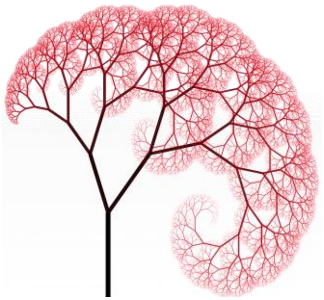

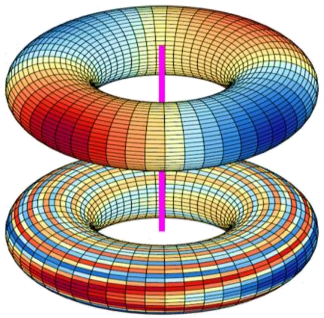

Barriers and Classifications of Robust Koopman Learning

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 $F: \mathcal{X} \to \mathcal{X}$ – 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: $\left\{\left(x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right) : m = 1, \dots, M\right\}$

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

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Data
21st century

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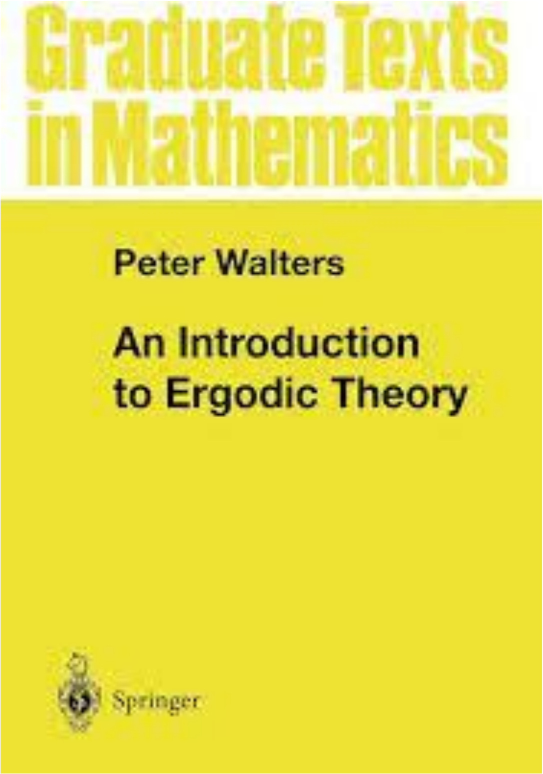
Why should you care?

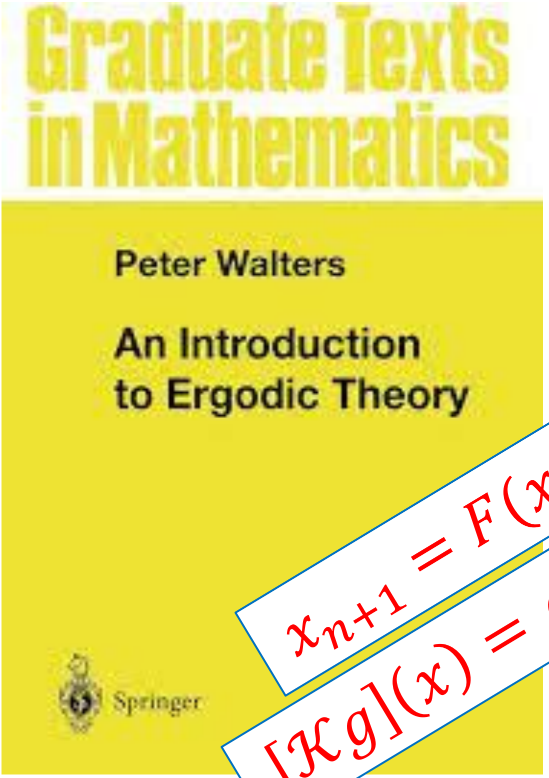
Fundamental in ergodic theory



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

Why should you care?

Fundamental in ergodic theory



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

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

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

Can provide a *diagonalization* of a nonlinear system.

eigenfunction of $\mathcal{K}$

continuous spectrum

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

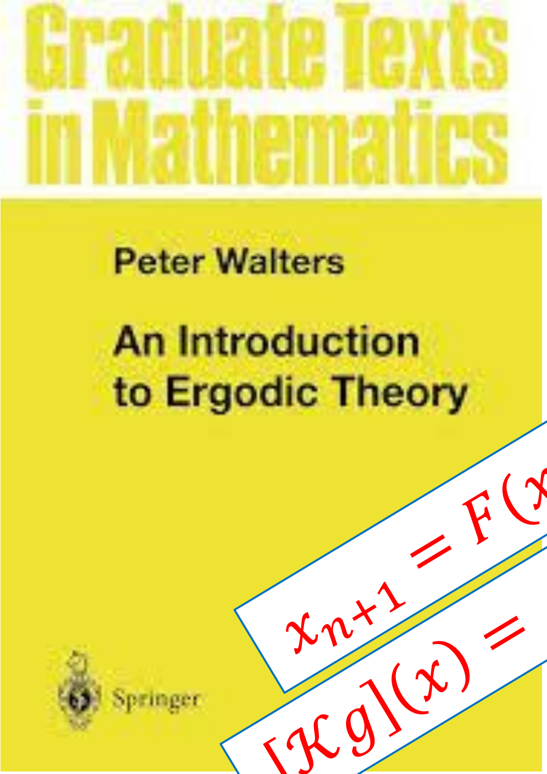
$$g(x_n) = [\mathcal{K}^n g](x_0)$$

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

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

Why should you care?

