

Barriers and Classifications of Robust Koopman Learning

Matthew Colbrook

University of Cambridge

15/08/2024

Ask at end ;)

“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>

What on earth is a Koopman operator?

- 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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20th century

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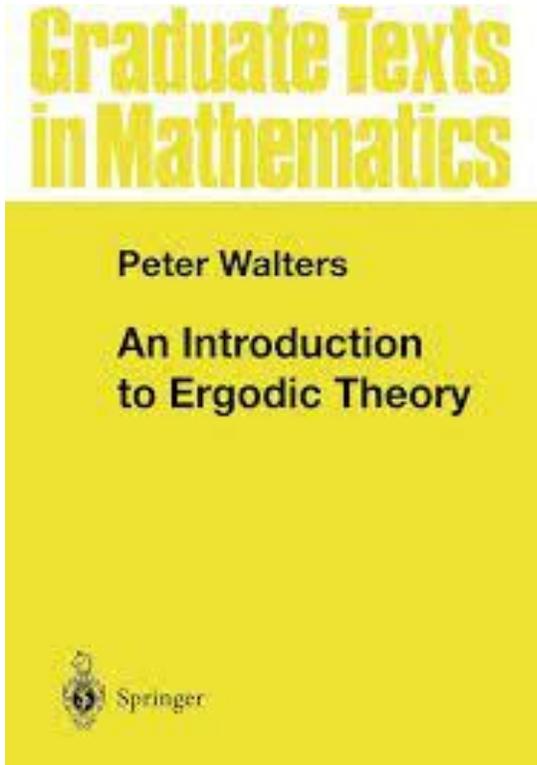
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- Analysis
20th century
- Data
21st century

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Why should you care?

Fundamental in ergodic theory

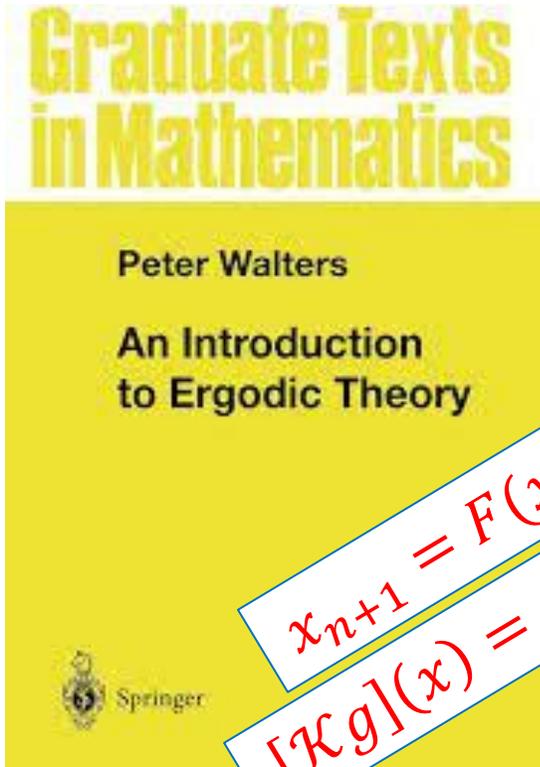


E.g., key to ergodic theorems of Birkhoff and von Neumann.

Why should you care?

Fundamental in ergodic theory

Can provide a *diagonalization* of a nonlinear system.



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

$$[K g](x) = g(F(x))$$

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

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

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

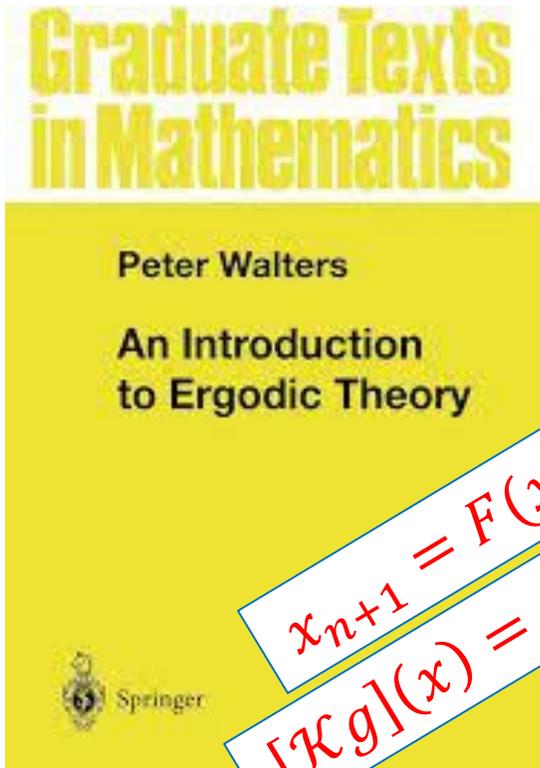
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Spectral properties encode: geometric features, invariant measures, transient behavior, long-time behavior, coherent structures, quasiperiodicity, etc.

Why should you care?

