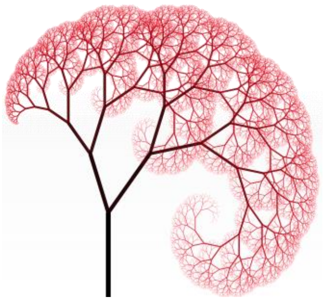

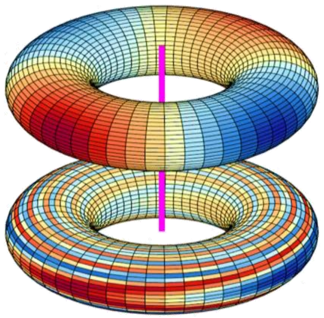

Classifications of Data-Driven Koopman Learning

Matthew Colbrook

University of Cambridge

9/07/2024

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

C., Mezić, Stepanenko *"Limits and Powers of Koopman Learning,"* preprint, 2024.
Will appear on arXiv this evening. If you cannot wait – visit
https:/www.damtp.cam.ac.uk/user/mjc249/home.html

The objects

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

cts $F: \mathcal{X} \to \mathcal{X}$ – 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 $\mathcal{K}_F: L^2 \to L^2$; $[\mathcal{K}_F g](x) = g(F(x))$
- ***Available*** Snapshot data: $\left\{\left(x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right): m = 1, \ldots, M\right\}$

NB: Pointwise definition of $\mathcal{K}_F$ needs $F\#\omega \ll \omega$ – this will hold throughout.
NB: $\mathcal{K}_F$ bounded equivalent to $\mathrm{d}F\#\omega/\mathrm{d}\omega \in L^\infty$ – this will hold throughout (can be dropped).

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Analysis
20th century

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The objects

- Compact metric space $(\mathcal{X}, d)$ – the state space
- $x \in \mathcal{X}$ – the state
- ***Unknown*** cts $F: \mathcal{X} \to \mathcal{X}$ – 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 $\mathcal{K}_F: L^2 \to L^2$; $[\mathcal{K}_F g](x) = g(F(x))$

