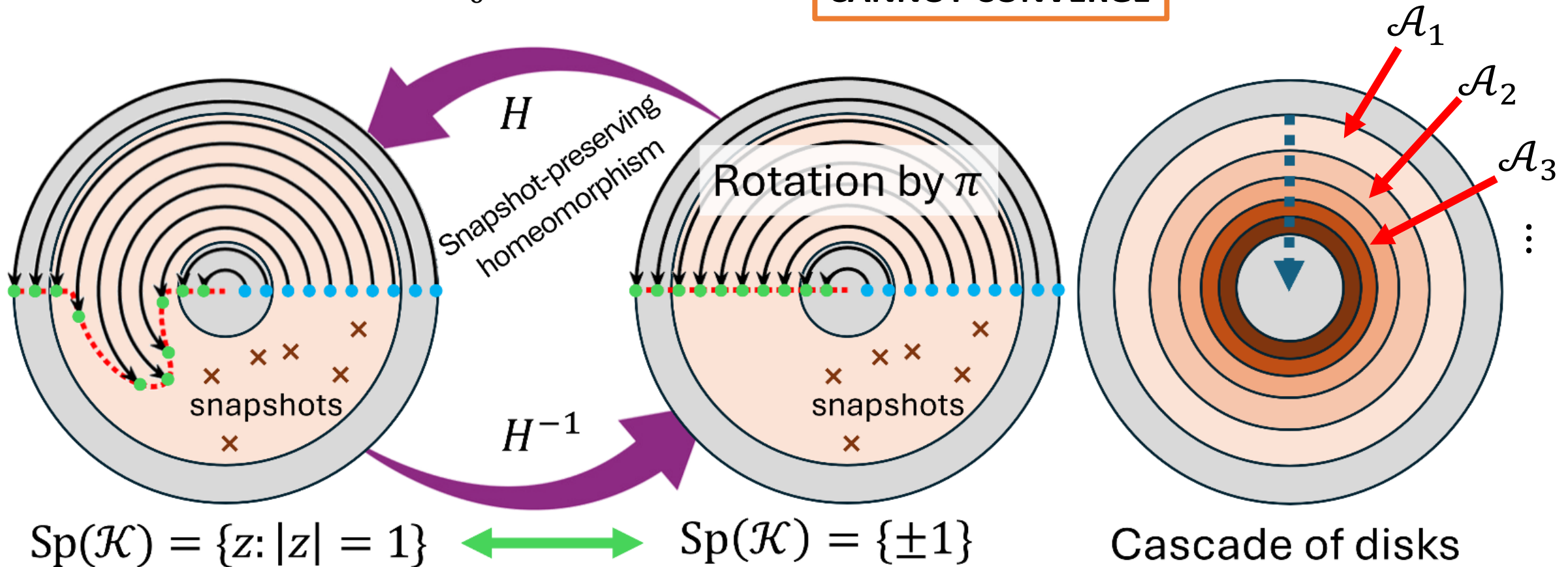
# Proof idea: Constructing an adversary

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

Consistent data  $\Rightarrow \Gamma_{n_k}(F) = \Gamma_{n_k}(\widetilde{F}_k)$ ,  $\text{dist}(i, \Gamma_{n_k}(F)) \leq 1$ ,  $n_k \rightarrow \infty$

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

**CANNOT CONVERGE**



## Theorem B (possibility)

$\Omega_{\mathcal{X}}^m = \{F: \mathcal{X} \rightarrow \mathcal{X} \mid F \text{ cts, measure preserving}\}.$

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

**Theorem B:** There **exists deterministic** algorithms  $\{\Gamma_{n_2, n_1}\}$  using input data  $\mathcal{T}_F$  such that  $\lim_{n_2 \rightarrow \infty} \lim_{n_1 \rightarrow \infty} \Gamma_{n_2, n_1}(F) = \text{Sp}(\mathcal{K}_F) \quad \forall F \in \Omega_{\mathcal{X}}^m.$

Double limit  $\lim_{n_2 \rightarrow \infty} \lim_{n_1 \rightarrow \infty}$

# Extended Dynamic Mode Decomposition (EDMD)

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

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

- Schmid, “*Dynamic mode decomposition of numerical and experimental data*,” **J. Fluid Mech.**, 2010.
- Rowley, Mezić, Bagheri, Schlatter, Henningson, “*Spectral analysis of nonlinear flows*,” **J. Fluid Mech.**, 2009.
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# Extended Dynamic Mode Decomposition (EDMD)