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

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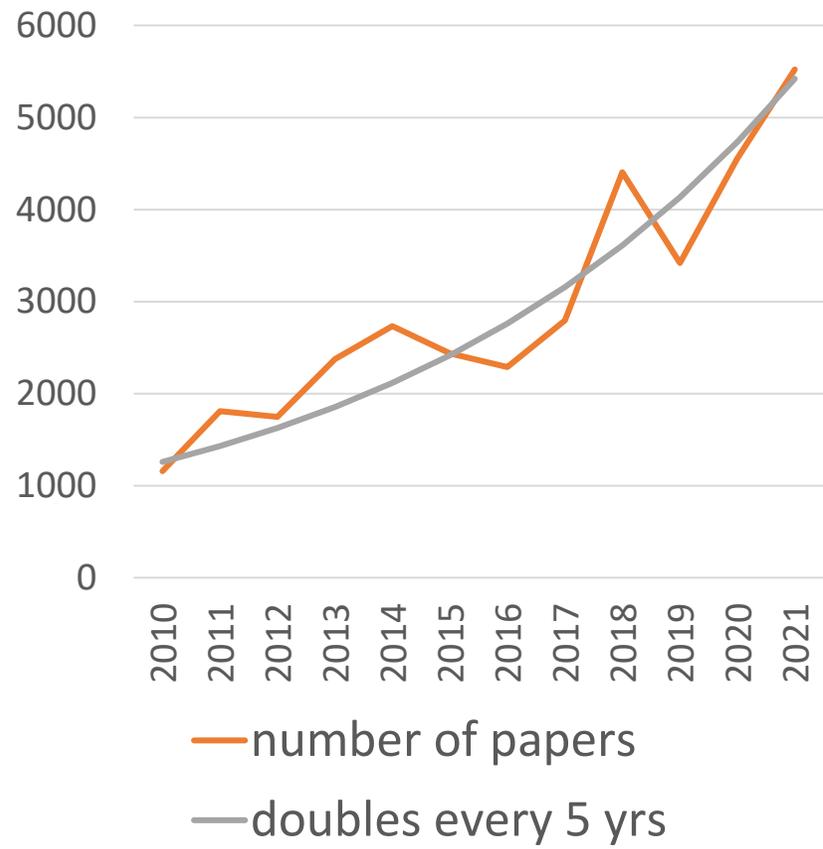
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Birkhoff and v

+ interest in their spectral properties... me
....., etc.

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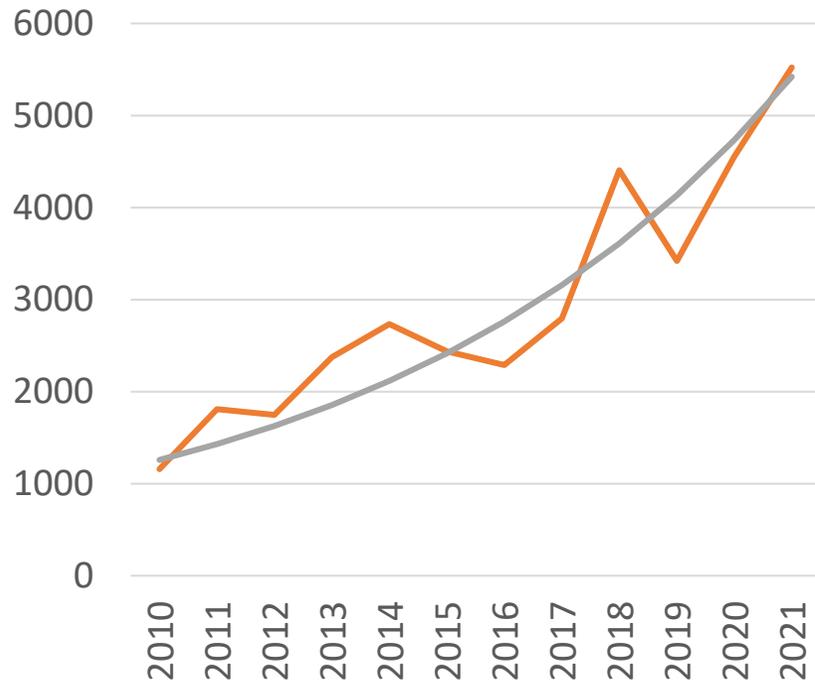
Google scholar New Papers on "Koopman Operators"



Ubiquitous in data-driven era

Loads of applications!!!

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— number of papers
 — doubles every 5 yrs

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2012

CHAOS 22, 047510 (2012)



Applied Koopmanism^{a)}

Marko Budišić, Ryan Mohr, and Igor Mezic
 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 engine “big data” measurements. This overview article presents an systems, based on the “dynamics of observables” picture. The 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 com 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: Ko eigenquotients, and continuous indicators of ergodicity. For ei 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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SIAM Review
 Vol. 64, No. 2, pp. 229–340

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Modern Koopman Theory for Dynamical Systems*

Steven L. Brunton[†]
 Marko Budišić[‡]
 Eureka 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 is prediction, estimation, and control of nonlinear systems developed for linear systems. However, obtaining and embeddings in which the dynamics appear open challenge. The success of Koopman analysis (1) there exists rigorous theory connecting it to classical systems; (2) the approach is formulated in terms leveraging big data and machine learning techniques; (3) algorithms, such as the dynamic mode decomposition extended to reduce Koopman theory to practice (e.g., we provide an overview of modern Koopman spectral and algorithmic developments and highlight key applications. We also discuss key advances and of machine learning that are likely to drive future research in the theoretical landscape of dynamical systems.