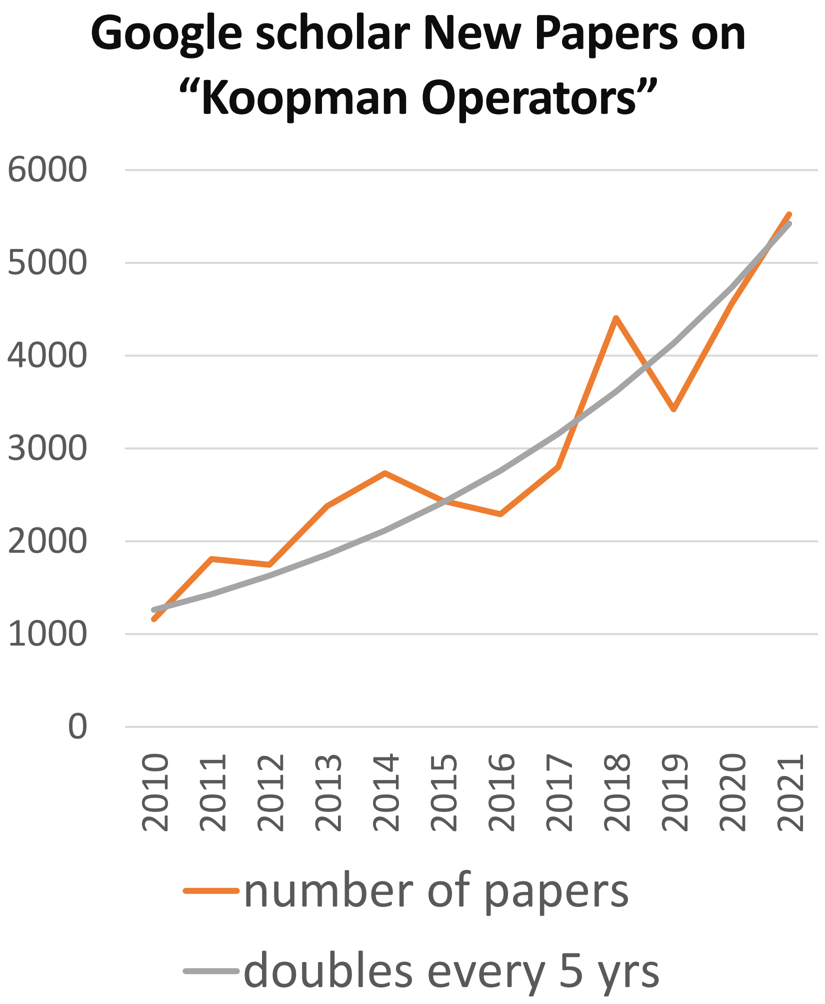
Analysis
20th century

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

Data
21st century

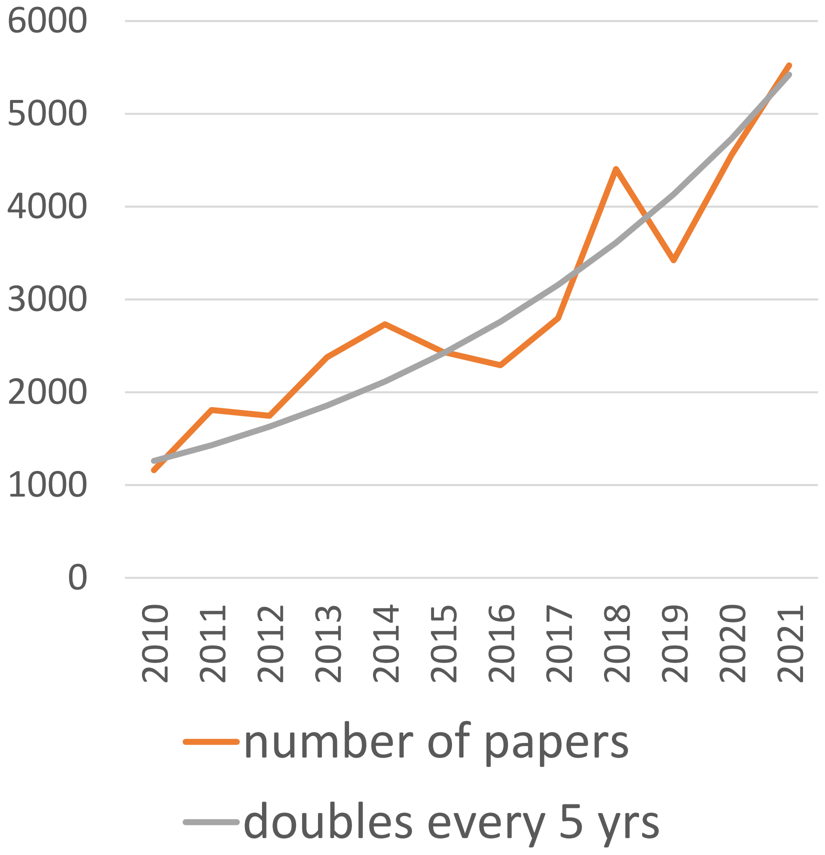
NB: Pointwise definition of $\mathcal{K}_F$ needs $F\#\omega \ll \omega$ – this will hold throughout.
NB: $\mathcal{K}_F$ bounded equivalent to $\mathrm{d}F\#\omega/\mathrm{d}\omega \in L^\infty$ – this will hold throughout (can be dropped).

The question



The question

Google scholar New Papers on "Koopman Operators"



2022

SIAM Review
Vol. 64, No. 2, pp. 229–340

Modern Koopman Theory for Dynamical Systems*

Steven L. Brunton†
Marko Budišić‡
Eurika Kaiser†
J. Nathan Kutz§

Abstract. The field of dynamical systems is being transformed by the mathematical tools and algorithms emerging from modern computing and data science. First-principles derivations and asymptotic reductions are giving way to data-driven approaches that formulate models in operator-theoretic or probabilistic frameworks. Koopman spectral theory has emerged as a dominant perspective over the past decade, in which nonlinear dynamics are represented in terms of an infinite-dimensional linear operator acting on the space of all possible
This linear representation of nonlinear dynamics
ie prediction, estimation, and control of nonlinear
ods developed for linear systems. However, obtain-
ns and embeddings in which the dynamics appear
open challenge. The success of Koopman analysis
1) there exists rigorous theory connecting it to clas-
al systems; (2) the approach is formulated in terms
veraging big data and machine learning techniques;
l algorithms, such as the dynamic mode decompo-
d extended to reduce Koopman theory to practice
iew, we provide an overview of modern Koopman
retical and algorithmic developments and highlight-
of applications. We also discuss key advances and
of machine learning that are likely to drive future
m the theoretical landscape of dynamical systems.

or, data-driven discovery, control theory, spectral
le decomposition, embeddings

0, 37M10, 37M99, 37N35, 47A35, 47B33

2012

CHAOS 22, 047510 (2012)

CrossMark

Applied Koopmanism[a)]

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 21 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 uncertain systems, which are more and more common in engin
"big data" measurements. This overview article presents an a
systems, based on the "dynamics of observables" picture. T
operator: an infinite-dimensional, linear operator that is nonet
nonlinear dynamics. The first goal of this paper is to make it
different papers and contexts all relate to each other through
operator. The second goal is to present these methods in a con
framework accessible to researchers who would like to apply
them. Finally, we aim to provide a road map through the lite
described in detail. We describe three main concepts: K
eigenquotients, and continuous indicators of ergodicity. For e
of theoretical concepts required to define and study them,
developed for their analysis, and, when possible, applicati
Koopman framework is showing potential for crossing over fr
industrial practice. Therefore, the paper highlights its strength
Additionally, we point out areas where an additional research p
adopted as an off-the-shelf framework for analysis and des
Physics. [http://dx.doi.org/10.1063/1.4772195]

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2024

The multiverse of dynamic mode decomposition algorithms

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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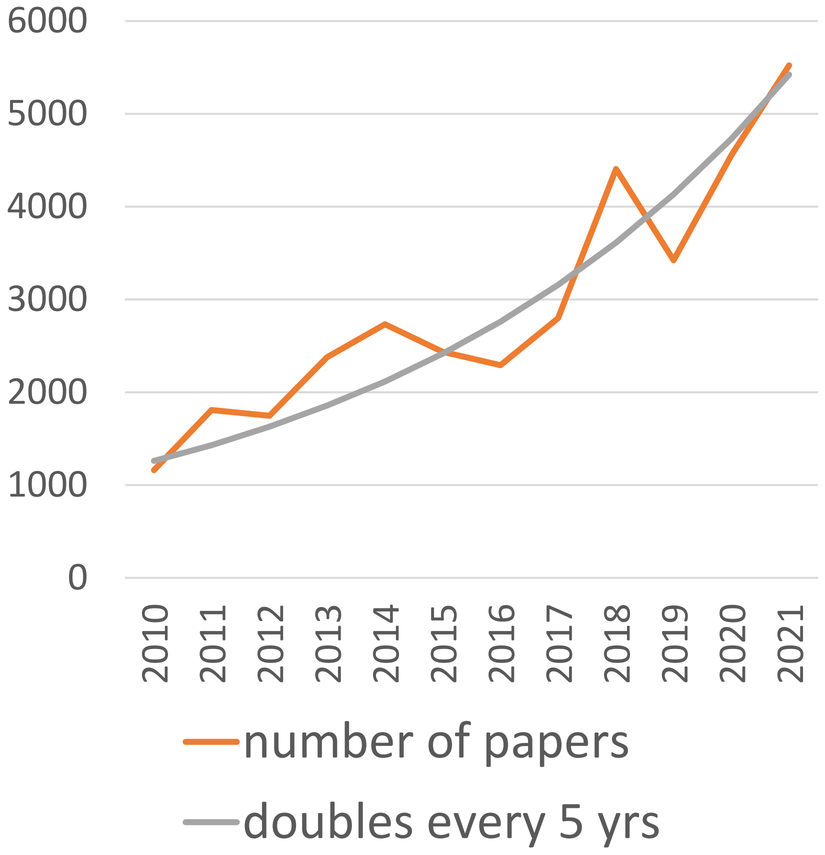