Fundamental in ergodic theory



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E.g., key to erg

Birkhoff and v

Spectral properties encode: geometric features,

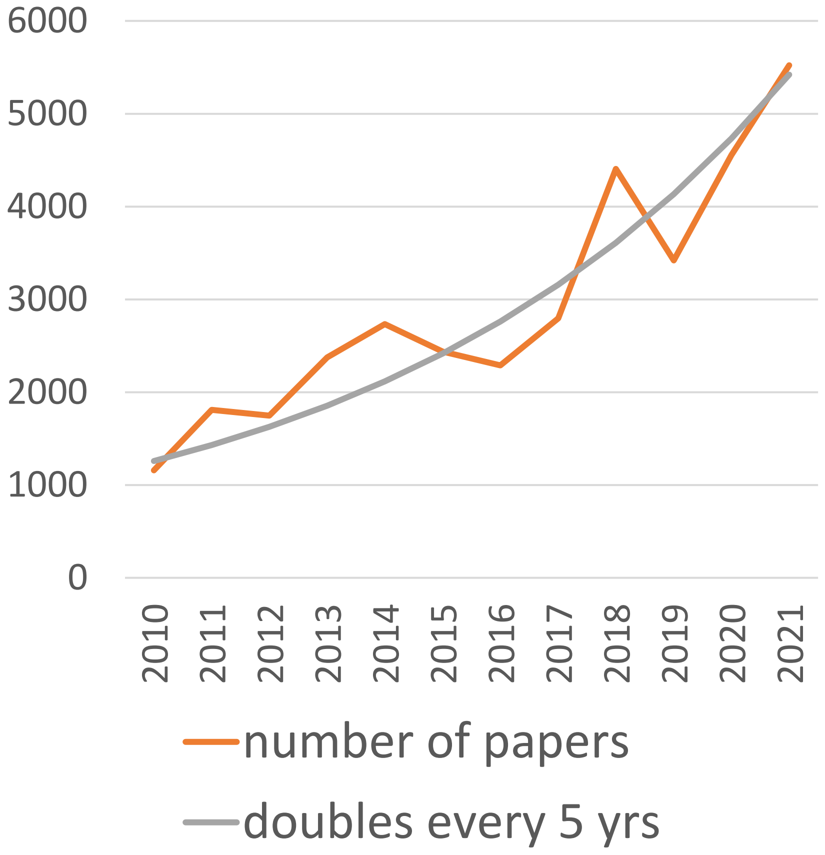
me

/, etc.

+ interest in their spectral properties...

Ubiquitous in data-driven era

Google scholar New Papers on "Koopman Operators"



Loads of applications!!!

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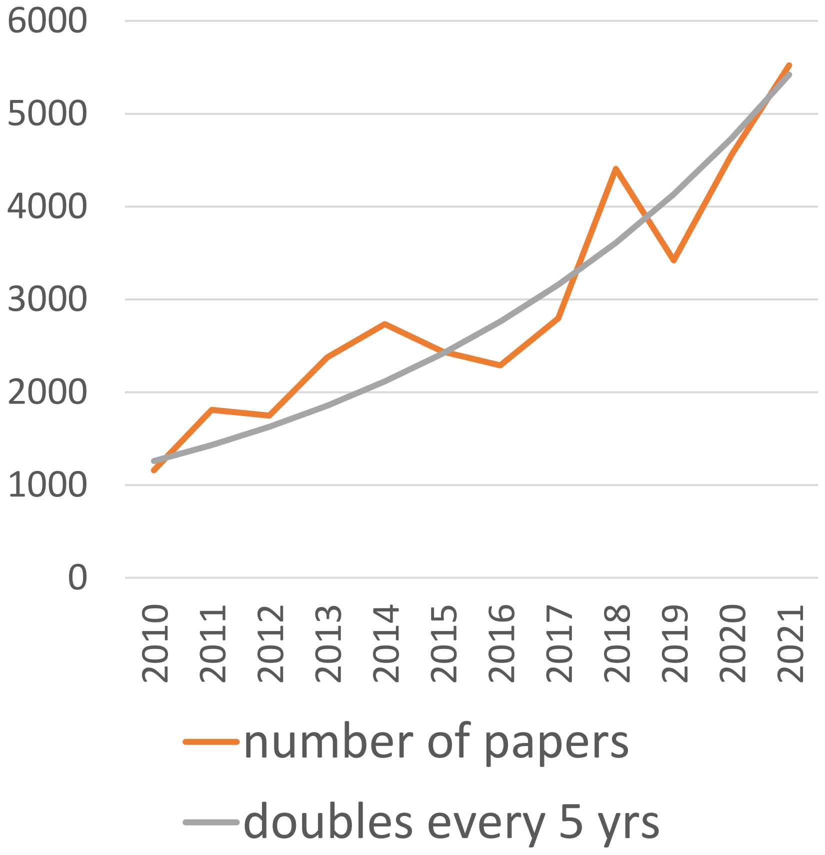

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Open question: *When can we learn spectral properties of Koopman operators from trajectory data, and when can we not?*

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

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

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

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

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

Proof idea

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

Lemma: Let $X = \{x_1, \dots, x_N\}, Y = \{y_1, \dots, y_N\}$ be distinct points in annulus $\mathcal{A} = \{x \in \mathbb{D} | 0 < R < \|x\| < r < 1\}$ 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