for, data-driven discovery, control theory, spectral decomposition, embeddings

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

The multiverse of dynamic mode decomposition algorithms

2024

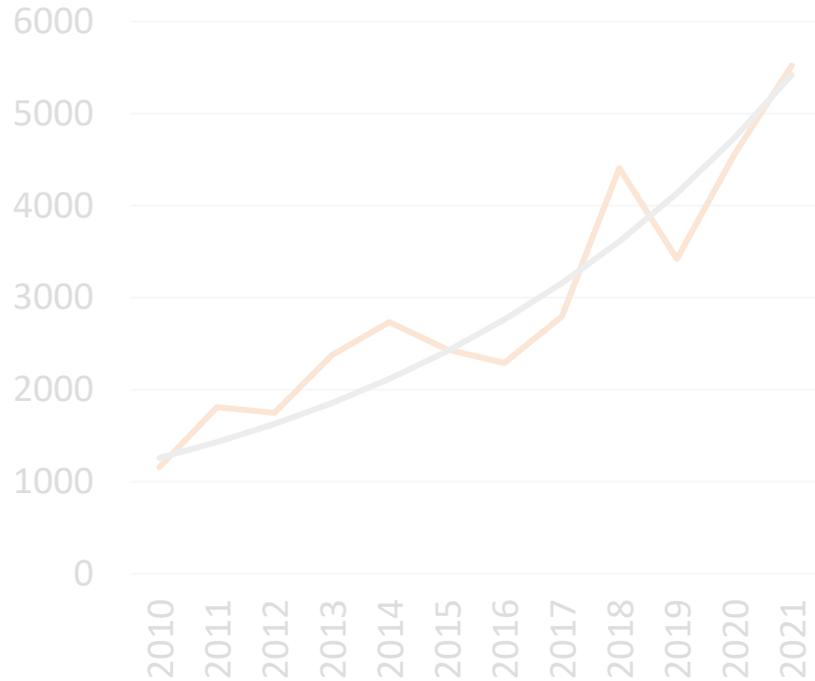
Matthew J. Colbrook

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2.2	The fundamental DMD algorithm	141	3.2	Compression and randomized linear algebra
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Open question: *When can we learn spectral properties of Koopman operators from trajectory data, and when can we not?*

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2.2.1	The linear case				

Outline

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

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

Example: Theorem A (impossibility)

Implies \mathcal{K} is unitary



$\Omega_{\mathbb{D}} = \{F: \mathbb{D} \rightarrow \mathbb{D} \mid F \text{ cts, measure preserving, invertible}\}.$

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

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: Impossibility extends to random algorithms converging with probability $> 1/2$.

Proof idea

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

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

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

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 ...

Proof idea

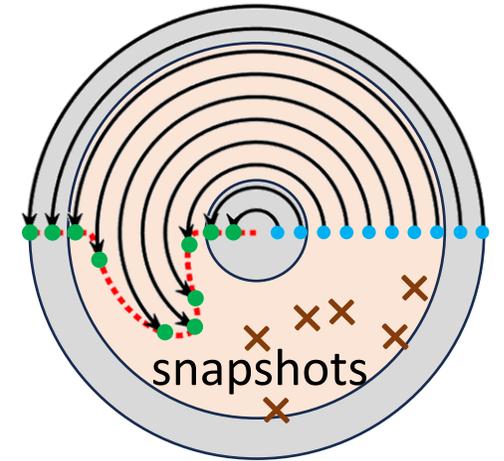
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Build an **adversarial** F ...

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

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



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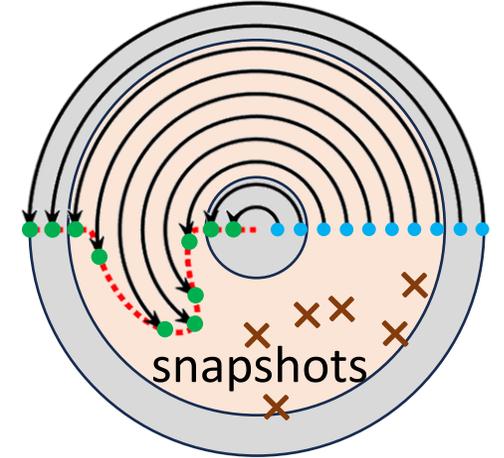
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$$\lim_{n \rightarrow \infty} \Gamma_n(\widetilde{F}_1) = \text{Sp}(\mathcal{K}_{\widetilde{F}_1}) \Rightarrow \exists n_1 \text{ s.t. } \text{dist}(i, \Gamma_{n_1}(\widetilde{F}_1)) \leq 1.$$

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

Let X, Y correspond to these snapshots.



Proof idea

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

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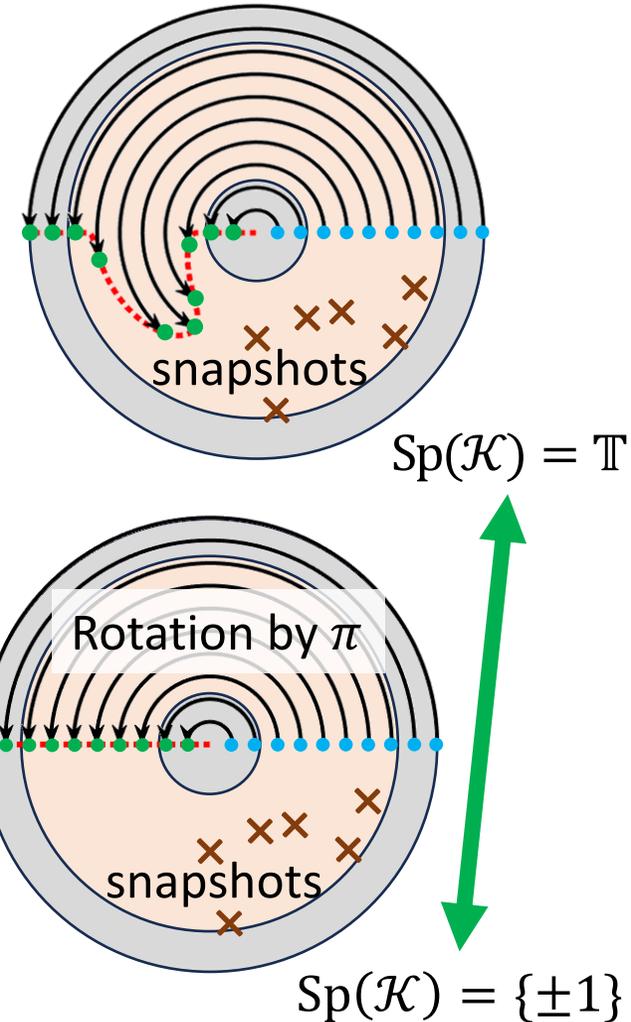
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Lemma: $F_1 = H_1^{-1} \circ F_0 \circ H_1$ on annulus \mathcal{A}_1 .