The question

2012

2022

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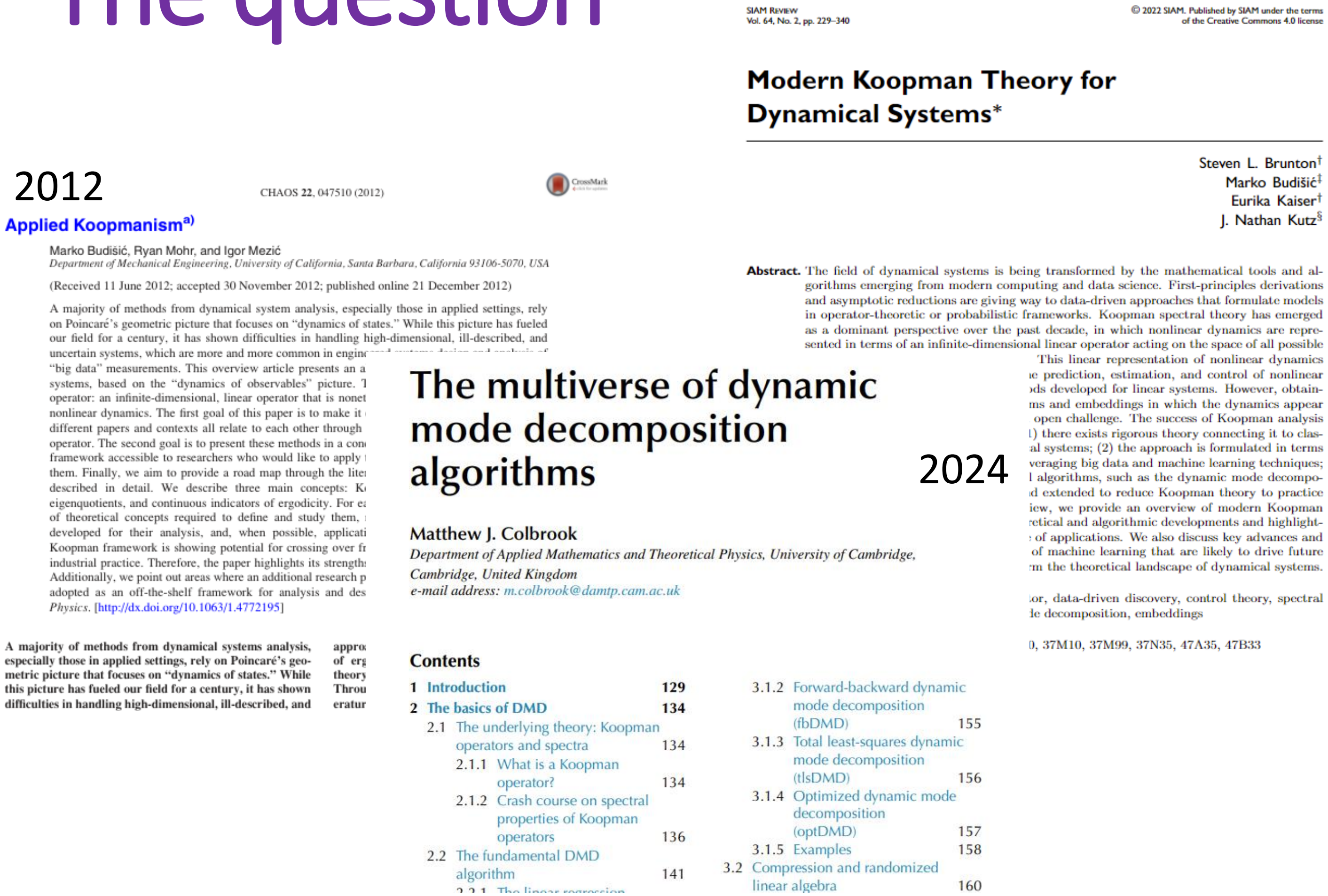

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The multiverse of dynamic mode decomposition algorithms

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Open question: ***When can we learn spectral properties of Koopman operators from trajectory data, and when can we not?***

Outline

- Constructing adversaries – *impossibility theorem*
- Towers of algorithms – *possibility theorem*
- The Solvability Complexity Index Hierarchy – *classifications*
- Where does this leave us?

Example: Theorem A (impossibility)

<u>*Class:*</u> $\Omega_{\mathbb{D}} = \{F: \mathbb{D} \to \mathbb{D} \text{ s.t. } F \text{ cts, measure preserving, invertible}\}$.

<u>*Perfect measurement device:*</u> $\mathcal{T}_F = \{(x, y_m): x \in \mathbb{D}, \|F(x) - y_m\| \leq 2^{-m}\}$.

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

- For **any** sequence of *random* algorithms $\{\Gamma_n\}$ that uses $\mathcal{T}_F$

$$\inf_{F\in\Omega_{\mathbb{D}}} \mathbb{P}\left(\lim_{n\to\infty} \Gamma_n(F) = \mathrm{Sp}(\mathcal{K}_F)\right) \leq 1/2.$$

No better than random chance

- Universal - any type of algorithm or computational model.
- Phase transition at $\mathbb{P} = 1/2$ optimal.
- Can learn statistics for $\Omega_{\mathbb{D}}$, doesn't help!
- Extends to other $\mathcal{X}$.