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

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

Build an adversarial F…

Proof idea

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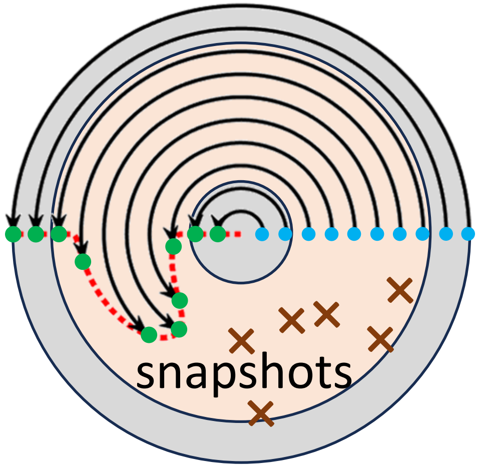

$\widetilde{F_1}(r, \theta) = \big(r, \theta + \pi + \phi(r)\big)$, $\mathrm{supp}(\phi) \subset$ [1/4, 3/4]

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

Proof idea

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

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

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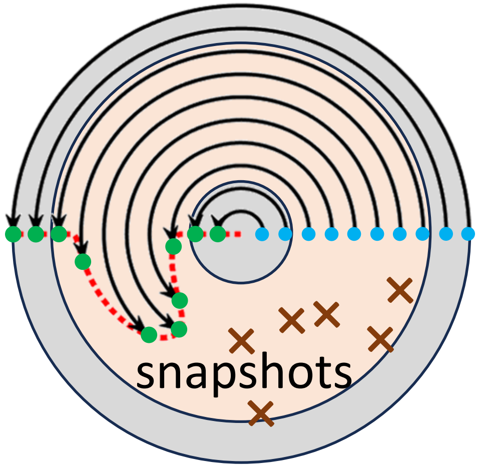

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$\mathrm{Sp}(\mathcal{K}_{\widetilde{F_1}}) = \mathbb{T}$ (unit circle).

$\lim_{n\to\infty} \Gamma_n(\widetilde{F_1}) = \mathrm{Sp}(\mathcal{K}_{\widetilde{F_1}}) \Rightarrow \exists n_1$ s.t. $\mathrm{dist}(i, \Gamma_{n_1}(\widetilde{F_1})) \leq 1$.

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

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

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

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

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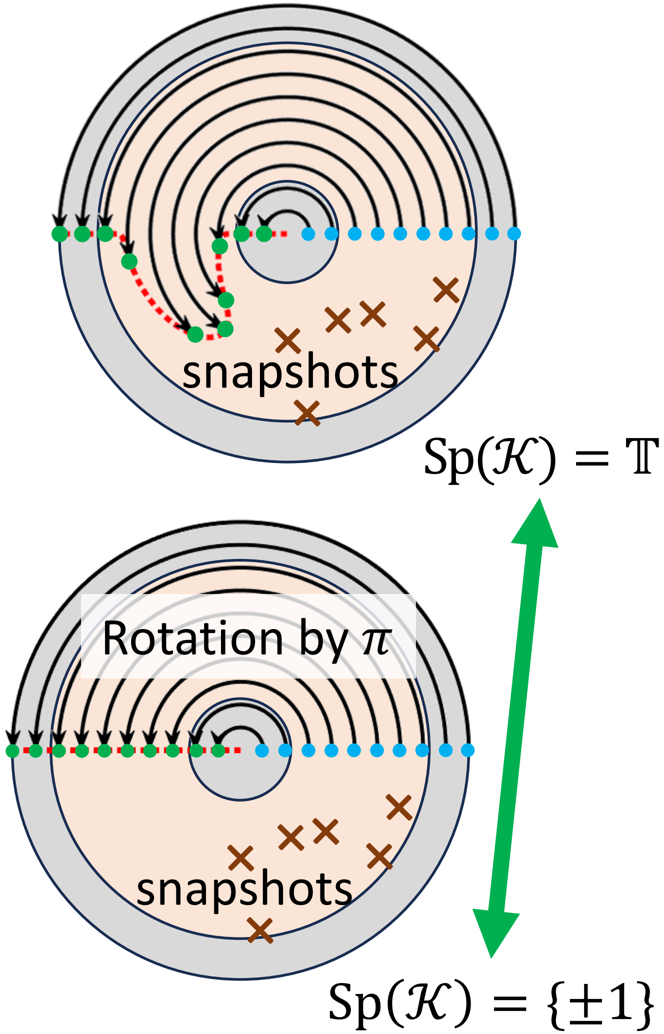
BUT Γ_{n_1} uses finite amount of info to output $\Gamma_{n_1}\big(\widetilde{F_1}\big)$.

Let X, Y correspond to these snapshots.

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

Consistent data $\Rightarrow \Gamma_{n_1}(F_1) = \Gamma_{n_1}\big(\widetilde{F_1}\big)$, $\mathrm{dist}(i, \Gamma_{n_1}(F_1)) \leq 1$