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

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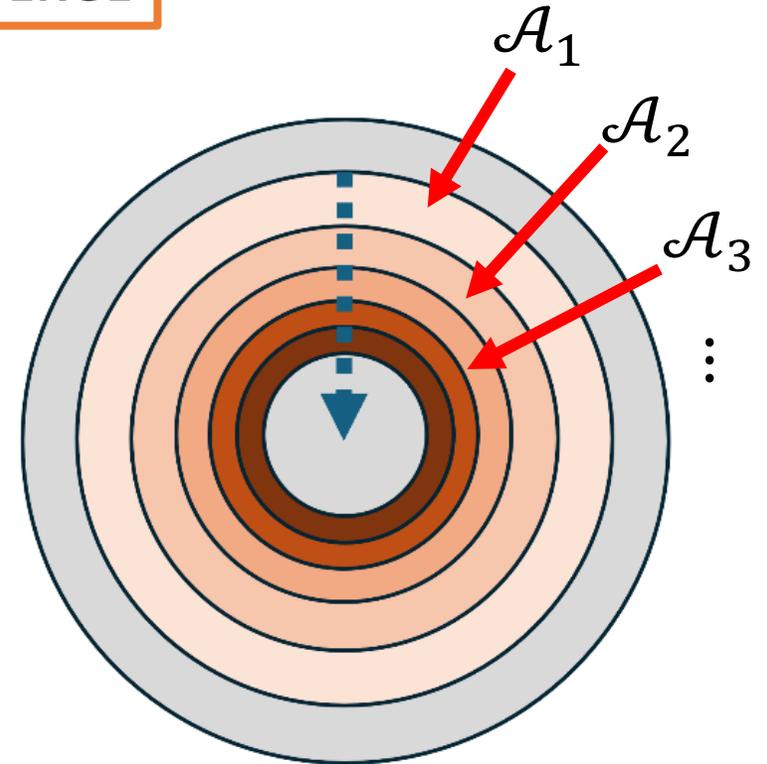
Proof idea (deterministic case)

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

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CANNOT CONVERGE



Cascade of disks

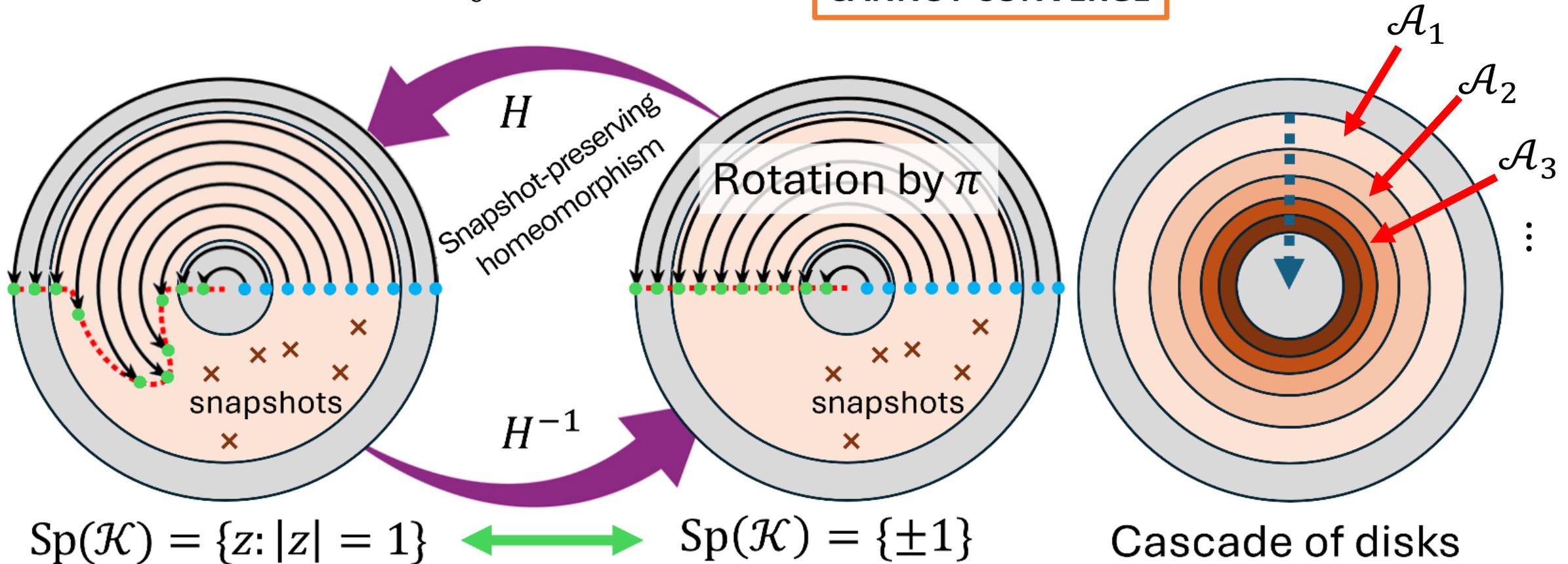
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CANNOT CONVERGE



Example: Theorem B (possibility)

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

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

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

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

Proof sketch

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

N = size of basis, M = number of snapshots (quadrature).

Proof sketch

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- Measure-preserving $\Rightarrow \|(\mathcal{K}_F - zI)^{-1}\|^{-1} = \text{dist}(z, \text{Sp}(\mathcal{K}_F))$.