Proof idea (deterministic case)

F_0: rotation by π, $\mathrm{Sp}(\mathcal{K}_{F_0}) = \{\pm 1\}$ (easy exercise using Lap. efuns)

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 data ($x_j \to y_j$) 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 (deterministic case)

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

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

Inductively define an adversarial F.

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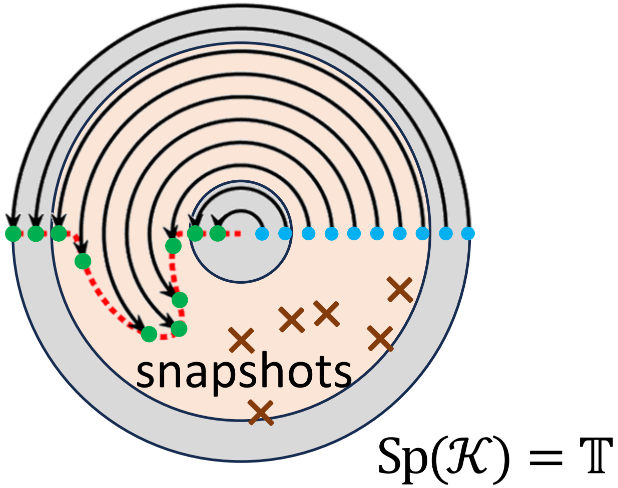
Inductively define an adversarial F.

Base: $\widetilde{F_1}(r,\theta) = \big(r, \theta + \pi + \phi(r)\big)$, $\mathrm{supp}(\phi) \subset [1/4, 3/4]$

Easy exercise: $\mathrm{Sp}(\mathcal{K}_{\widetilde{F_1}}) = \mathbb{T}$ (unit circle).



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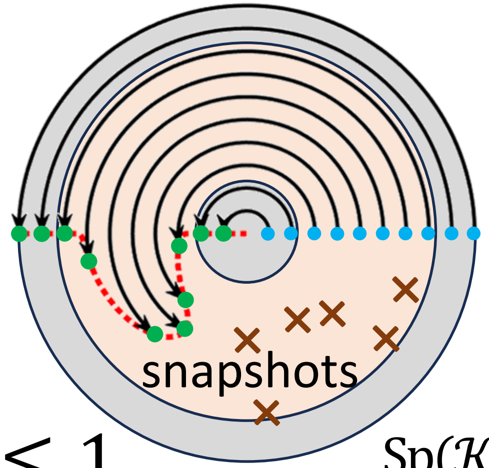

<u>Convergence</u> $\Gamma_n\big(\widetilde{F_1}\big) \to \mathrm{Sp}(\mathcal{K}_{\widetilde{F_1}}) \Rightarrow \exists n_1$ s.t. $\mathrm{dist}(i, \Gamma_{n_1}\big(\widetilde{F_1}\big)) \leq 1$.
BUT Γ_{n_1} reads finite amount of info when outputs $\Gamma_{n_1}\big(\widetilde{F_1}\big)$.
Let *X*, *Y* correspond to these finitely many snapshots.

Proof idea (deterministic case)

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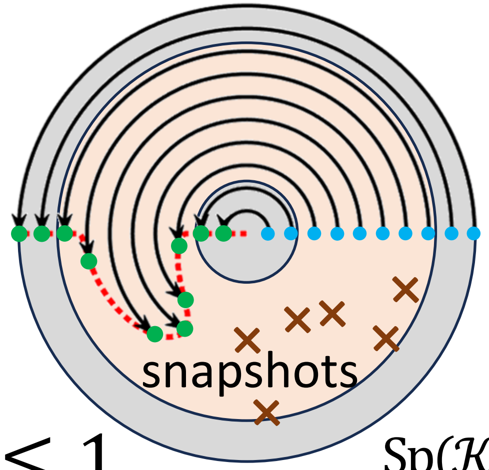

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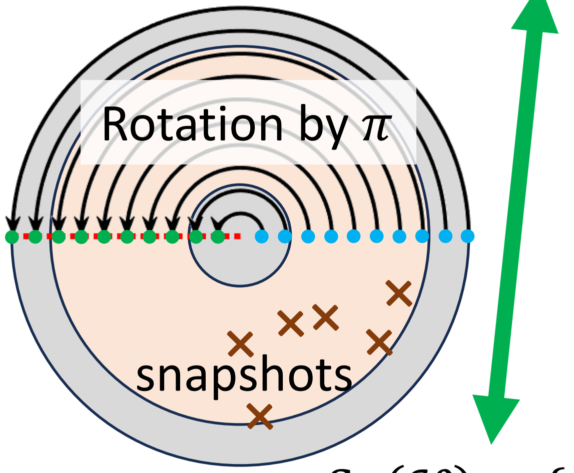


Apply lemma: $F_1 = H_1^{-1} \circ F_0 \circ H_1$ on annulus $\mathcal{A}_1$.
<u>Consistent data</u> $\Rightarrow \Gamma_{n_1}(F_1) = \Gamma_{n_1}(\widetilde{F_1})$, $\mathrm{dist}(i, \Gamma_{n_1}(F_1)) \leq 1$
BUT $\mathrm{Sp}(\mathcal{K}_{F_1}) = \mathrm{Sp}(\mathcal{K}_{F_0}) = \{\pm 1\}$