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

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

quadrature points

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

quadrature weights

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

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

Galerkin  
Approximation

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

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



Caution

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

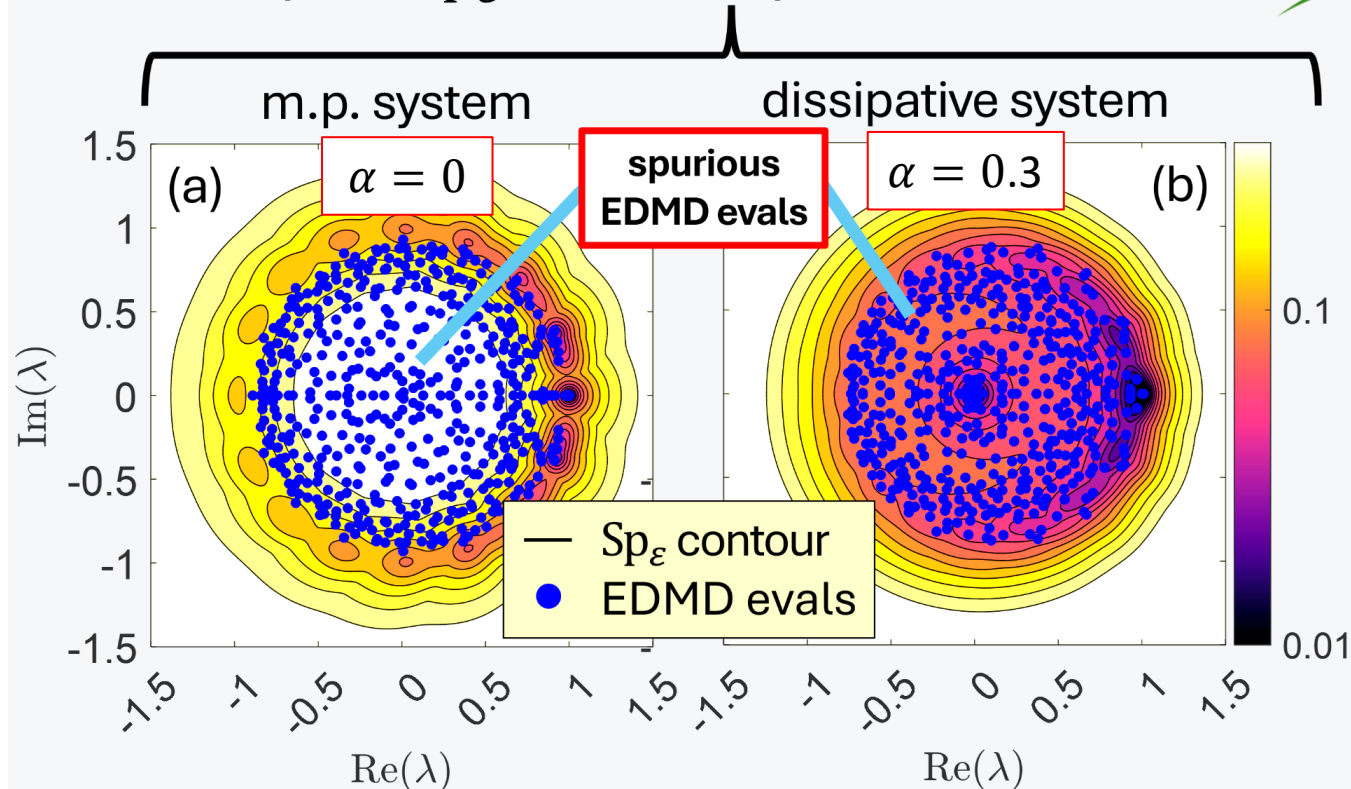
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- Williams, Kevrekidis, Rowley "A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition," **J. Nonlinear Sci.**, 2015.