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- 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 $\text{Sp}(\mathcal{K}_F)$

Proof sketch

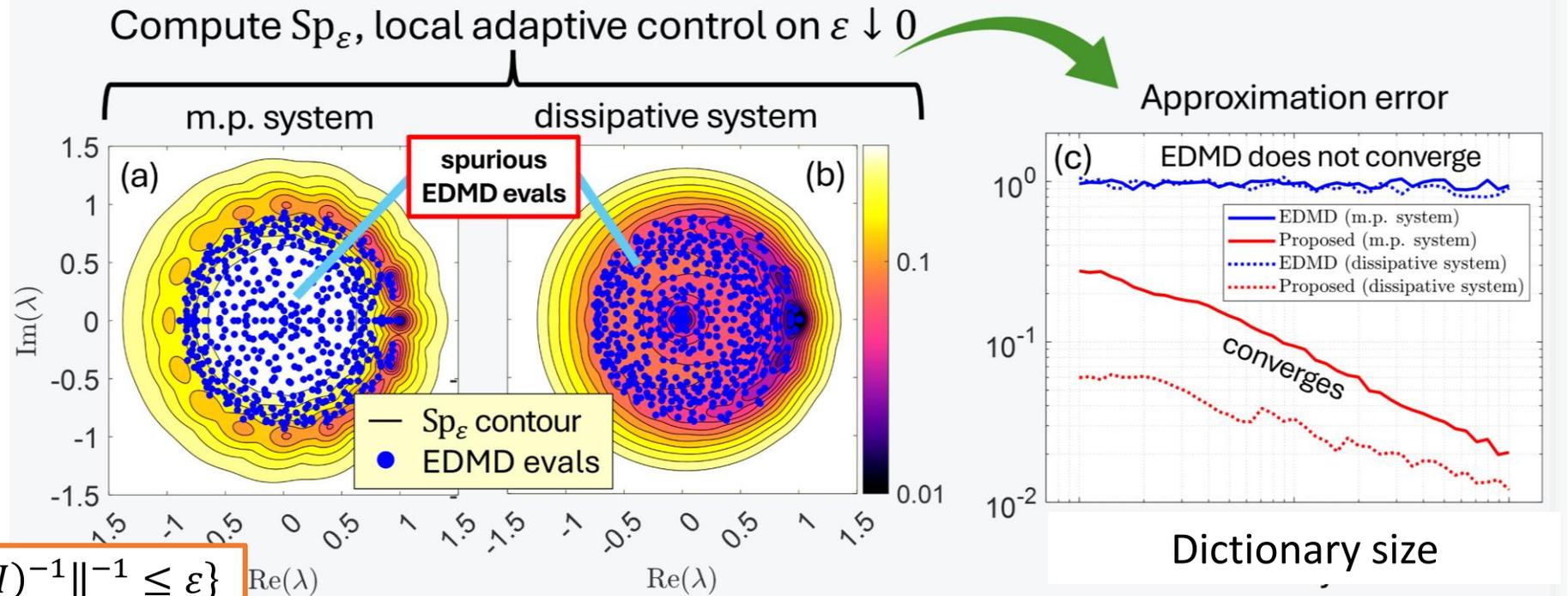
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- Local N -adaptive minimisation of $\gamma_{N,M}(F, z)$ to approximate $\text{Sp}(\mathcal{K}_F)$

“Extended Dynamic Mode Decomposition” is essentially the finite section method.



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:

algorithm



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.

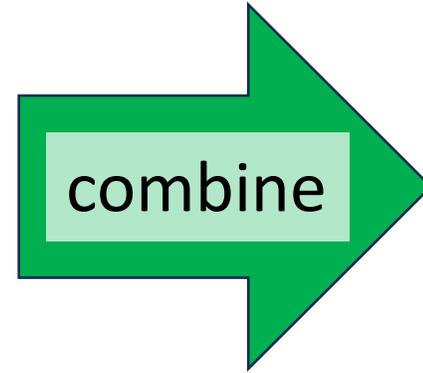
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Theorem A: $SCI > 1$

Theorem B: $SCI \leq 2$



$SCI = 2$

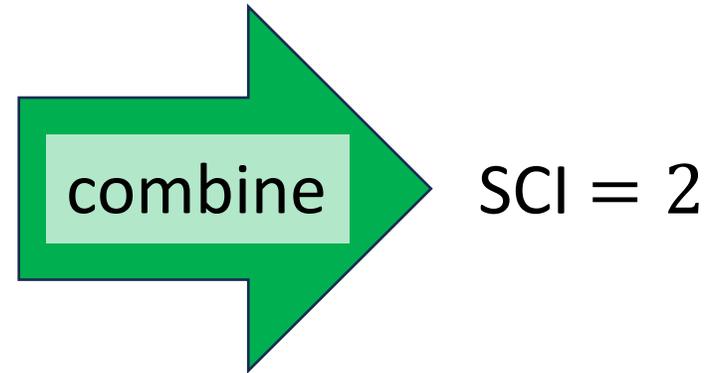
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So far literature has only proven upper bounds, that need not be sharp...