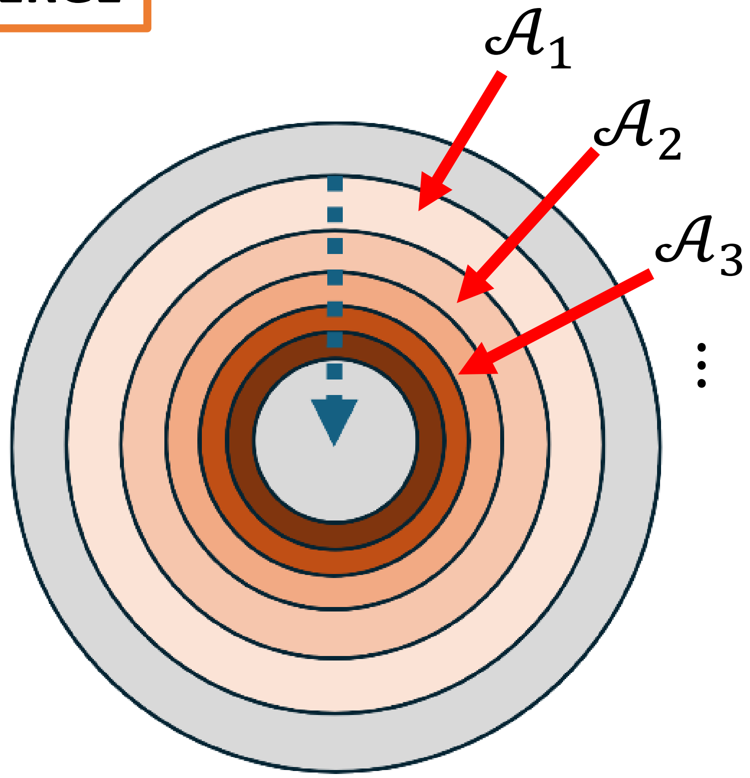
Proof idea (deterministic case)

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 (deterministic case)

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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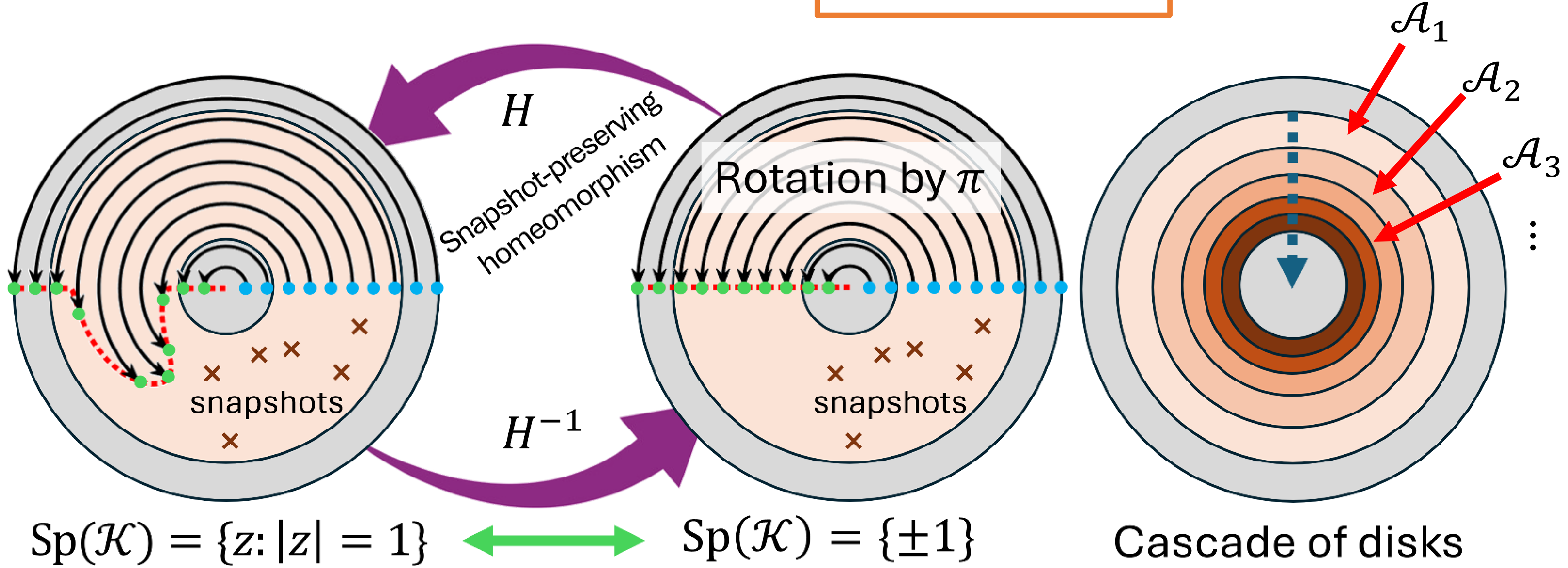

Example: Theorem B (possibility)

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Perfect measurement device: $\mathcal{T}_F = \{(x, y_m): x \in \mathcal{X}, \|F(x) - y_m\| \le 2^{-m}\}$.

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

Note the double limit $\lim_{n_2\to\infty}\lim_{n_1\to\infty}$

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

Proof sketch

- Apply a double limit: $\lim_{N\to\infty} \lim_{M\to\infty} \gamma_{N,M}(F,z) = \|(\mathcal{K}_F - zI)^{-1}\|^{-1}$.

$\boldsymbol{N}$ = size of dictionary, $\boldsymbol{M}$ = number of snapshots.

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  N = size of dictionary, M = number of snapshots.

- For measure-preserving systems: $\|(\mathcal{K}_F - zI)^{-1}\|^{-1} = \mathrm{dist}(z, \mathrm{Sp}(\mathcal{K}_F))$.

