

A classification theory for data-driven Koopman Spectral Computations

Matthew Colbrook

University of Cambridge

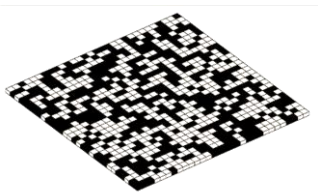
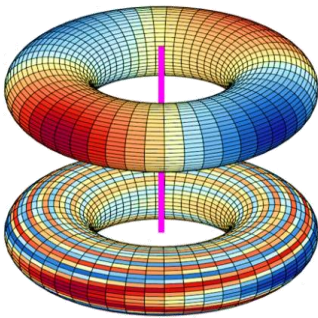
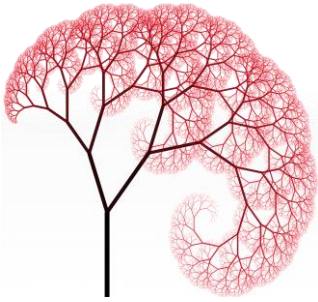
12/12/2024



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

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)
19th century

- Borel measure ω 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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Analysis
20th century

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Data-driven dynamical systems

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- } Dynamics (geometry)
19th century
- } Analysis
20th century
- } Data
21st century

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Why should you 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.

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

Why should you care about Koopman?

Fundamental in ergodic theory

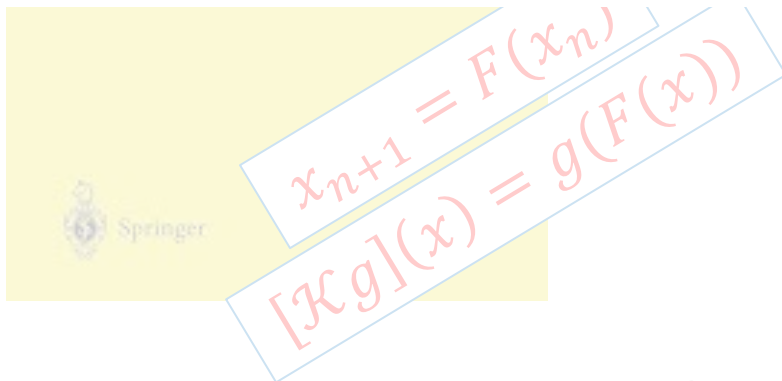
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$$g(x) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \underbrace{\varphi_{\lambda_j}(x)}_{\text{eigenfunction of } \mathcal{K}} + \int_{-\pi}^{\pi} \underbrace{\phi_{\theta,g}(x)}_{\text{continuous spectrum}} d\theta$$

+ HUGE recent interest in their spectral properties...



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

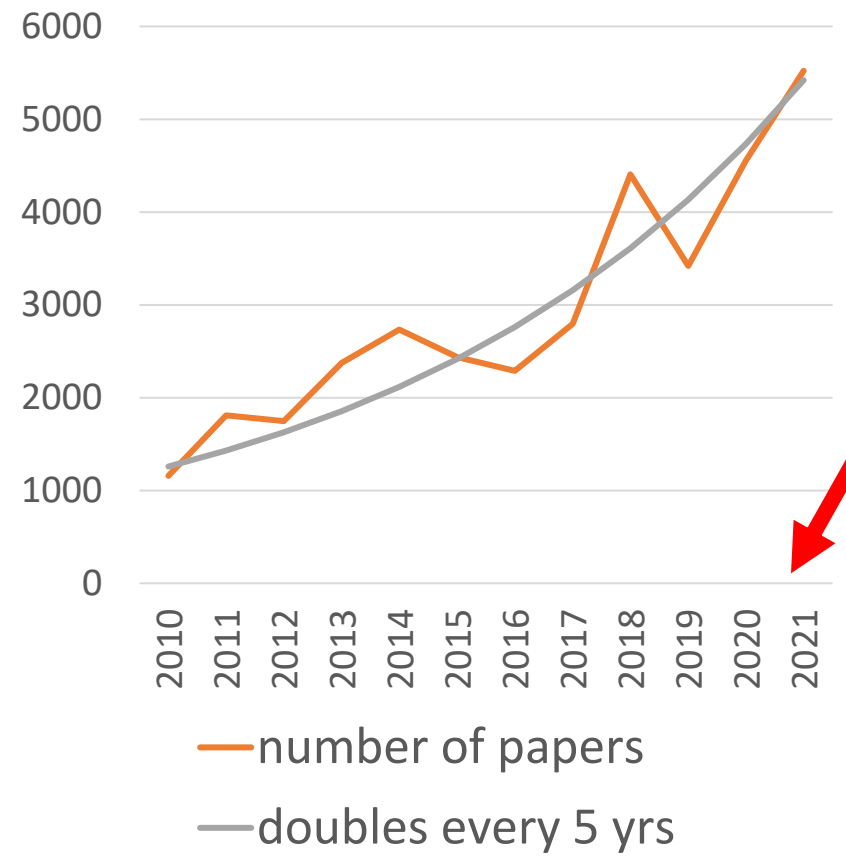
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New Papers on "Koopman Operators"

Central in data-driven era

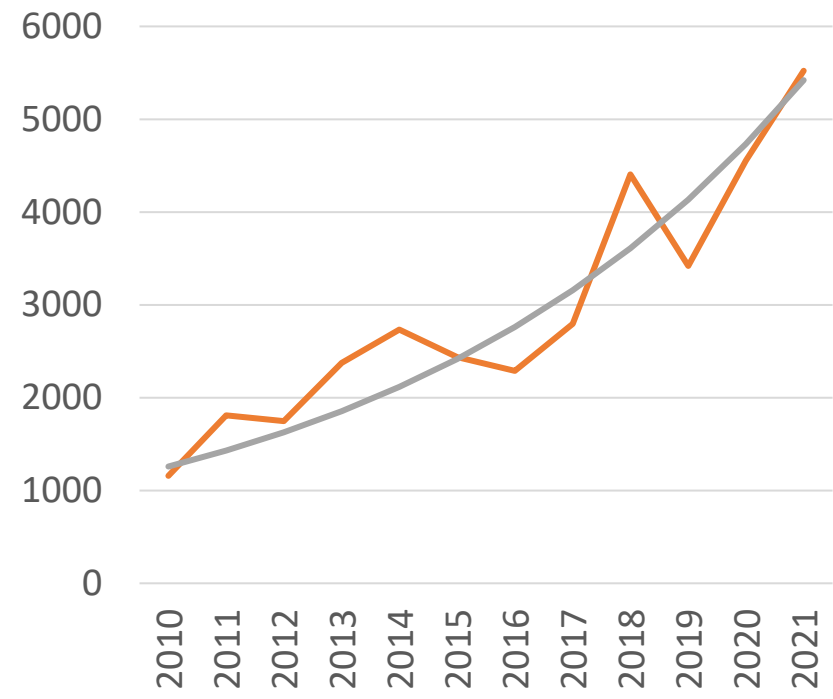


When I got into Koopman and had too much time during covid to produce this plot. The trend continues...