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Classifications: Solvability Complexity Index (SCI)

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

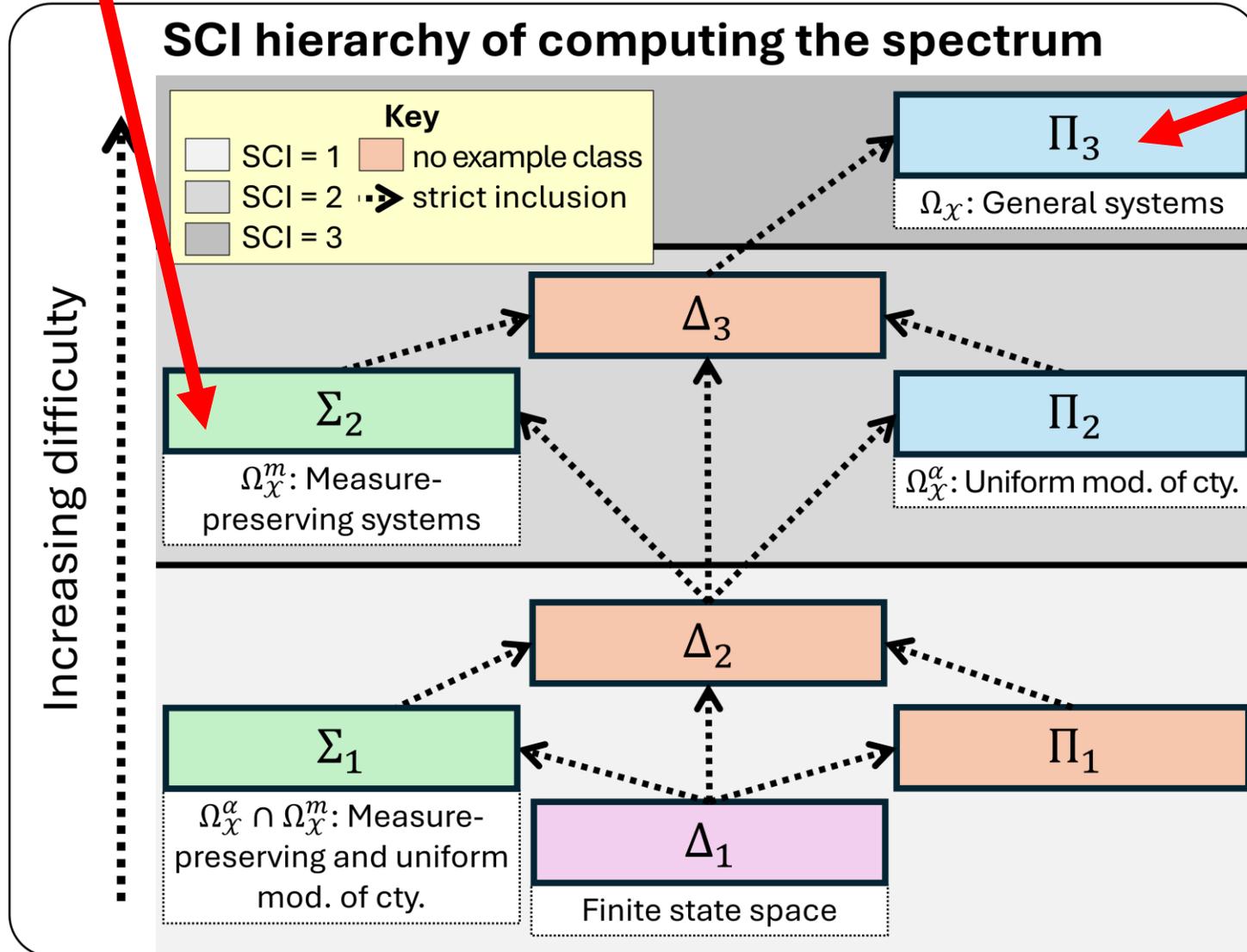
covers spectrum

- 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

SCI for Koopman I

3 limits needed
in general!



Different classes:

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

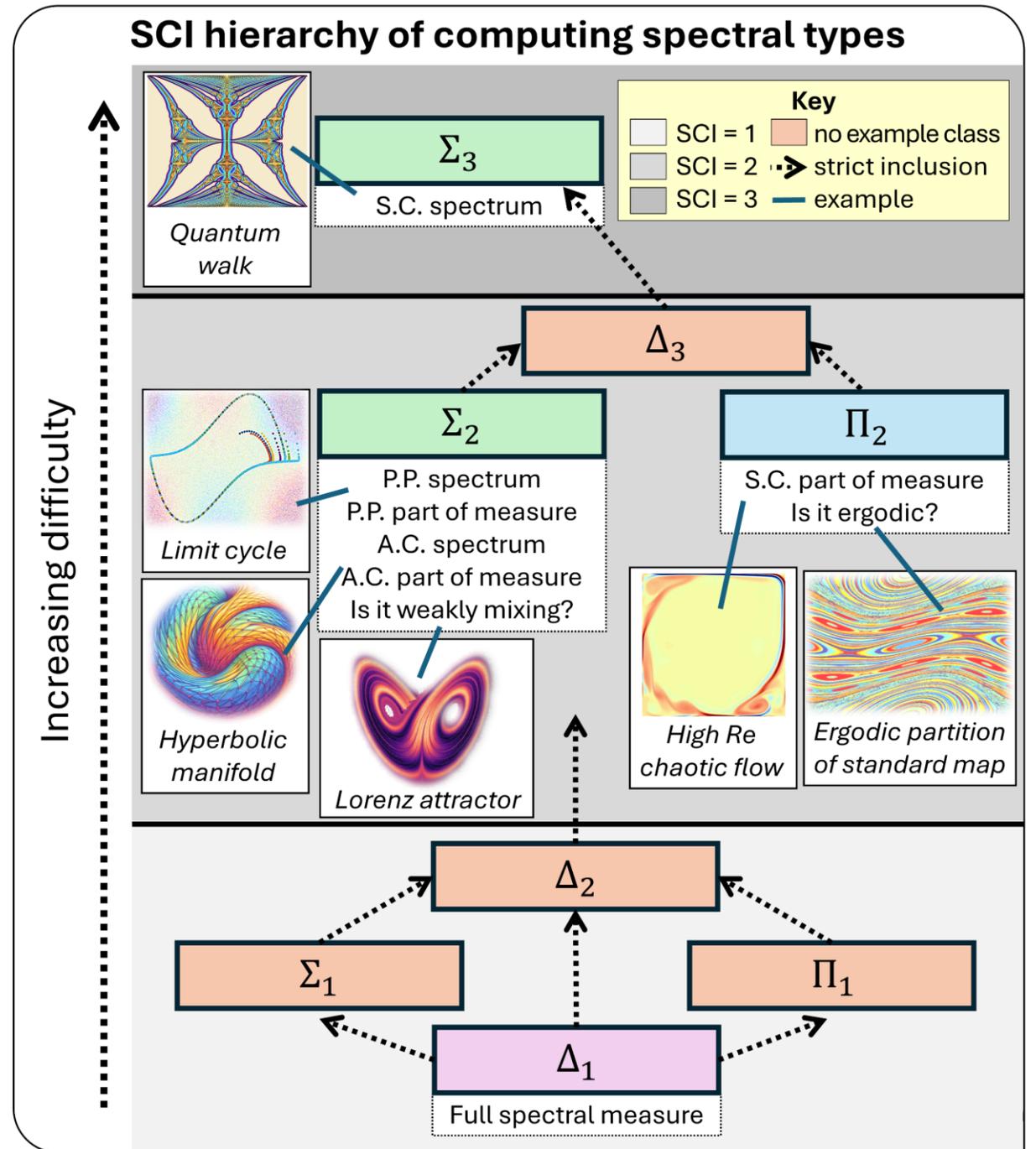
$$\Omega_{\mathcal{X}}^m = \{F: \mathcal{X} \rightarrow \mathcal{X} \mid F \text{ cts, m. p.}\}$$