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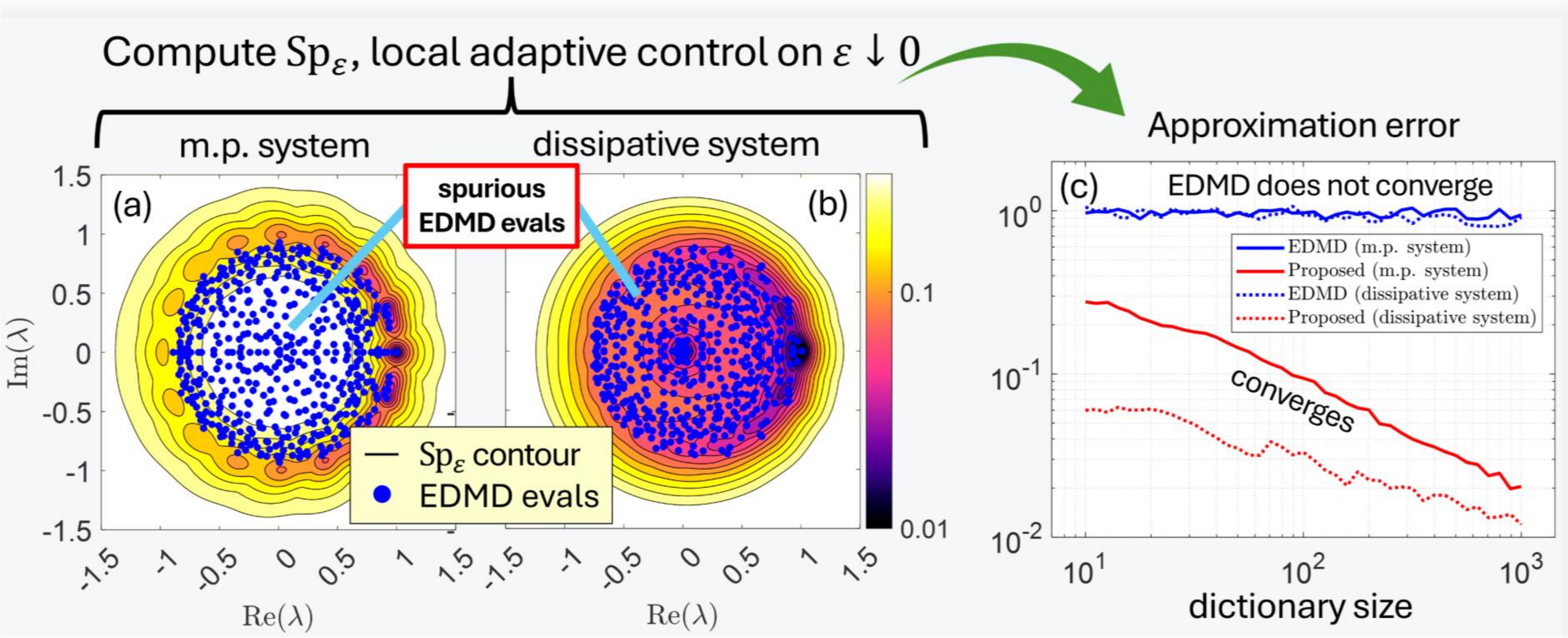

Towers of algorithms

Call $\{\Gamma_{n_k,\dots,n_1}\}$ with $\lim_{n_k\to\infty} \dots \lim_{n_1\to\infty} \Gamma_{n_k,\dots,n_1}$ convergent a **tower of algorithms.**

algorithm

First appeared in dynamical systems theory:

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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Theorem A: $\text{SCI} > 1$

Theorem B: $\text{SCI} \leq 2$

combine → $\text{SCI} = 2$

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combine

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

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

Previous techniques prove upper bounds on SCI. "N/C": method need not converge without additional strong assumptions (e.g., observable inside a known finite-dimensional invariant subspace) "n/a": indicates algorithm not applicable to problem.

Appears also in Ulam's method, computation of SRB measures, control,…

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

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

- Hansen, "On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators." **J. Am. Math. Soc.**, 2011.
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verification

trust output

covers spectrum

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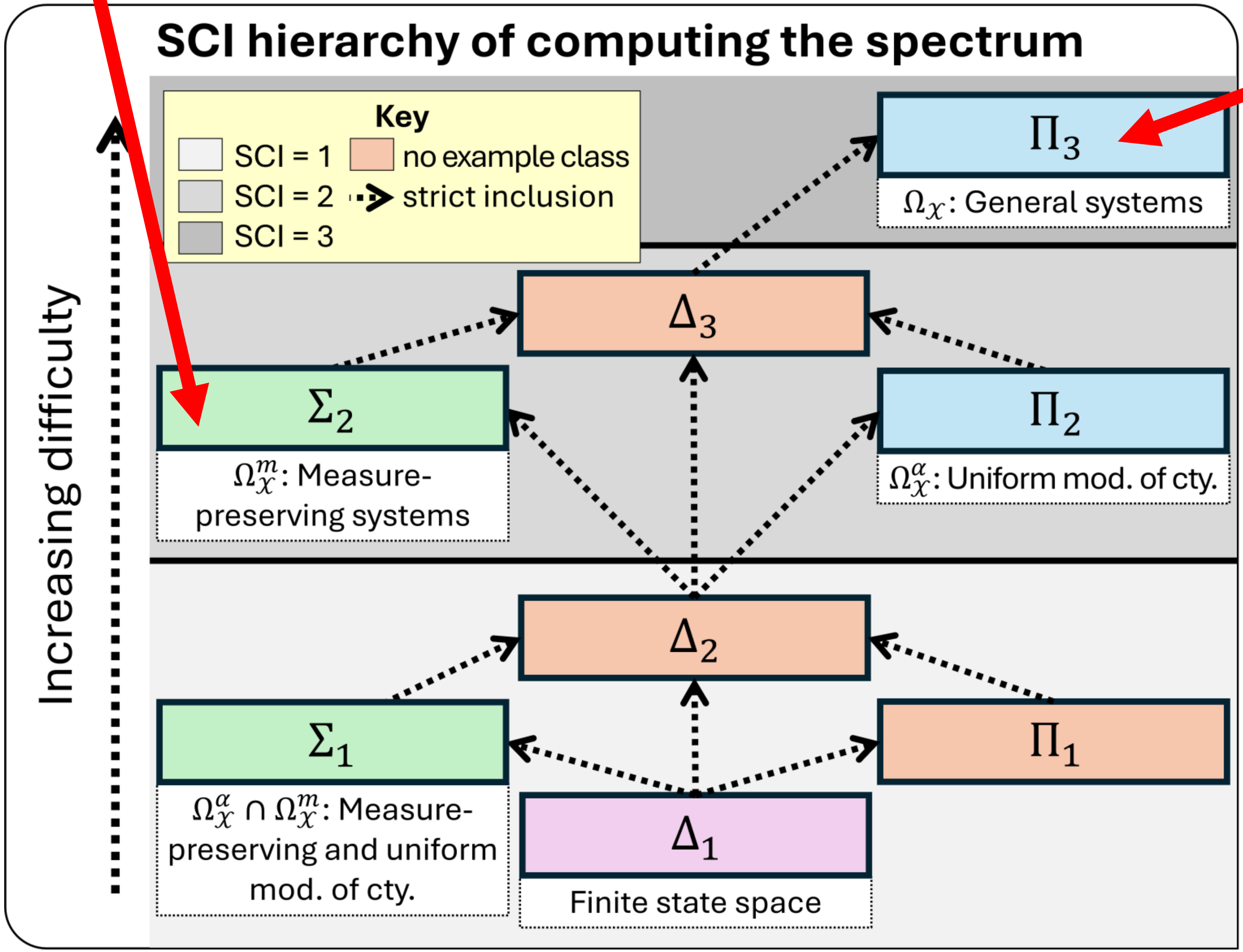
SCI for Koopman I