# Example: EDMD does NOT converge

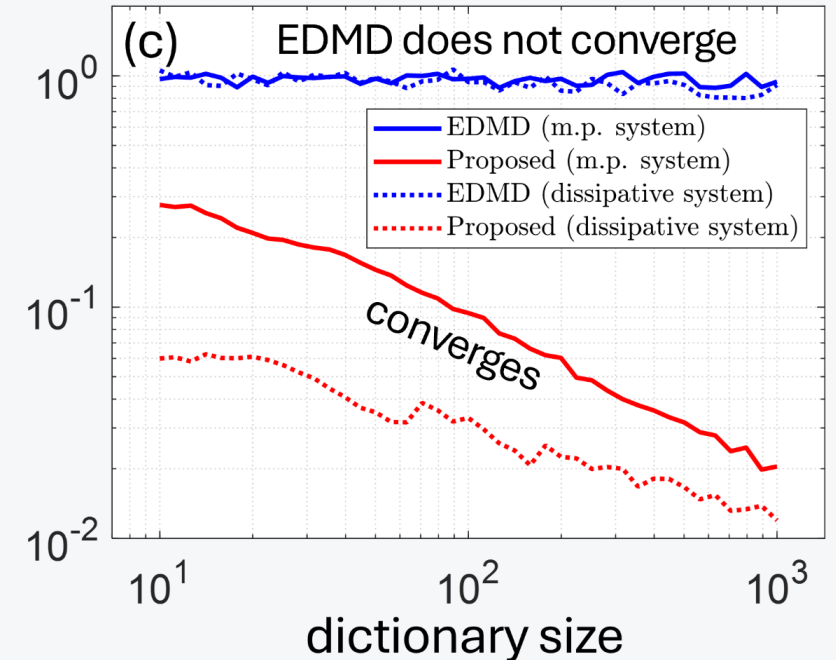
- Duffing oscillator:  $\dot{x} = y, \dot{y} = -\alpha y + x(1 - x^2)$ , sampled  $\Delta t = 0.3$ .
- Gaussian radial basis functions, Monte Carlo integration ( $M = 50000$ )

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

Compute  $\text{Sp}_\varepsilon$ , local adaptive control on  $\varepsilon \downarrow 0$



Approximation error



# Residual DMD (ResDMD)

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

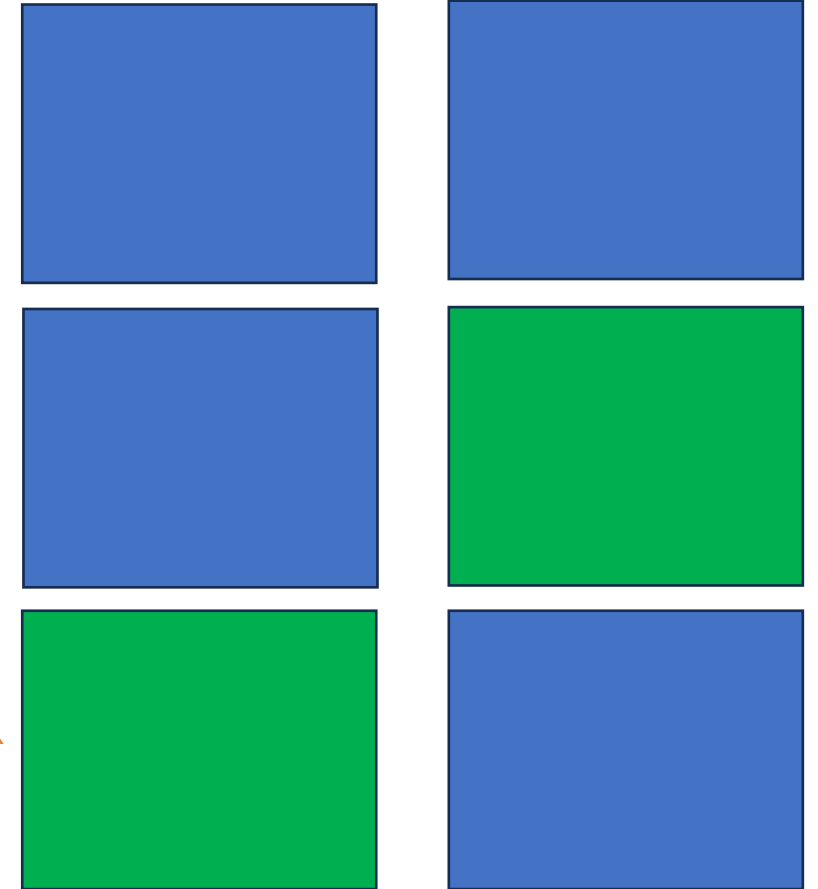
$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[ \underbrace{\Psi_X^* W \Psi_Y}_{K_1} \right]_{jk}$$