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



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

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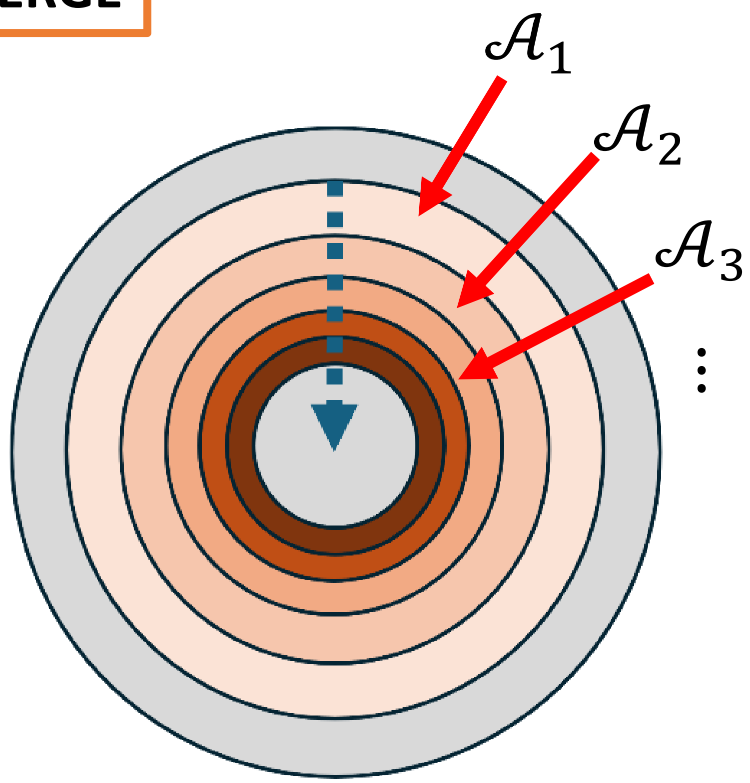
CANNOT CONVERGE



Cascade of disks

Proof idea (deterministic case)

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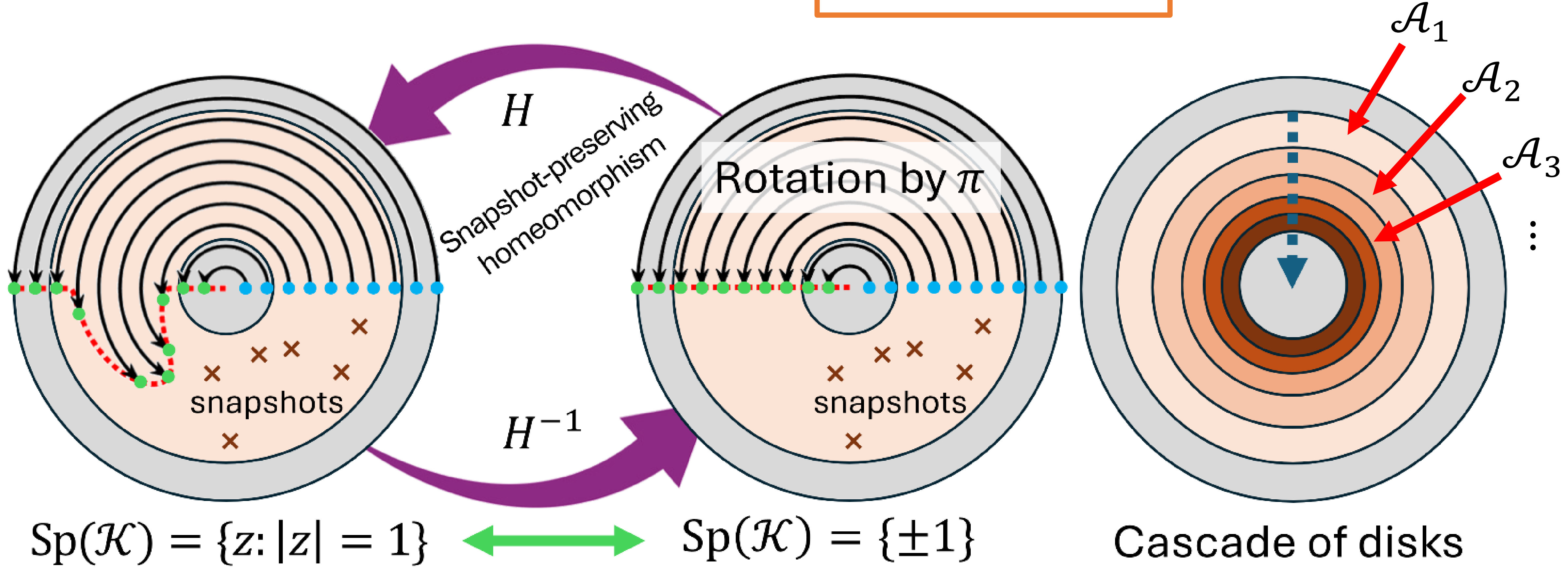

Example: Theorem B (possibility)

$\Omega_{\mathcal{X}}^{m} = \{F\colon \mathcal{X} \to \mathcal{X} \mid F \text{ cts, measure preserving}\}.$
$\mathcal{T}_F = \{(x, y_m) | x \in \mathcal{X}, \|F(x) - y_m\| \leq 2^{-m}\}.$

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

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

Proof sketch

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

$\boldsymbol{N}$ = size of basis, $\boldsymbol{M}$ = number of snapshots (quadrature).

Proof sketch

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

  $\boldsymbol{N}$ **= size of basis,** $\boldsymbol{M}$ **= number of snapshots (quadrature).**

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

Proof sketch

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  $\boldsymbol{N}$ **= size of basis,** $\boldsymbol{M}$ **= number of snapshots (quadrature).**
- Measure-preserving $\Rightarrow \|(\mathcal{K}_F - zI)^{-1}\|^{-1} = \mathrm{dist}(z, \mathrm{Sp}(\mathcal{K}_F))$.
- Local N-adaptive minimisation of $\gamma_{N,M}(F,z)$ to approximate $\mathrm{Sp}(\mathcal{K}_F)$