Theorems A + B

3 limits needed in general!



Different classes:

$$\Omega_{\mathcal{X}} = \{F: \mathcal{X} \to \mathcal{X} \text{ s.t. } F \text{ cts}\}$$

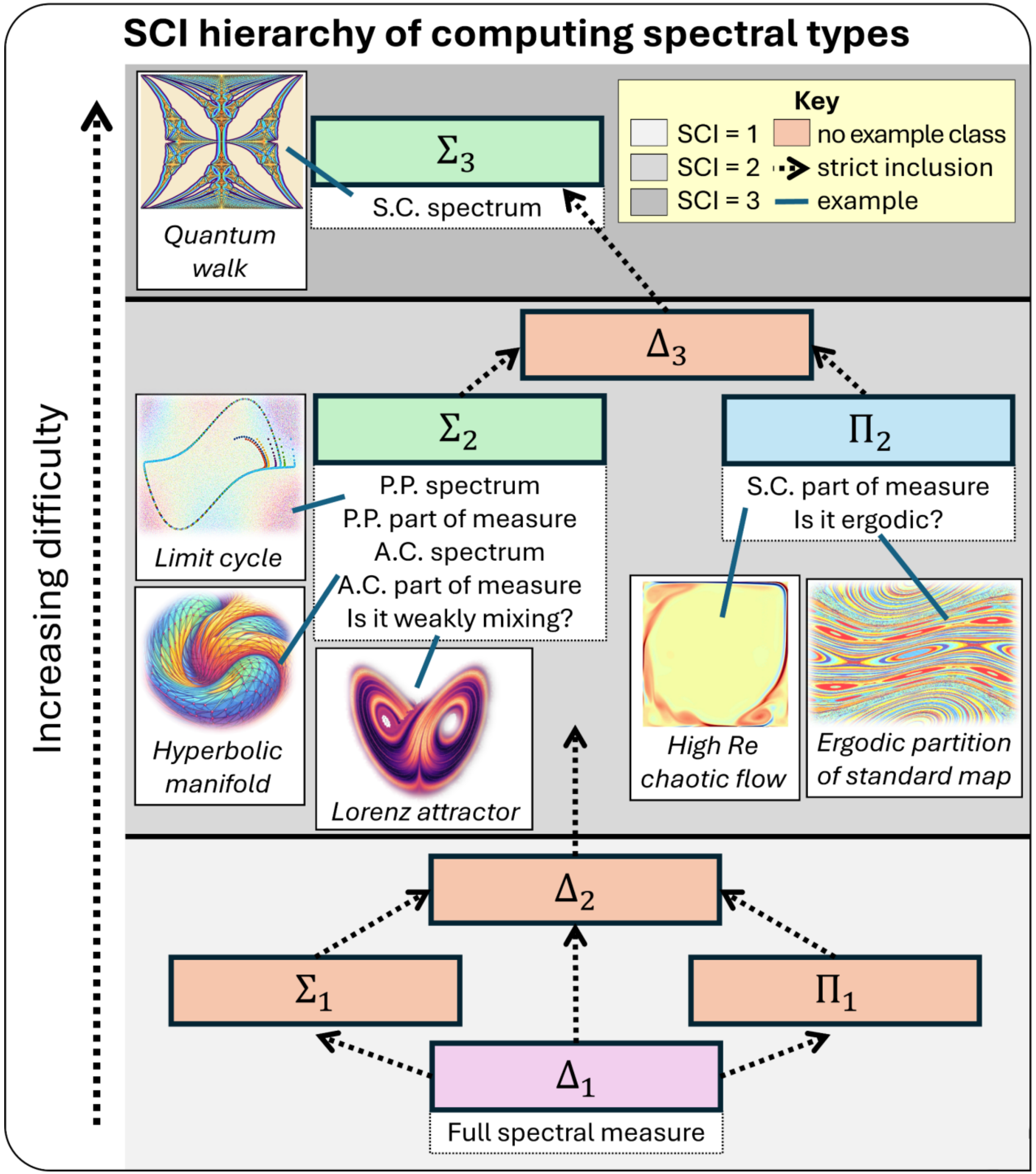
$$\Omega_{\mathcal{X}}^m = \{F: \mathcal{X} \to \mathcal{X} \text{ s.t. } F \text{ cts, m.p.}\}$$

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

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

Optimal algorithms and classifications of dynamical systems.