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

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

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- Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>

# Residual DMD (ResDMD)

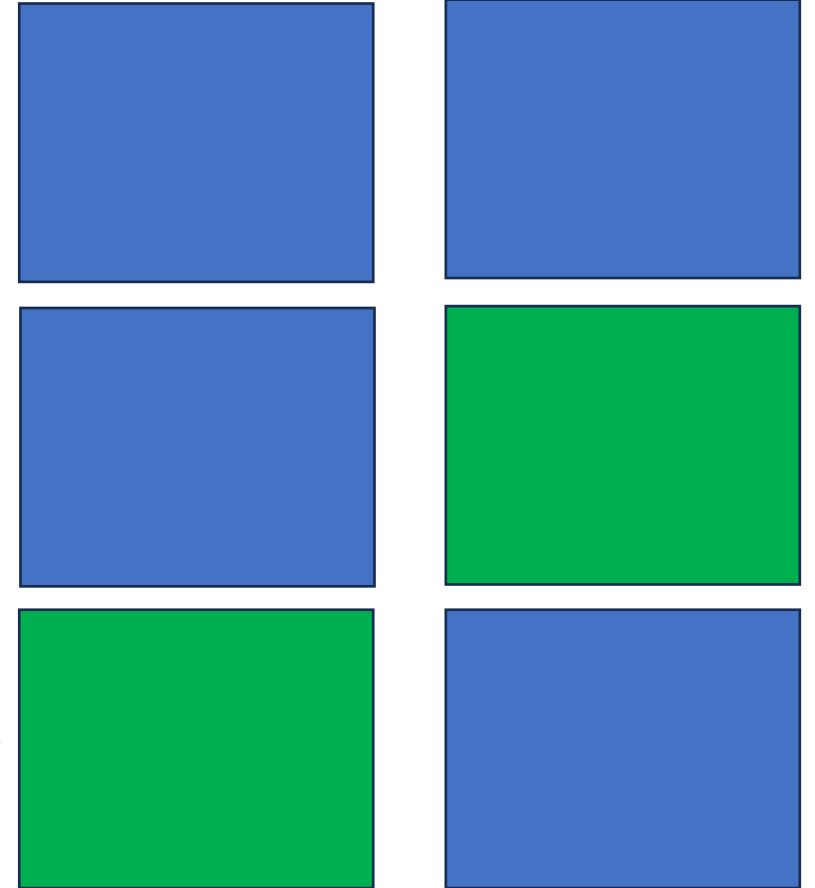
What's the missing



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

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

adjoint



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

# Residual DMD (ResDMD)

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

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

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



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

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

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



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

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# Proof sketch

**Theorem B:** There **exists** *deterministic* algorithms  $\{\Gamma_{n_2, n_1}\}$  using input data  $\mathcal{T}_F$  such that  $\lim_{n_2 \rightarrow \infty} \lim_{n_1 \rightarrow \infty} \Gamma_{n_2, n_1}(F) = \text{Sp}(\mathcal{K}_F) \quad \forall F \in \Omega_{\mathcal{X}}^m$ .

- *Residuals*  $\rightarrow \lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} \gamma_{N, M}(F, z) = \|(\mathcal{K}_F - zI)^{-1}\|^{-1}$ .

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

- Measure-preserving  $\Rightarrow \|(\mathcal{K}_F - zI)^{-1}\|^{-1} = \text{dist}(z, \text{Sp}(\mathcal{K}_F))$ .
- Local  $N$ -adaptive minimisation of  $\gamma_{N, M}(F, z)$  to approximate  $\text{Sp}(\mathcal{K}_F)$ .

**Double limit  $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$**

# Limits of limits: Towers of algorithms

**Def:**  $\{\Gamma_{n_k, \dots, n_1}\}$  with  $\lim_{n_k \rightarrow \infty} \dots \lim_{n_1 \rightarrow \infty} \Gamma_{n_k, \dots, n_1}$  convergent a ***tower of algorithms***.

First appeared in dynamical systems theory: algorithms



Steve Smale

“Is there any purely iterative convergent rational map for polynomial zero finding?”