Proof sketch

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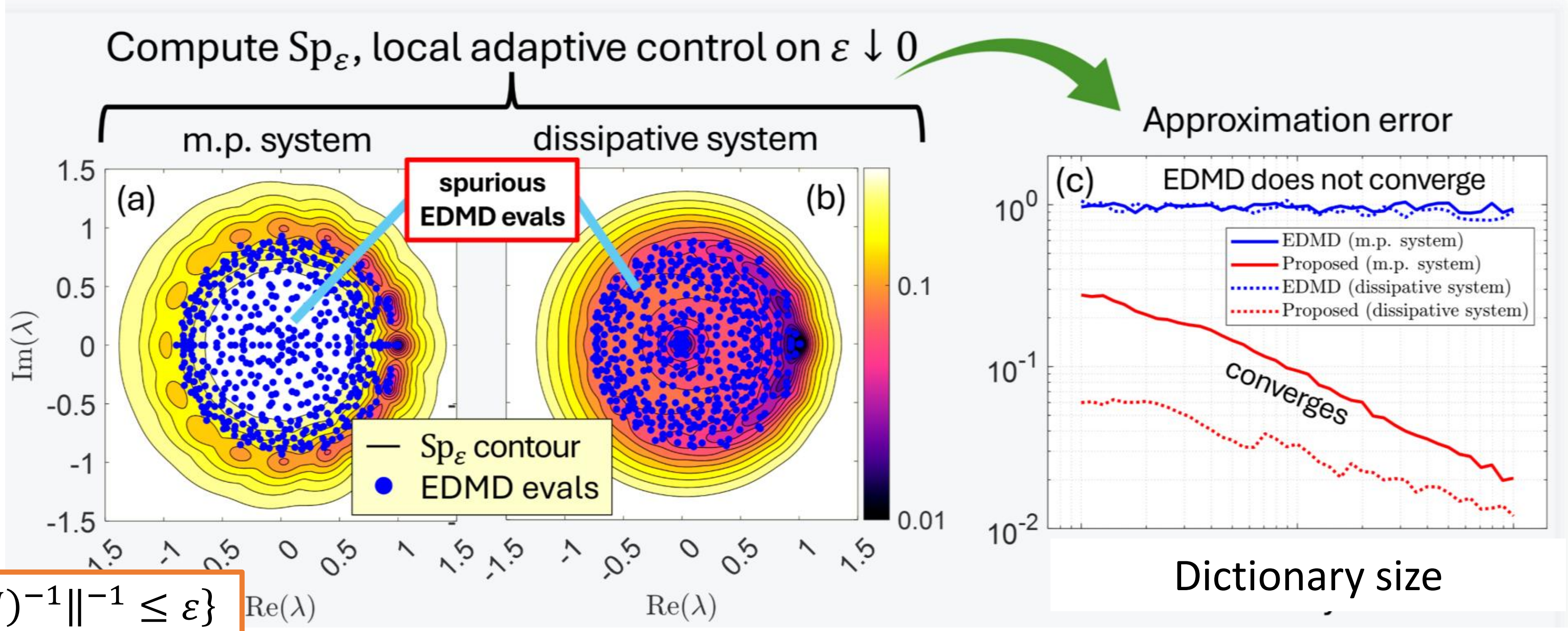
"Extended Dynamic Mode Decomposition" is essentially the finite section method.



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

Towers of algorithms

Def: $\{\Gamma_{n_k,\dots,n_1}\}$ 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.
- C., "*The foundations of infinite-dimensional spectral computations,*" **PhD diss.**, University of Cambridge, 2020.
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Theorem A: $\text{SCI} > 1$

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

combine

$\text{SCI} = 2$

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Theorem A: SCI > 1

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SCI $= 2$

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

Are these sharp?

Previous techniques prove upper bounds on SCI.
"N/C": method need not converge. "n/a": algorithm not applicable to problem.

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

Classifications: *Solvability Complexity Index (SCI)*

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

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

- Σ_m: SCI $\leq m$, final limit from below.
  E.g., Σ_1: $\Gamma_n(F) \subset \mathrm{Sp}(\mathcal{K}_F) + B_{2^{-n}}(0)$.
- Π_m: SCI $\leq m$, final limit from above.
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verification