SCI for Koopman II

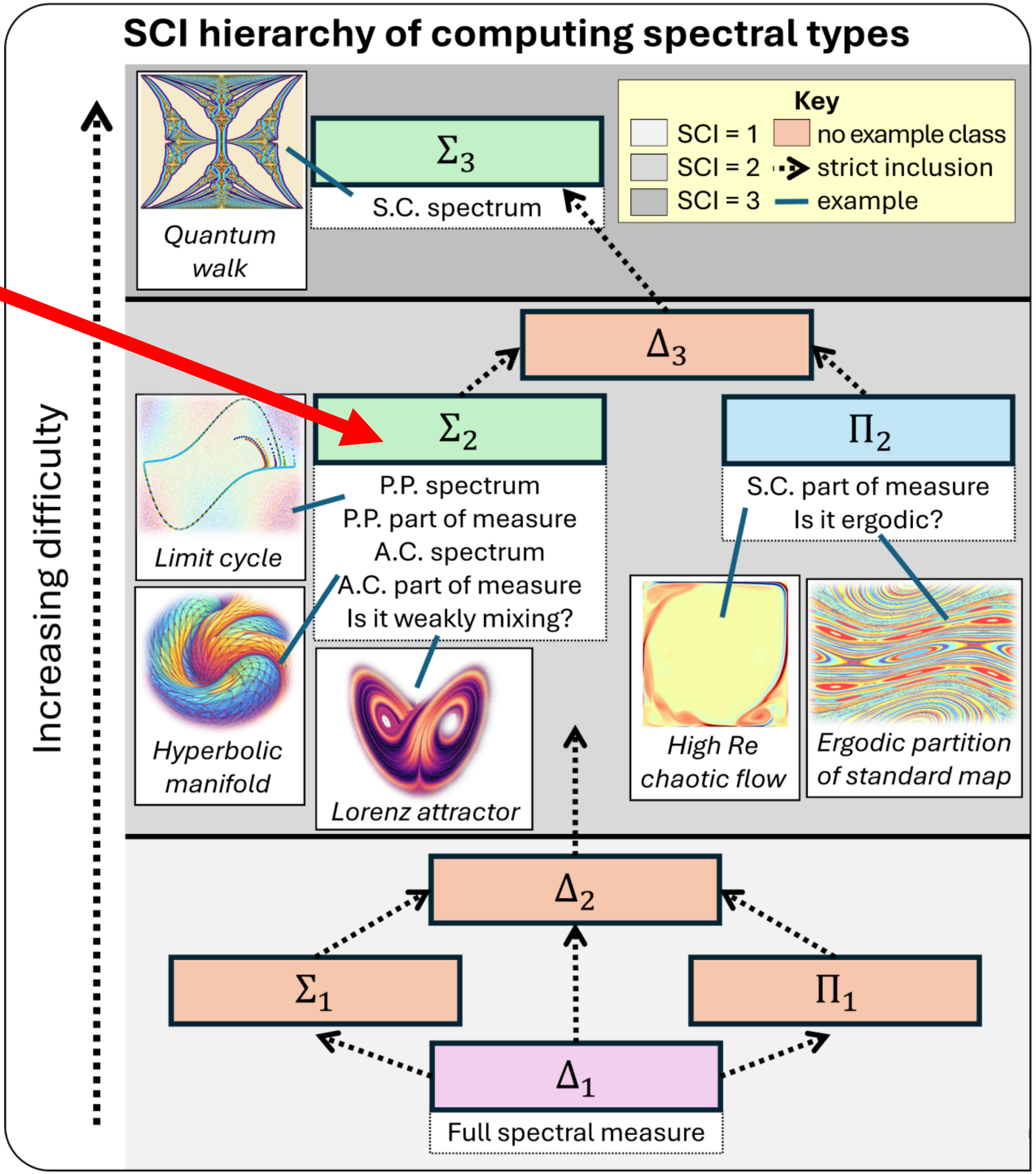


SCI for Koopman II

Example: Theorem C
For smooth, m.p. on a torus, learning non-trivial eigenfunctions or even determining if there are any has $\mathrm{SCI} = 2$ (even if we can sample derivatives).

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

NB: Constant is trivial efun, others “non-trivial”!



Where does this leave us?

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

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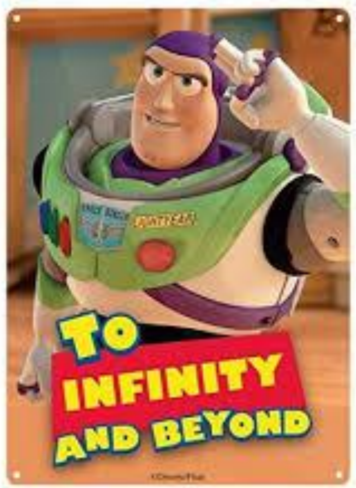

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- Future work:
  - Other function spaces.
  - Partial observations, continuous-time.
  - Control and uses of Koopman.
  - Other data-driven dynamical system methods.

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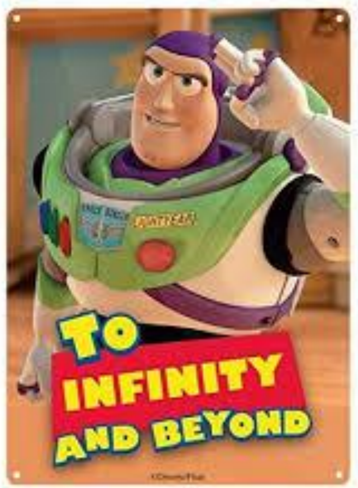

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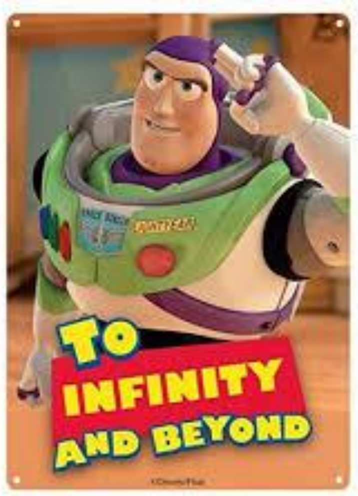

Where does your method fit into the SCI hierarchy? Is it optimal?

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