Curtis McMullen

“Yes for cubic, no for higher degree. Quartic and quintic can be solved using towers of algorithms. Sextic cannot be solved in any number of limits.”

- Smale, “On the efficiency of algorithms of analysis.” **Bull. Am. Math. Soc.**, 1985.
- McMullen, “Families of rational maps and iterative root-finding algorithms.” **Annals Math.**, 1987.
- McMullen, “Braiding of the attractor and the failure of iterative algorithms.” **Invent. Math.** 1988.
- Doyle, McMullen, “Solving the quintic by iteration.” **Acta Math.**, 1989.

# Classifications: *Solvability Complexity Index (SCI)*

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

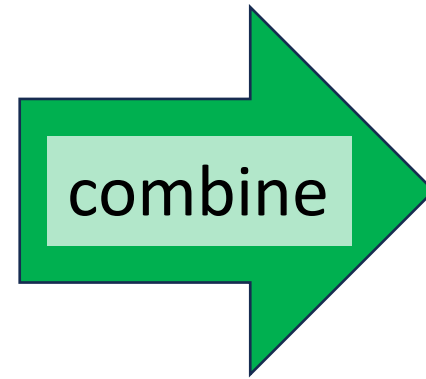
- 
- Hansen, "On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators." **J. Am. Math. Soc.**, 2011.
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# Classifications: *Solvability Complexity Index (SCI)*

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

**Theorem A:**  $SCI > 1$

**Theorem B:**  $SCI \leq 2$



$SCI = 2$

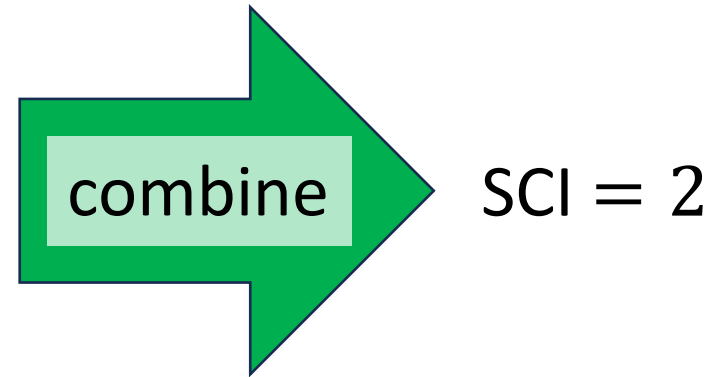
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So far literature has only proven upper bounds, that need not be sharp...

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- C., "The foundations of infinite-dimensional spectral computations," **PhD diss.**, University of Cambridge, 2020.
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# Results from Koopman literature

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

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

# Classifications: *Solvability Complexity Index (SCI)*

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

- $\Delta_1$ : One limit, full error control. E.g.,  $d(\Gamma_n(F), \text{Sp}(\mathcal{K}_F)) \leq 2^{-n}$ .

- $\Delta_{m+1}$ :  $\text{SCI} \leq m$ .

- $\Sigma_m$ :  $\text{SCI} \leq m$ , final limit from below.

E.g.,  $\Sigma_1$ :  $\Gamma_n(F) \subset \text{Sp}(\mathcal{K}_F) + B_{2^{-n}}(0)$ .

- $\Pi_m$ :  $\text{SCI} \leq m$ , final limit from above.