Loads of applications!!!

New Papers on "Koopman Operators"

Central in data-driven era



— number of papers
 — doubles every 5 yrs

Loads of applications!!!

2012

Applied Koopmanism⁹⁾

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*

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 Marko Budišić[†]
 Eureka Kaiser[†]
 J. Nathan Kutz[‡]

2022

Abstract. The field of dynamical systems is being transformed by the mathematical tools and algorithms emerging from modern computing and data-driven methods. Asymptotic reductions are giving way to data-driven operator-theoretic or probabilistic frameworks, as a dominant perspective over the past decade, is centered in terms of an infinite-dimensional linear operator measurement functions of the system. This linear has tremendous potential to enable the prediction systems with standard textbook methods developing finite-dimensional coordinate systems and emulating approximately linear remains a central open challenge due primarily to three key factors: (1) there exist classical geometric approaches for dynamical systems; of 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 an operator theory, describing recent theoretical and computational challenges in the rapidly growing field of machine learning and significantly transform the theoretical

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

AMS subject classifications. 34A34, 37A30, 37C10, 37M10, 37M20

The multiverse of dynamic mode decomposition algorithms

2024

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Let's see an example!
Go to board...

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.
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Extended Dynamic Mode Decomposition (EDMD)

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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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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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Caution

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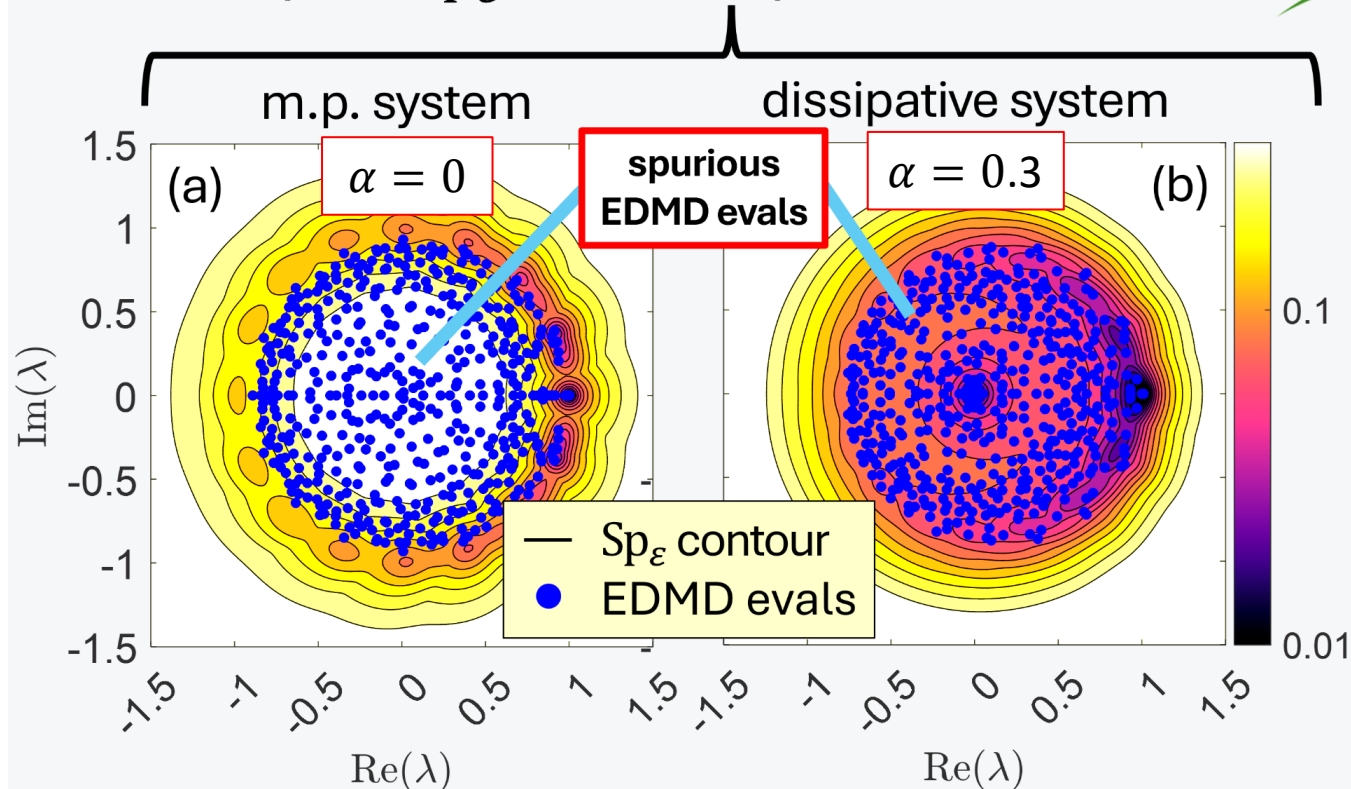
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Example: EDMD does NOT converge