trust output

covers spectrum

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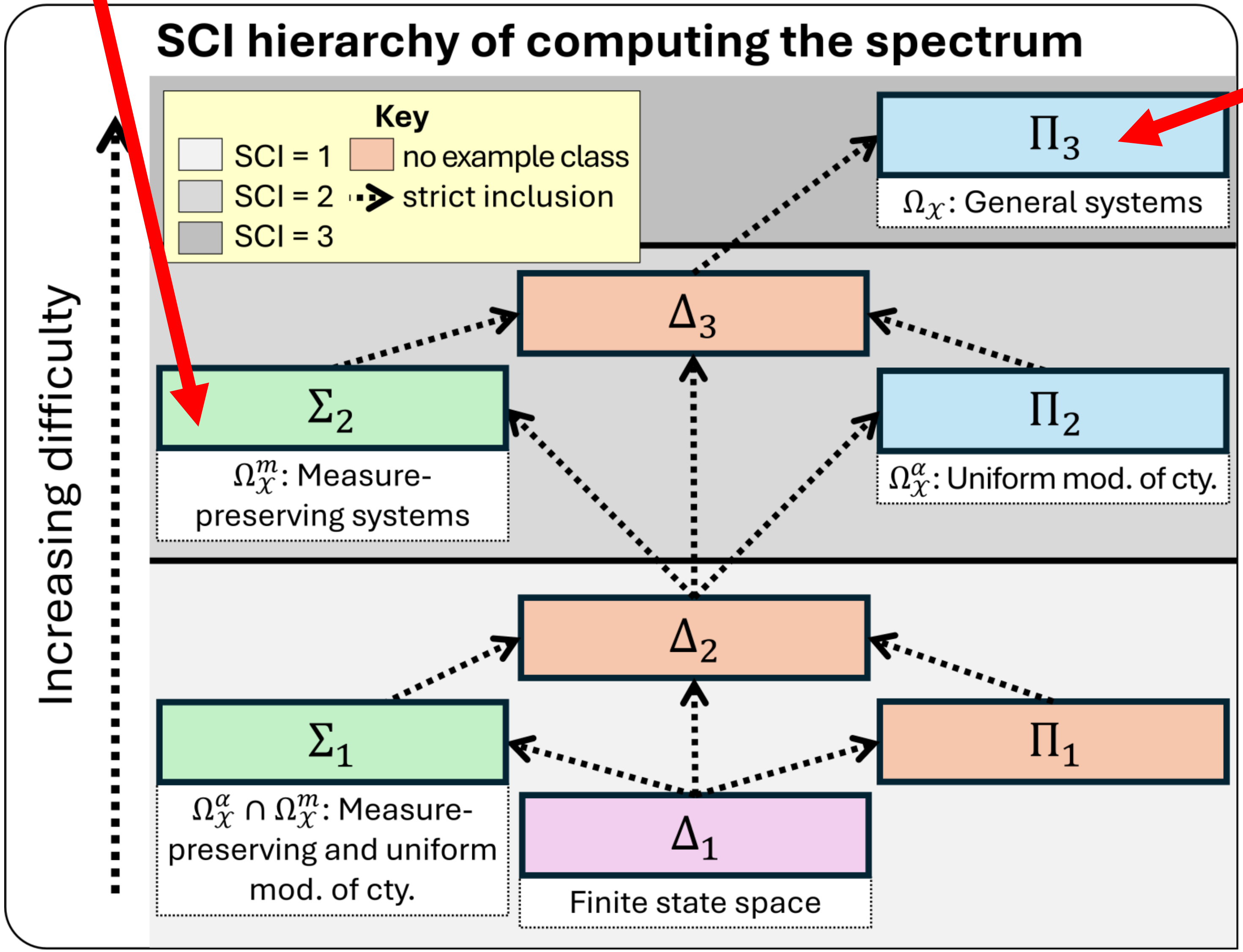
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "*On the solvability complexity index hierarchy and towers of algorithms,*" arXiv, 2020.

Theorems A + B

SCI for Koopman I

3 limits needed in general!



Different classes:

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

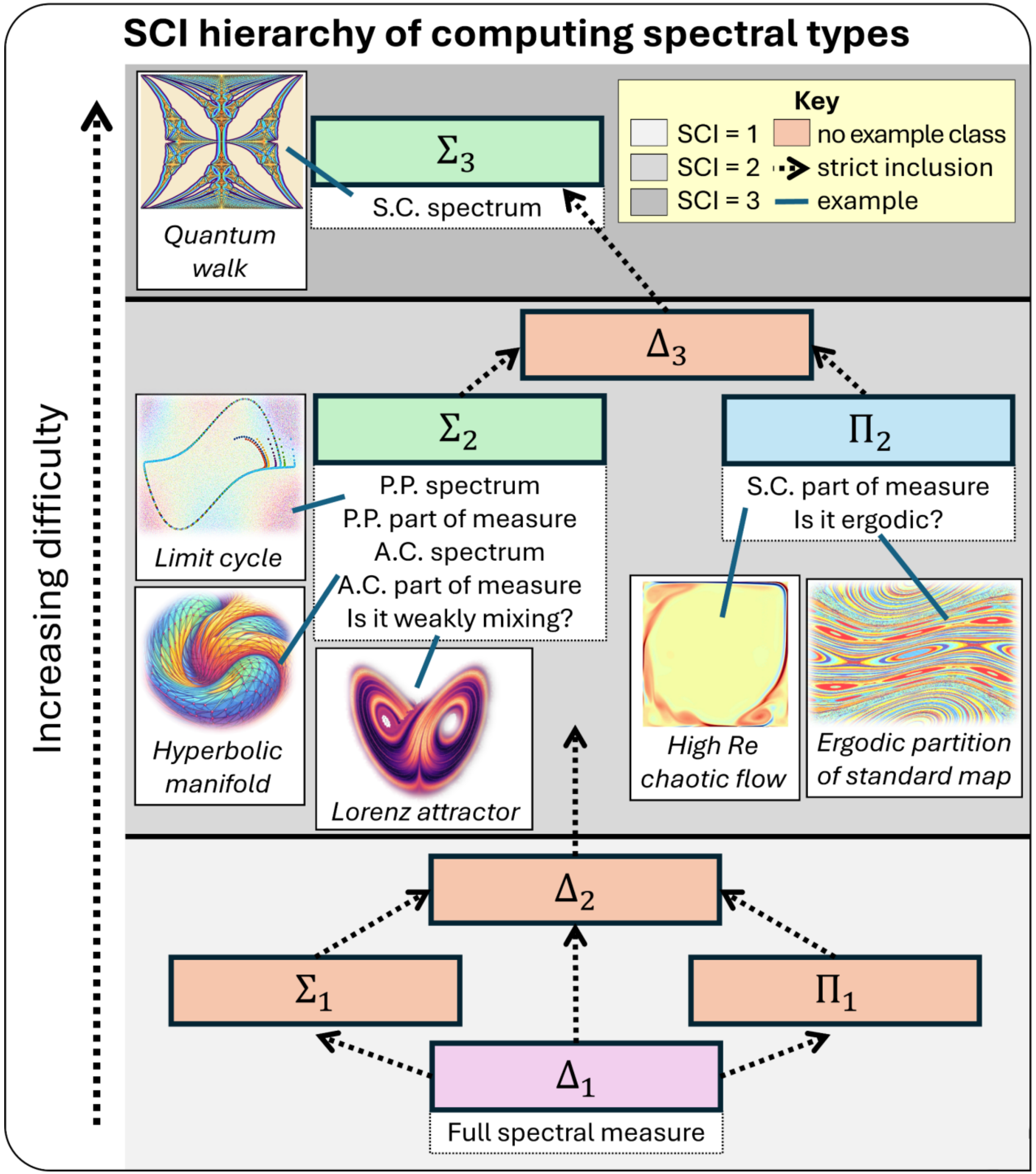
$$\Omega_\mathcal{X}^m = \{F: \mathcal{X} \to \mathcal{X} \mid F \text{ cts, m. p.}\}$$