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**verification**

**trust output**

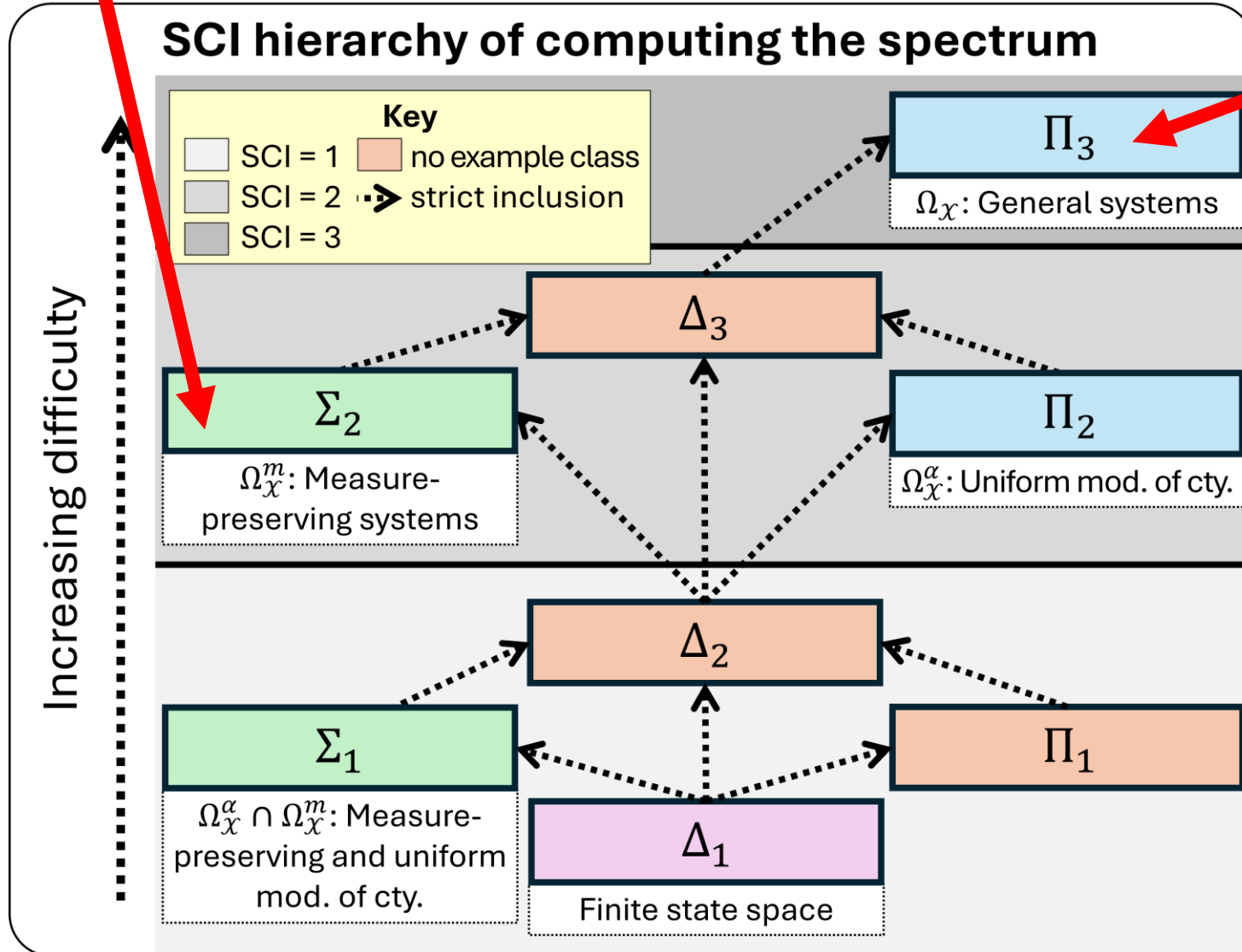
**covers spectrum**

- Hansen, "On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators." **J. Am. Math. Soc.**, 2011.
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## Theorems A + B

## Classification for Koopman I

3 limits needed  
in general!