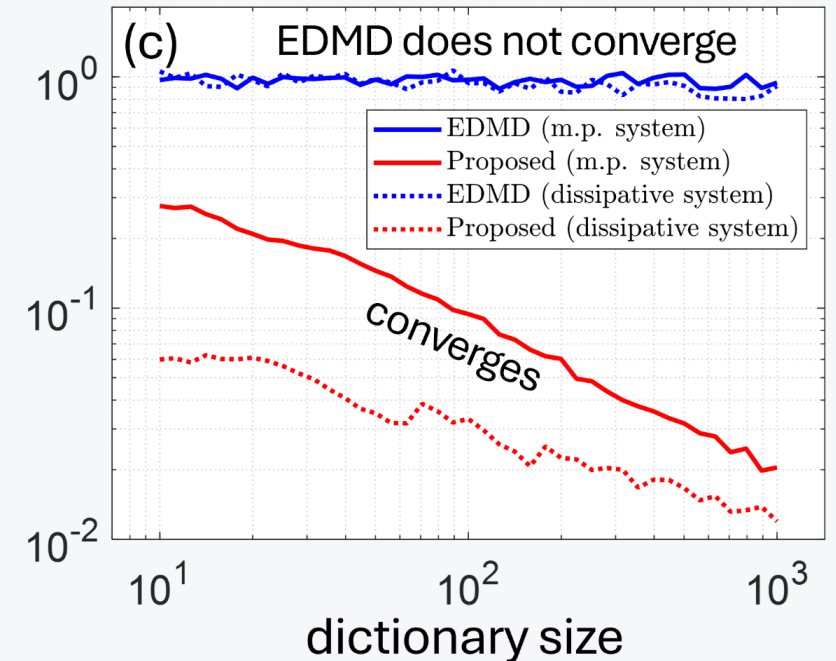
- Duffing oscillator: $\dot{x} = y, \dot{y} = -\alpha y + x(1 - x^2)$, sampled $\Delta t = 0.3$.
- Gaussian radial basis functions, Monte Carlo integration ($M = 50000$)

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

Compute Sp_ε , local adaptive control on $\varepsilon \downarrow 0$



Approximation error

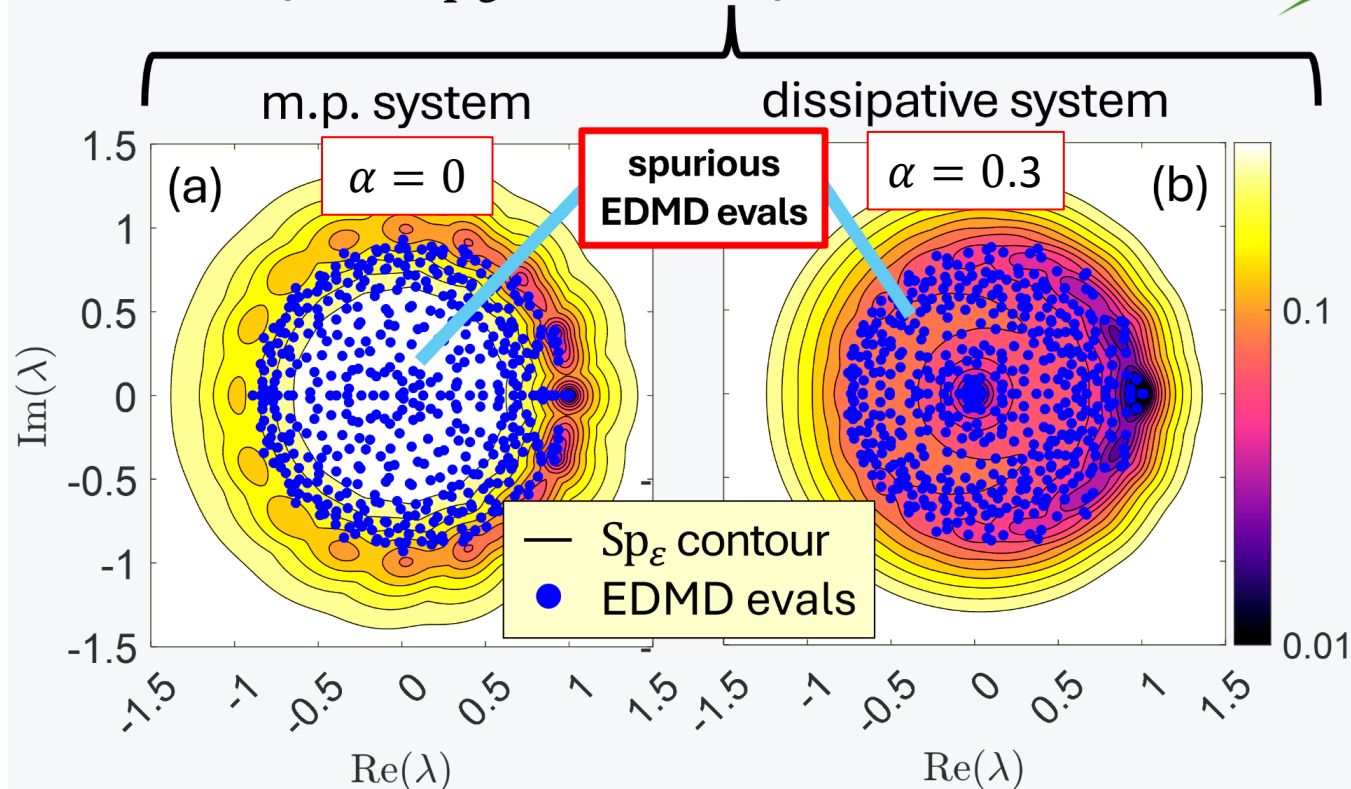


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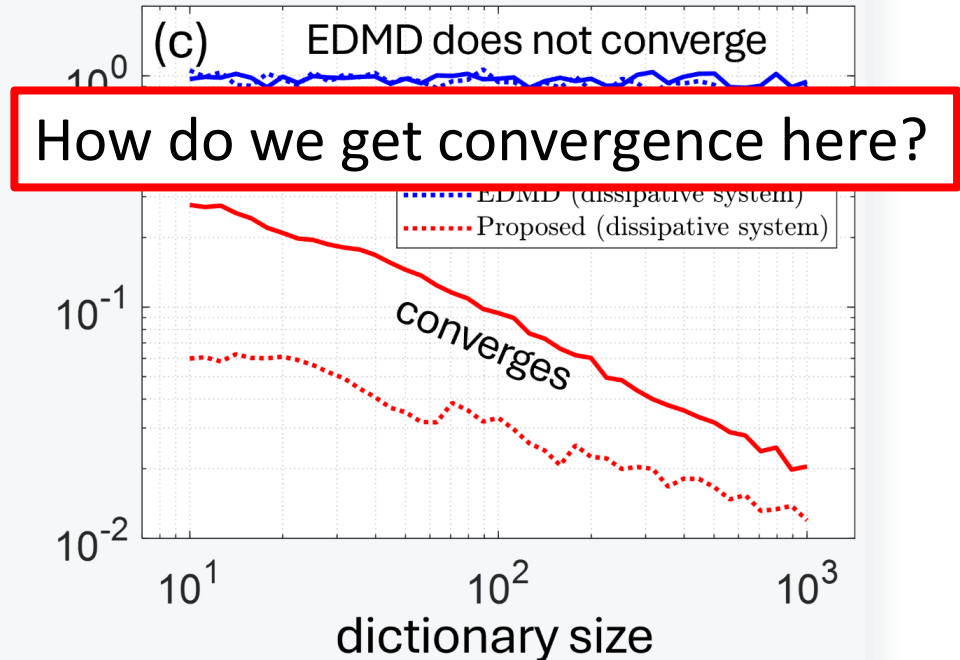
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Approximation error