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

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

Optimal algorithms and classifications of dynamical systems.

SCI for Koopman II

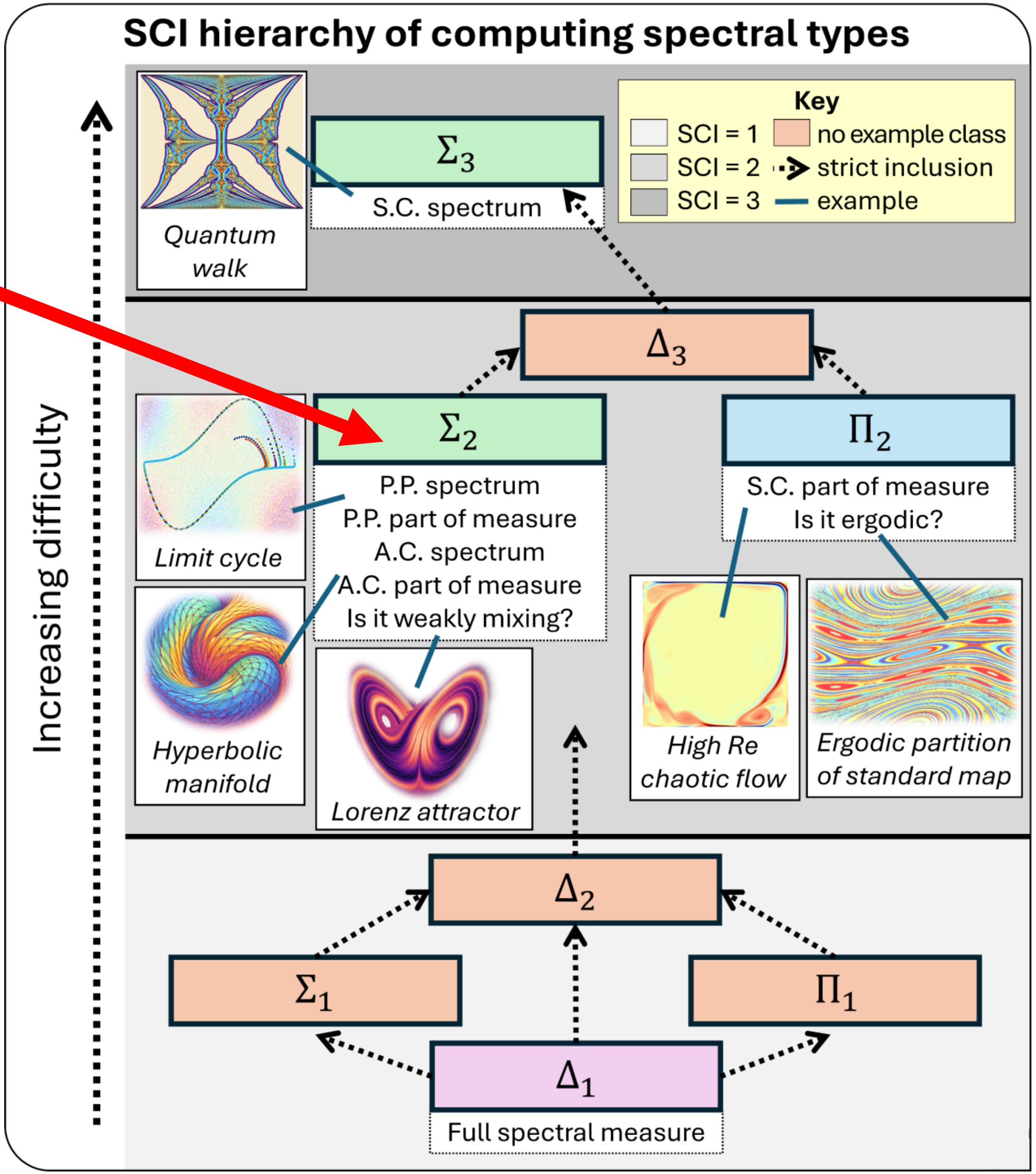


SCI for Koopman II

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"!



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)
  $\Rightarrow$ **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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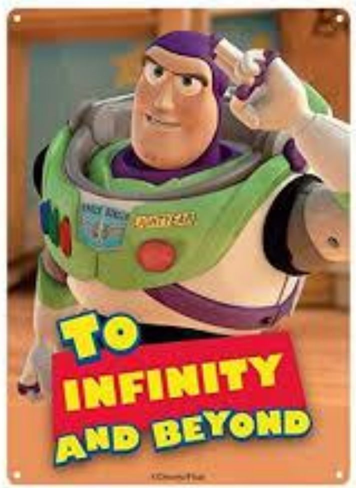
Buzz Lightyear was right!