## Different classes:

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

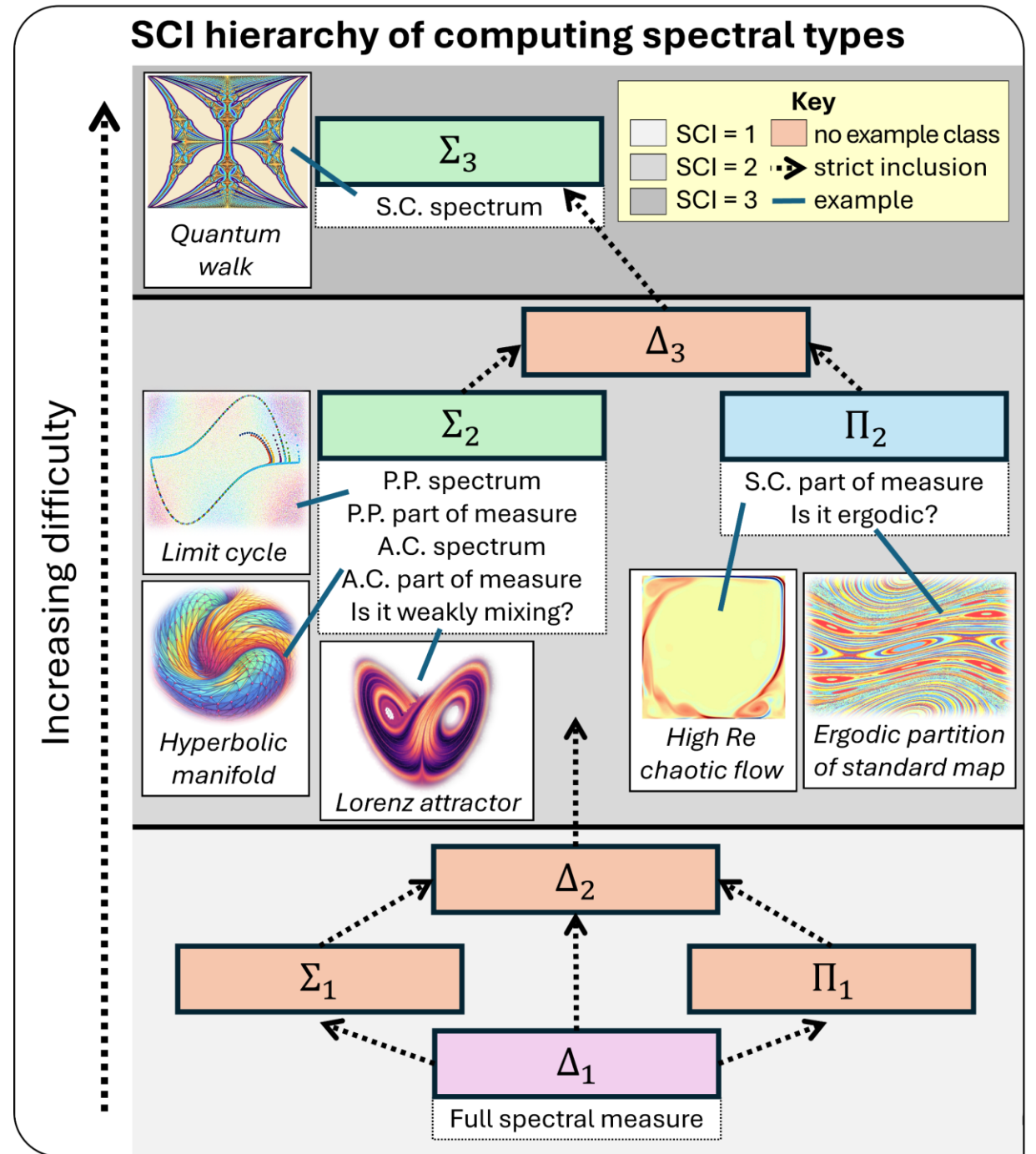
$$\Omega_{\mathcal{X}}^m = \{F: \mathcal{X} \rightarrow \mathcal{X} \mid F \text{ cts, m. p.}\}$$

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

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

Optimal algorithms and  
classifications of  
dynamical systems.