Residual DMD (ResDMD)

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

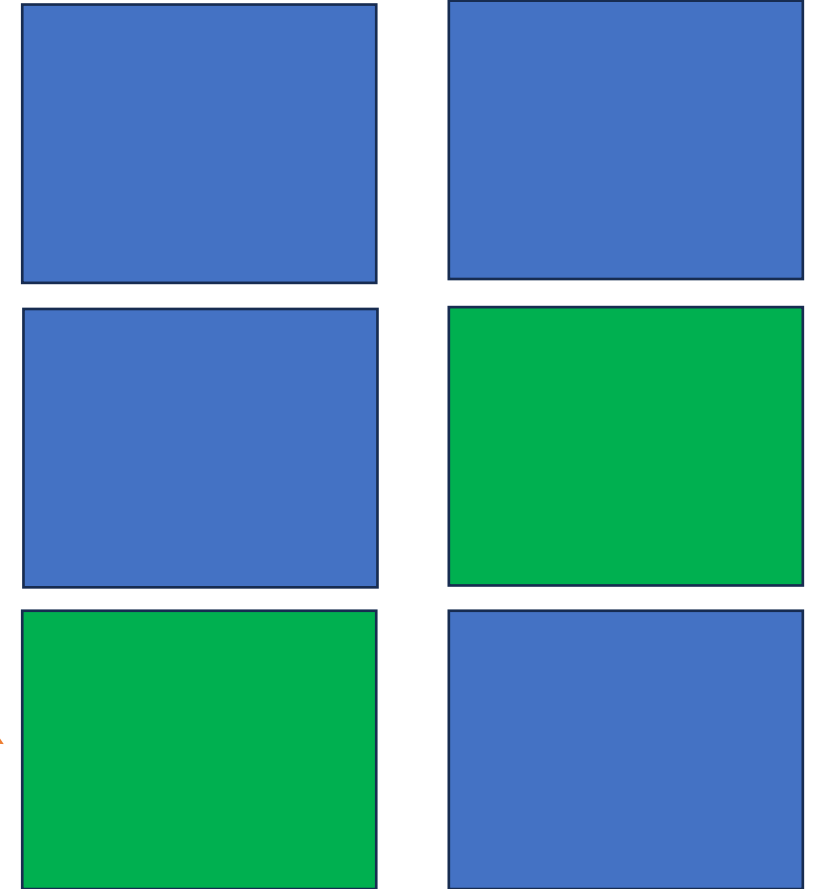
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- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," **Commun. Pure Appl. Math.**, 2023.
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- Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>

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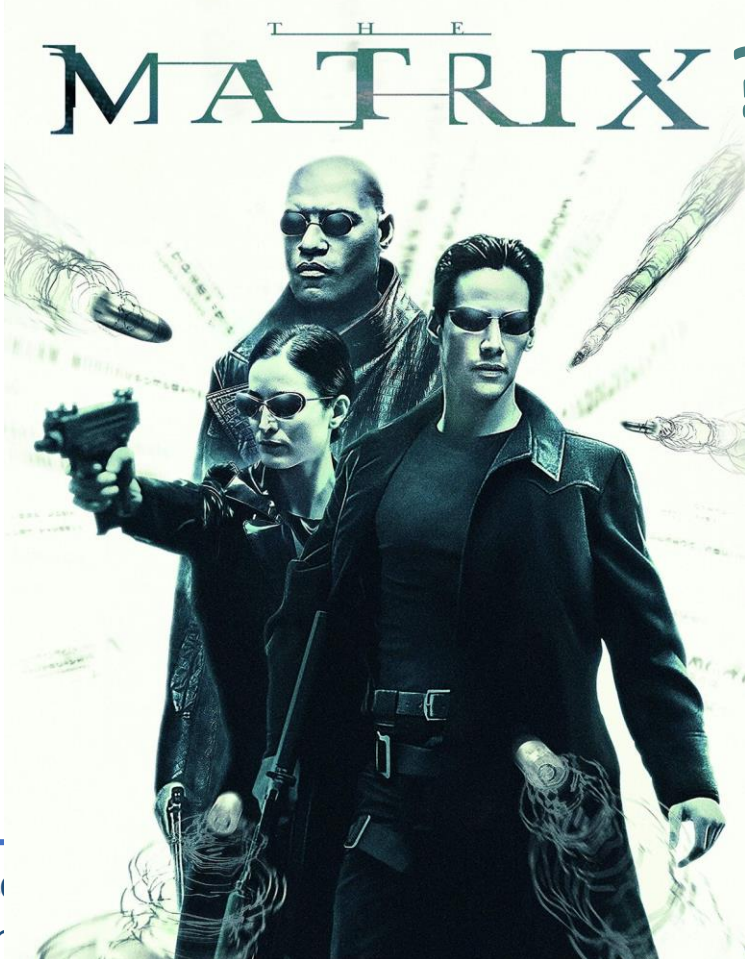
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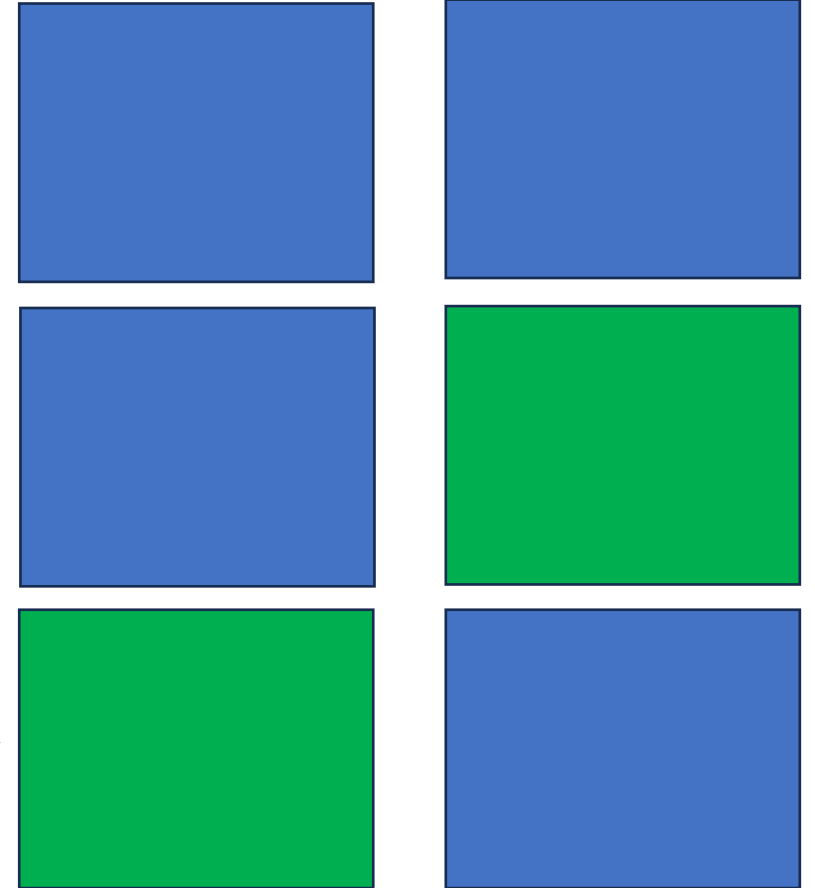
Residual DMD (ResDMD)