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

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

**Optimal algorithms and
classifications of
dynamical systems.**

SCI for Koopman II



SCI is everywhere, here is a shameless plug...

arXiv > math > arXiv:2407.20353

Search...

Help

Mathematics > Spectral Theory

[Submitted on 29 Jul 2024]

Optimal Algorithms for Quantifying Spectral Size with Applications to Quasicrystals

[Matthew J. Colbrook](#), [Mark Embree](#), [Jake Fillman](#)

We introduce computational strategies for measuring the "size" of the spectrum of bounded self-adjoint operators using various metrics such as the Lebesgue measure, fractal dimensions, the number of connected components (or gaps), and other spectral characteristics. Our motivation comes from the study of almost-periodic operators, particularly those that arise as models of quasicrystals. Such operators are known for intricate hierarchical patterns and often display delicate spectral properties, such as Cantor spectra, which are significant in studying quantum mechanical systems and materials science. We propose a series of algorithms that compute these properties under different assumptions and explore their theoretical implications through the Solvability Complexity Index (SCI) hierarchy. This approach provides a rigorous framework for understanding the computational feasibility of these problems, proving algorithmic optimality, and enhancing the precision of spectral analysis in practical settings. For example, we show that our methods are optimal by proving certain lower bounds (impossibility results) for the class of limit-periodic Schrödinger operators. We demonstrate our methods through state-of-the-art computations for aperiodic systems in one and two dimensions, effectively capturing these complex spectral characteristics. The results contribute significantly to connecting theoretical and computational aspects of spectral theory, offering insights that bridge the gap between abstract mathematical concepts and their practical applications in physical sciences and engineering. Based on our work, we conclude with conjectures and open problems regarding the spectral properties of specific models.



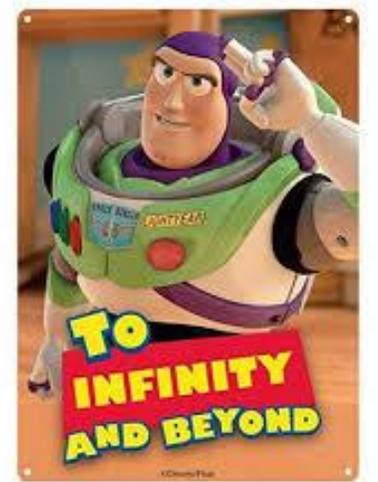
Where does this leave us?

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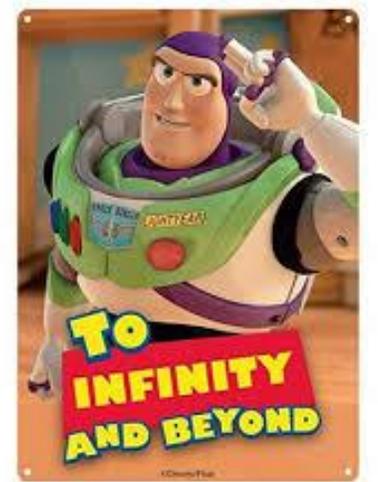
**Buzz
Lightyear
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- Future work:
 - Other function spaces.
 - Partial observations, continuous-time.
 - Control and uses of Koopman.
 - Other data-driven dynamical system methods.