# Classification for Koopman II

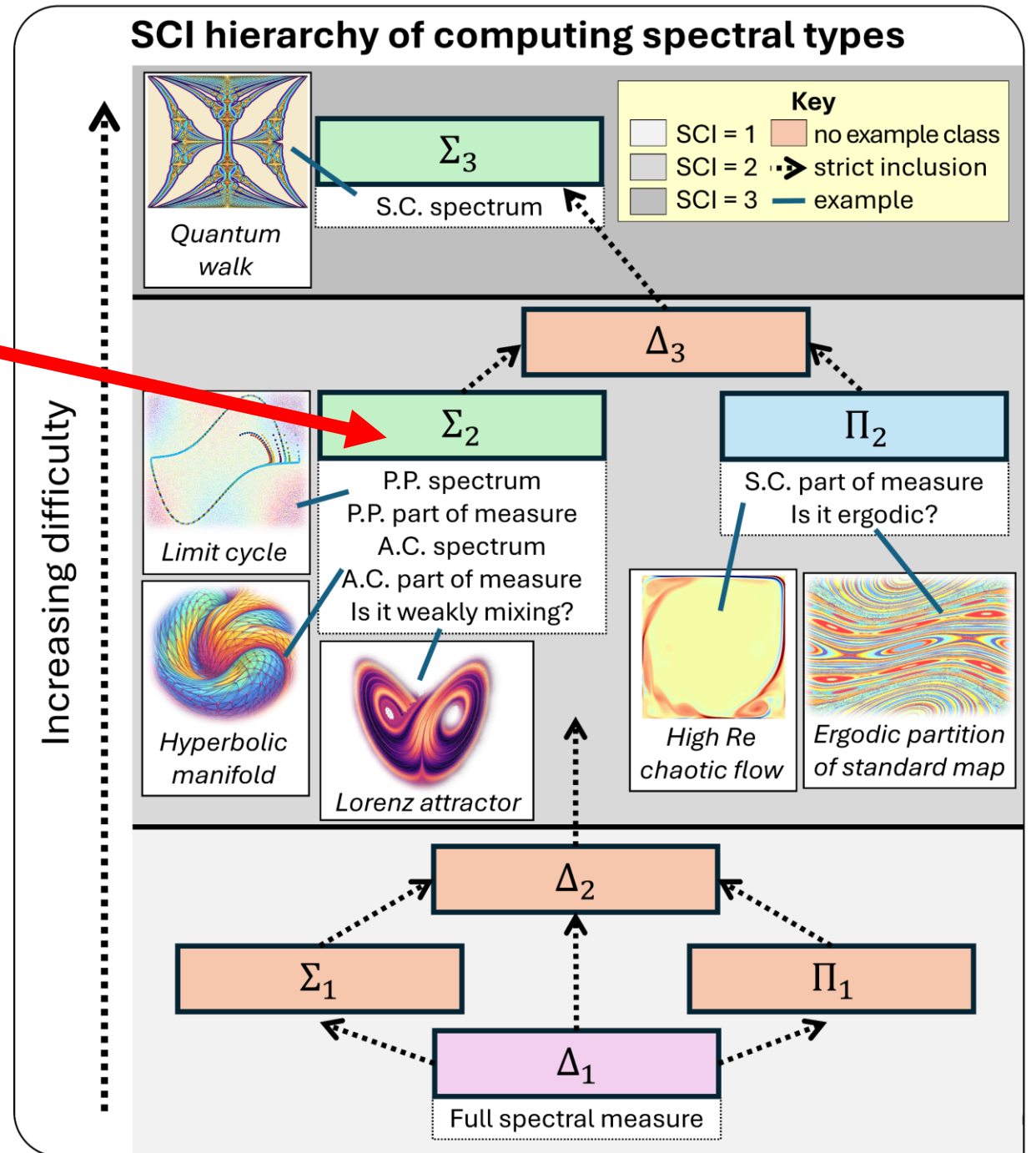


# Classification for Koopman II

## Example: Theorem C

For smooth, measure-preserving systems on a torus, learning eigenfunctions or even determining if there are any has  $SCI = 2$  (even if we can sample derivatives).

Finding finite-dimensional embeddings in which the dynamics are linear (e.g., autoencoders, latent space representation) is very hard!



# General tool in data-driven dynamical systems/PDEs

Adversarial arguments generalize to:

- “Learning the  $F$ ”. E.g., SINDy  $(x_{n+1} = F(x_n))$
- Solving PDEs with neural networks (PINNs)
- Learning PDEs from forcing-solution pairs (e.g., hyperbolic)

- 
- Brunton, Proctor, Kutz, “*Discovering governing equations from data by sparse identification of nonlinear dynamical systems,*” **Proc. Natl. Acad. Sci. USA**, 2016.
  - Karniadakis, Kevrekidis, Lu, Perdikaris, Wang, Yang, “*Physics-informed machine learning,*” **Nature Reviews Physics**, 2021.
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# Where does this leave us?

- Many problems **NECESSARILY** require multiple limits.
- New tools for **lower bounds** (impossibility results) for Koopman learning.
- Combine with **upper bounds** (algorithms)  
⇒ **classify difficulty** of problems + **prove optimality** of algorithms.
- Ergodic theory + approximation theory + computational analysis  
⇒ started to map out this terrain.

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  - Partial observations, continuous-time.
  - Control and uses of Koopman.
  - Other data-driven dynamical system methods.

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**Where does your problem/method fit into the SCI hierarchy? Is it optimal?**



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