What's the missing



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

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



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

Residual DMD (ResDMD)

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

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

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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- C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," *Commun. Pure Appl. Math.*, 2023.
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Let's get precise!
Go to board...

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 $> 1/2$.

*Let's define "algorithm"!
Go to board...*

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Implies \mathcal{K} is unitary



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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 ...

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

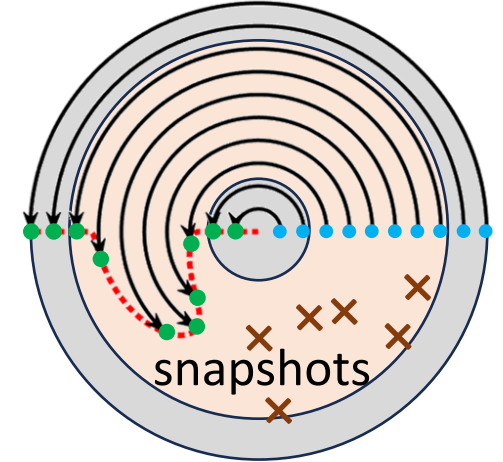
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Build an **adversarial** F ...

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

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



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

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

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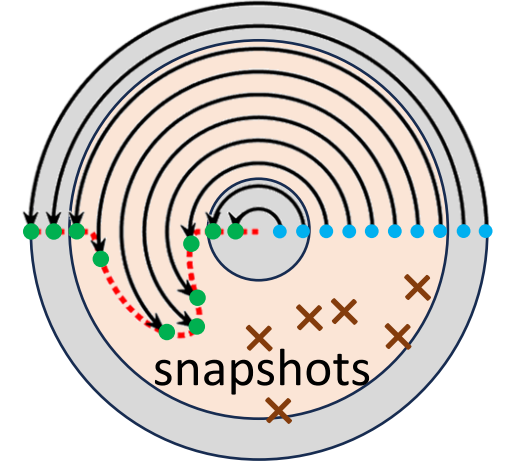
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$$\lim_{n \rightarrow \infty} \Gamma_n(\widetilde{F}_1) = \text{Sp}(\mathcal{K}_{\widetilde{F}_1}) \Rightarrow \exists n_1 \text{ s.t. } \text{dist}(i, \Gamma_{n_1}(\widetilde{F}_1)) \leq 1.$$

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

Let X, Y correspond to these snapshots.



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

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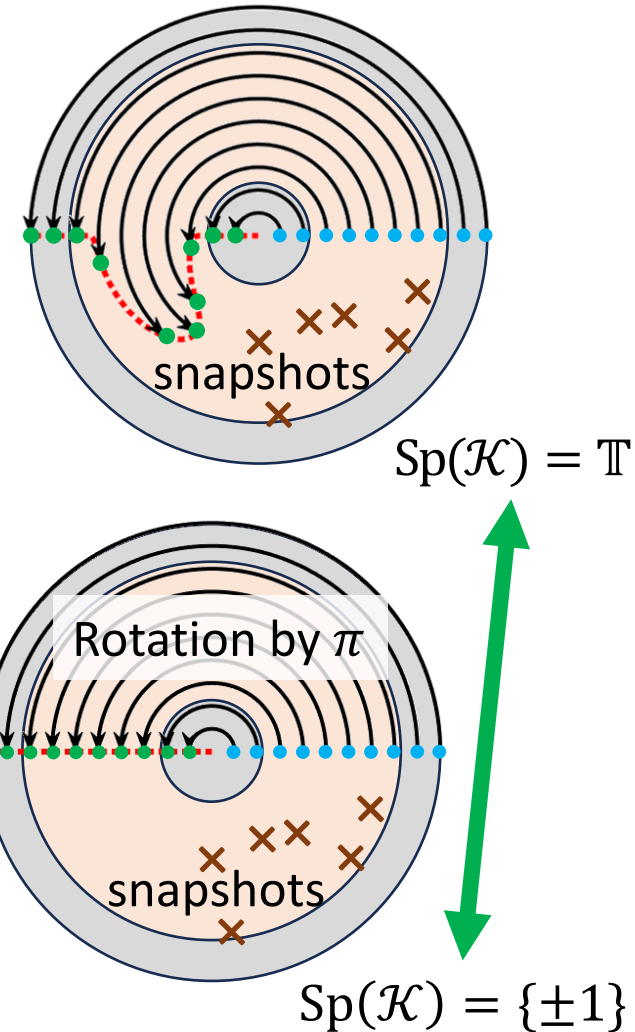
BUT Γ_{n_1} uses finite amount of info to output $\Gamma_{n_1}(\widetilde{F}_1)$.