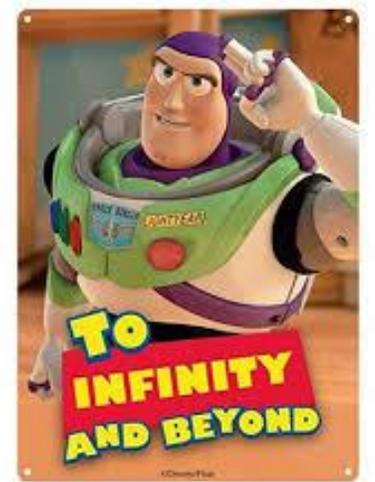
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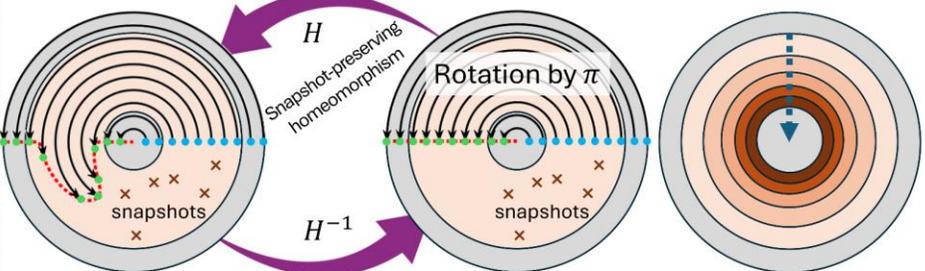
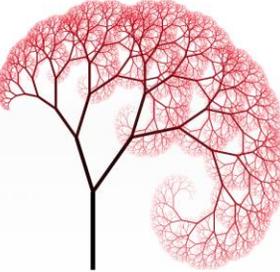
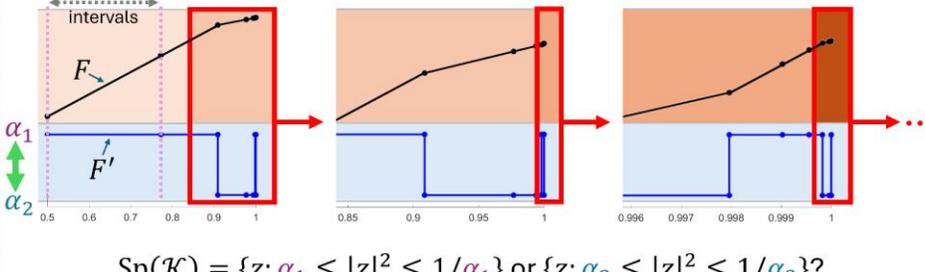
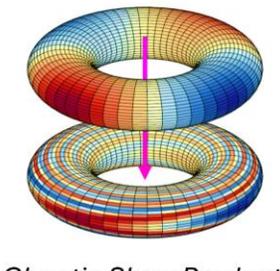
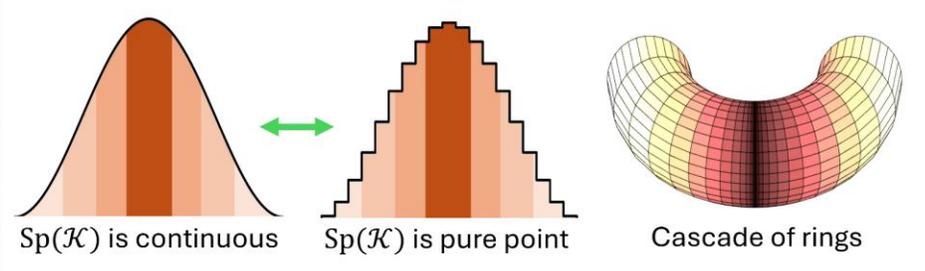
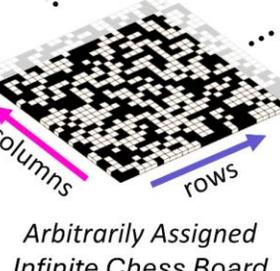
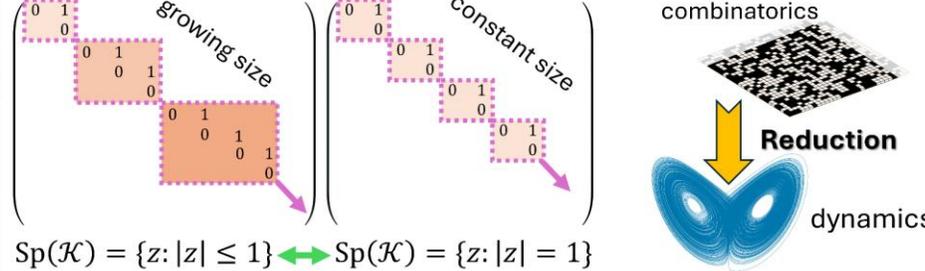
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Where does your problem/method fit into the SCI hierarchy? Is it optimal?

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	Motivation	Mechanism and Spectral Change (←→)
Sp for m.p.	 <p>Keplerian Disk</p>	 <p>Rotation by π</p> <p>Snapshot-preserving homeomorphism H</p> <p>H^{-1}</p> <p>snapshots</p> <p>snapshots</p> <p>Cascade of disks</p> <p>$\text{Sp}(\mathcal{K}) = \{z: z = 1\}$ ←→ $\text{Sp}(\mathcal{K}) = \{\pm 1\}$</p>
Sp for Lipschitz F	 <p>Fractal Curve</p>	 <p>intervals</p> <p>F</p> <p>F'</p> <p>α_1</p> <p>α_2</p> <p>$\text{Sp}(\mathcal{K}) = \{z: \alpha_1 \leq z ^2 \leq 1/\alpha_1\}$ or $\{z: \alpha_2 \leq z ^2 \leq 1/\alpha_2\}$?</p>
Non-trivial evals	 <p>Chaotic Skew Product</p>	 <p>$\text{Sp}(\mathcal{K})$ is continuous</p> <p>$\text{Sp}(\mathcal{K})$ is pure point</p> <p>Cascade of rings</p>
Sp for general F	 <p>Arbitrarily Assigned Infinite Chess Board</p> <p>columns</p> <p>rows</p>	 <p>growing size</p> <p>constant size</p> <p>combinatorics</p> <p>Reduction</p> <p>dynamics</p> <p>$\text{Sp}(\mathcal{K}) = \{z: z \leq 1\}$ ←→ $\text{Sp}(\mathcal{K}) = \{z: z = 1\}$</p>

Two definitions

Computational problem:

$$\mathbb{E}: \Omega \rightarrow \mathcal{M}$$

Λ : set of maps from Ω to a metric space (info algorithms can read).

E.g., $\mathbb{E} = \text{Sp}$, Ω class of dynamical systems, \mathcal{M} the Hausdorff metric, Λ training set

Don't need this slide