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



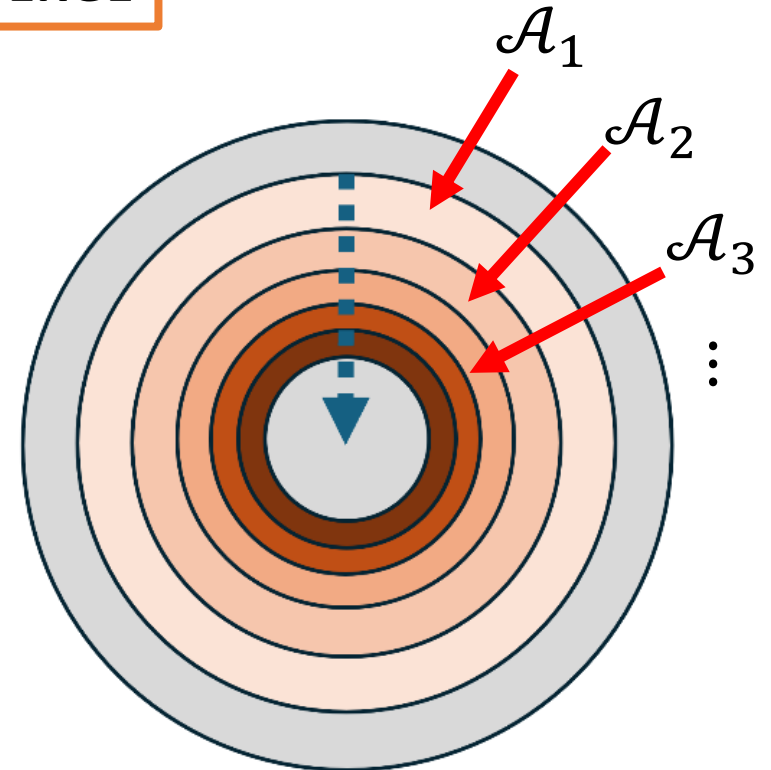
Proof idea: Constructing an adversary

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

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CANNOT CONVERGE



Cascade of disks

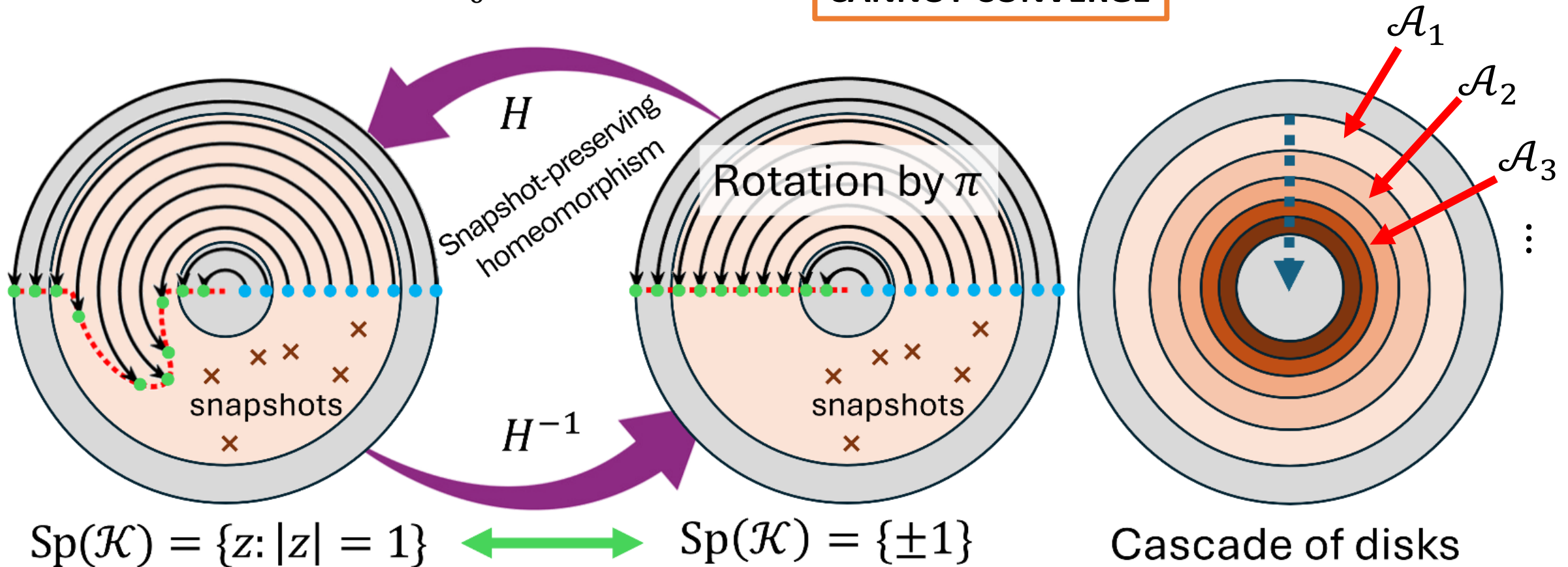
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BUT $\text{Sp}(\mathcal{K}_F) = \text{Sp}(\mathcal{K}_{F_0}) = \{\pm 1\}$

CANNOT CONVERGE



Theorem B (possibility using ResDMD ideas)

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

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

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

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.
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Classifications: *Solvability Complexity Index (SCI)*

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

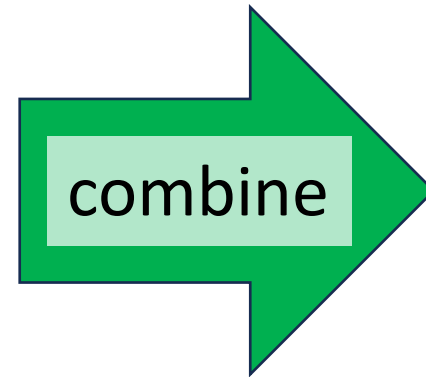
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Theorem A: $SCI > 1$

Theorem B: $SCI \leq 2$



$SCI = 2$

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

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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] 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) $\text{SCI} \leq 1$ (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. + ω 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 ∇F (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,...

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

- Δ_1 : One limit, full error control. E.g., $d(\Gamma_n(F), \text{Sp}(\mathcal{K}_F)) \leq 2^{-n}$.
- Δ_{m+1} : $\text{SCI} \leq m$.
- Σ_m : $\text{SCI} \leq m$, final limit from below.
E.g., $\Sigma_1: \Gamma_n(F) \subset \text{Sp}(\mathcal{K}_F) + B_{2^{-n}}(0)$.
- Π_m : $\text{SCI} \leq m$, final limit from above.
E.g., $\Pi_1: \text{Sp}(\mathcal{K}_F) \subset \Gamma_n(F) + B_{2^{-n}}(0)$.

-
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verification

trust output

covers spectrum

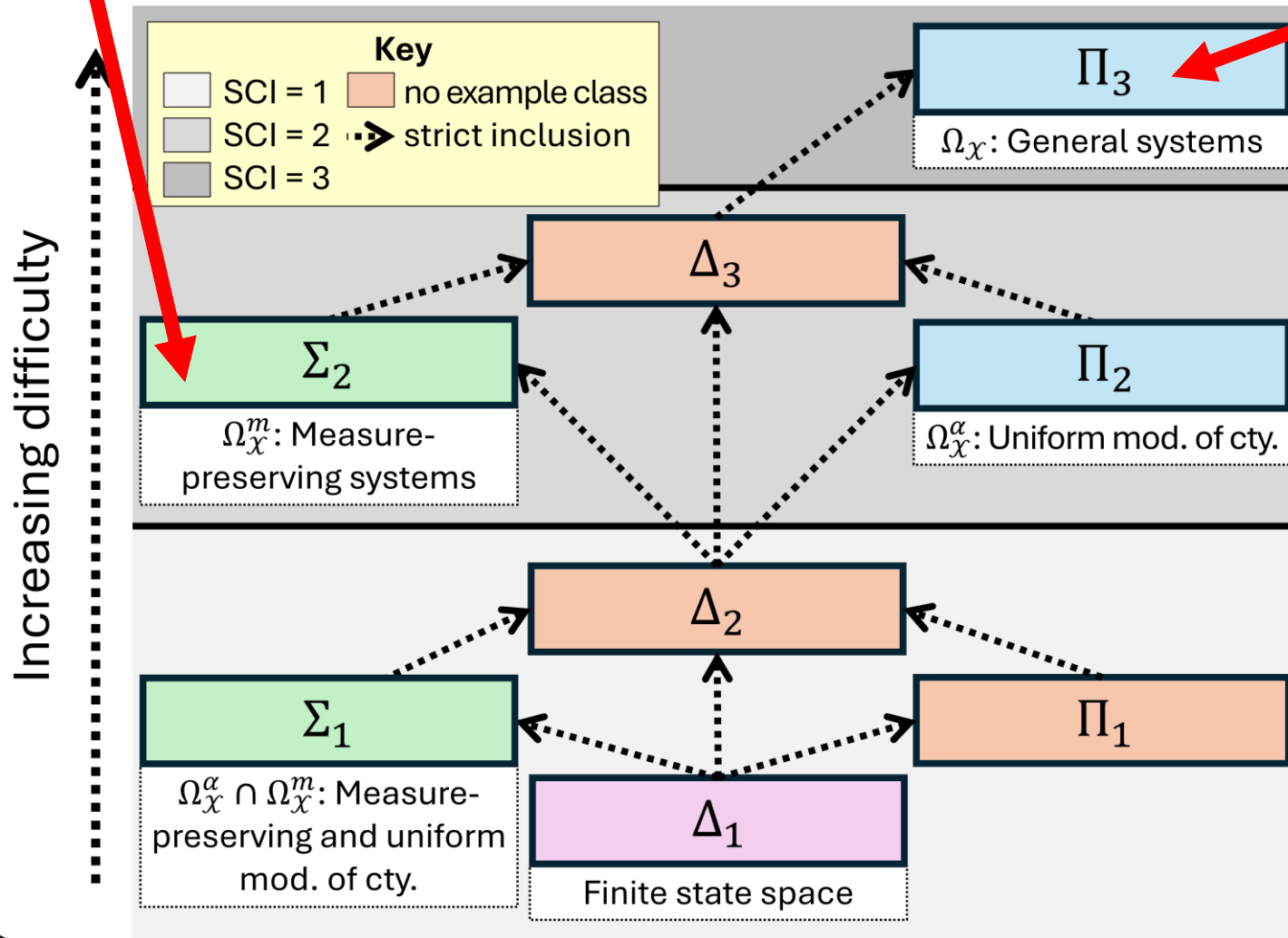
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Theorems A + B

Classification for Koopman I

3 limits needed
in general!

SCI hierarchy of computing the spectrum



Different classes:

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

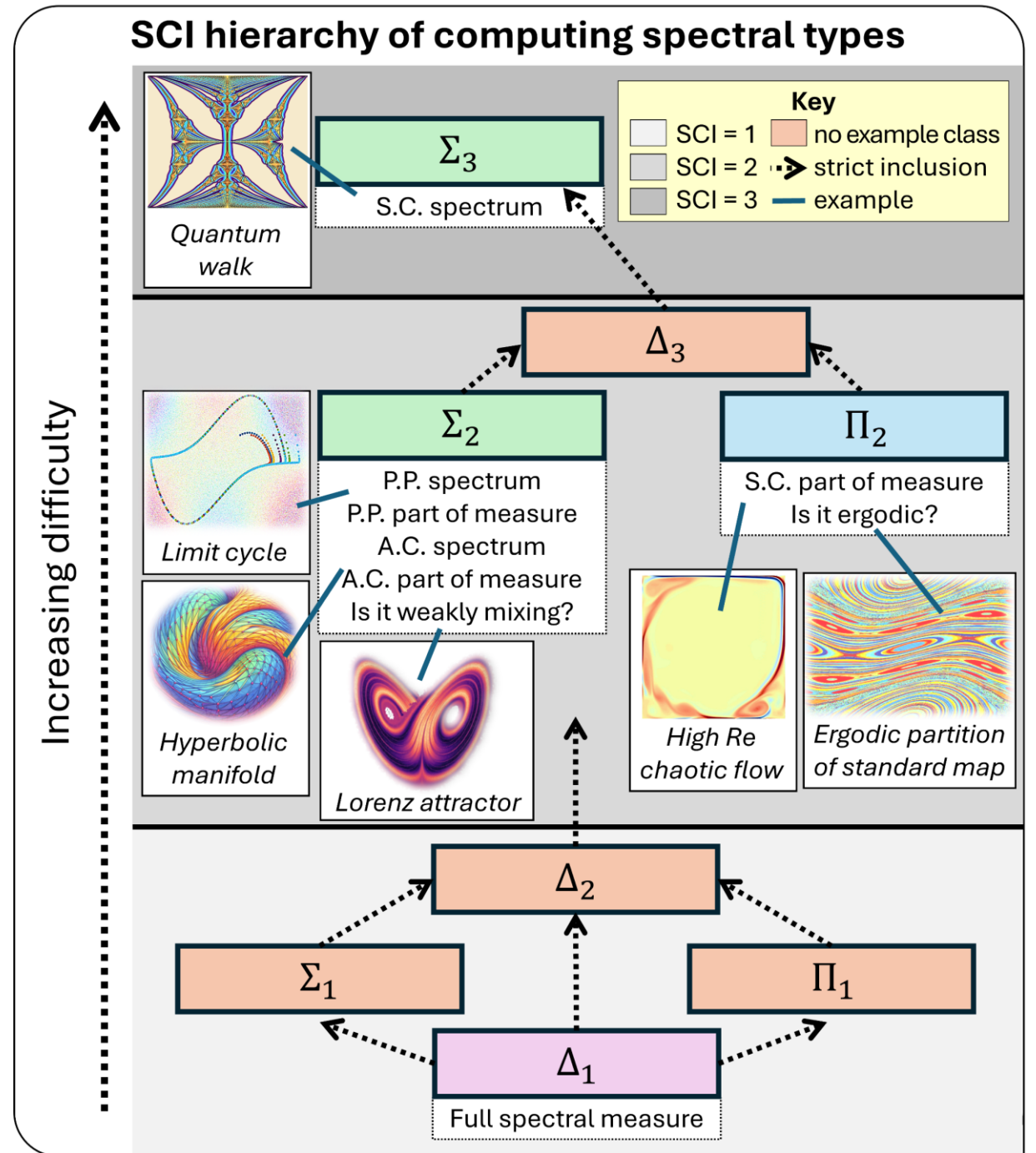
$$\Omega_X^m = \{F: X \rightarrow X \mid F \text{ cts, m. p.}\}$$

$$\Omega_X^\alpha = \{F: X \rightarrow X \mid F \text{ mod. ct'y. } \alpha\}$$

$$[d_X(F(x), F(y)) \leq \alpha(d_X(x, y))]$$

Optimal algorithms and
classifications of
dynamical systems.

Classification for Koopman II

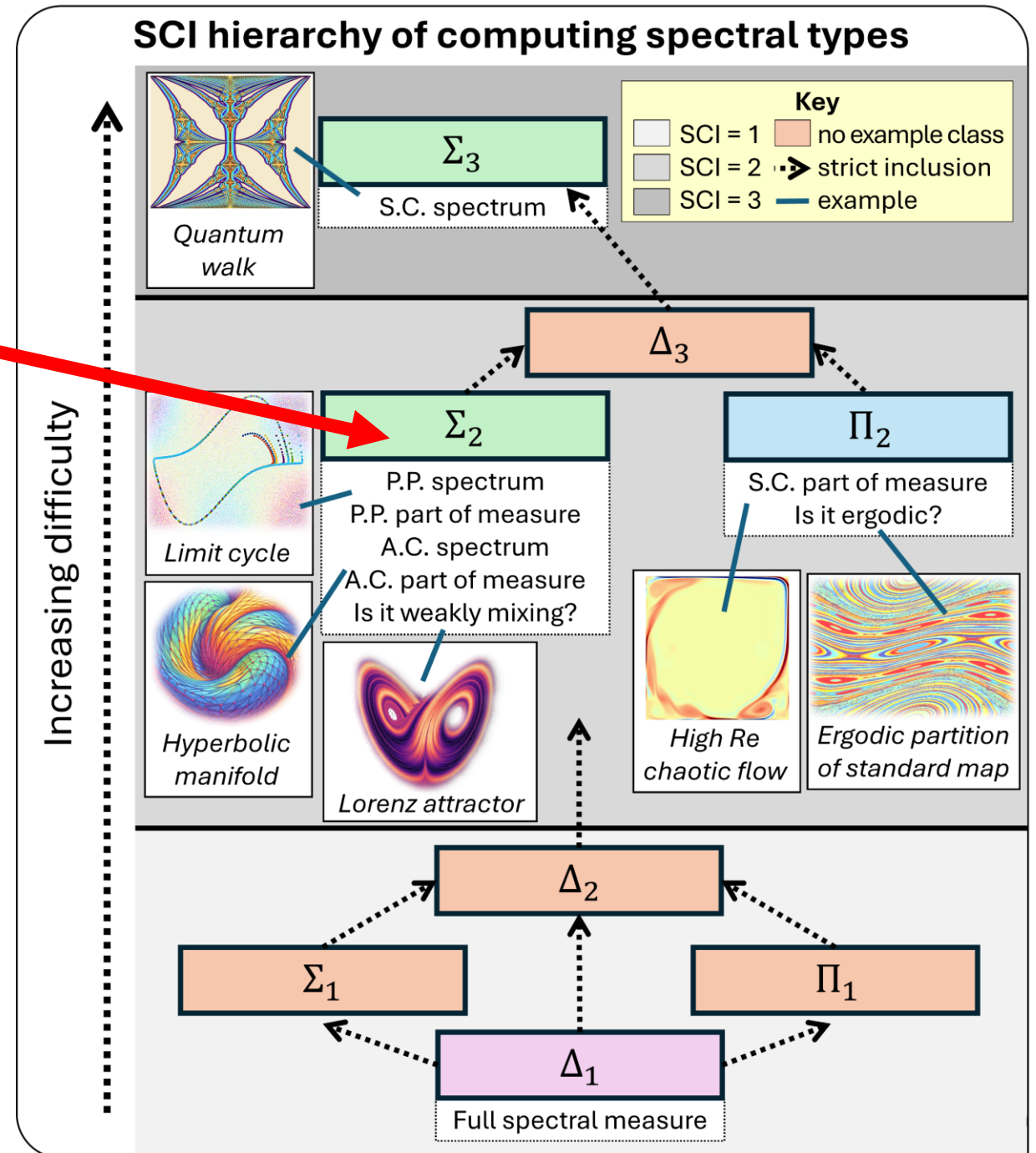


Classification for Koopman II

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)

-
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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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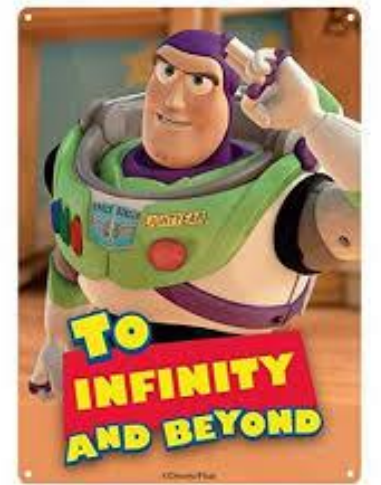
**Buzz
Lightyear
was right!**



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 - Partial observations, continuous-time.
 - Control and uses of Koopman.
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Where does your problem/method fit into the SCI hierarchy? Is it optimal?

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