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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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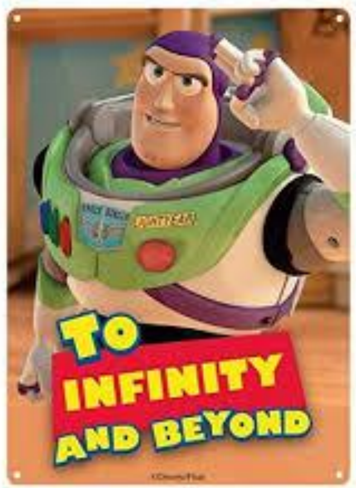

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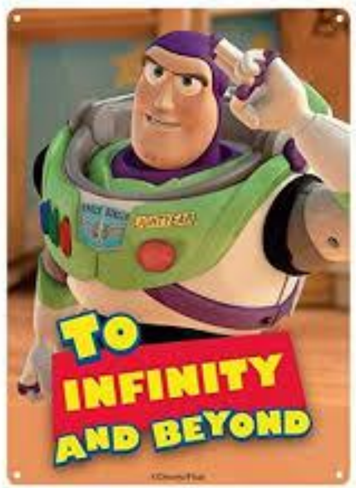

Where does your problem/method fit into the SCI hierarchy? Is it optimal?

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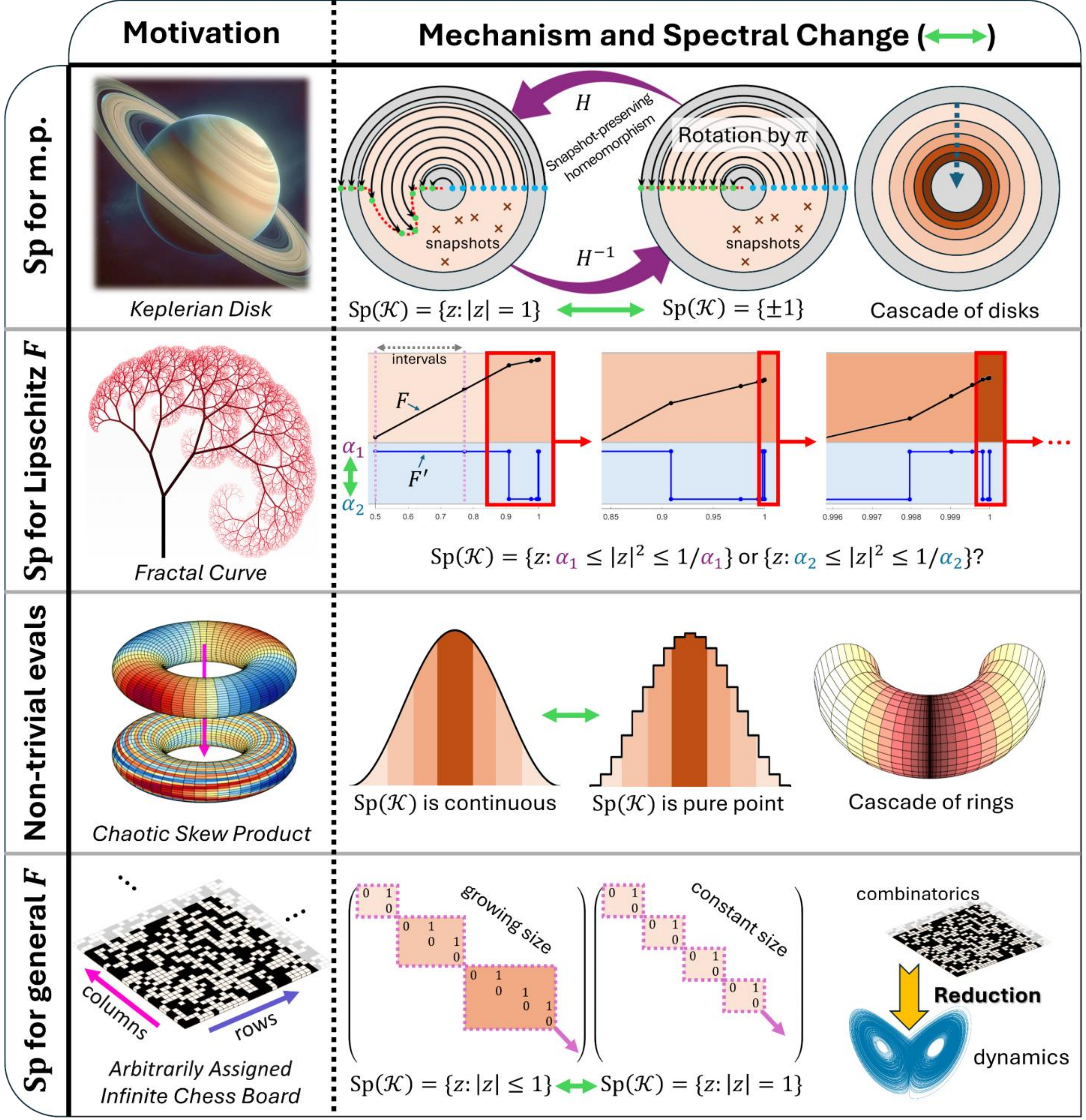
Motivation
Mechanism and Spectral Change
Sp for m.p.
Keplerian Disk
H
Snapshot-preserving homeomorphism
H^{-1}
Rotation by π
snapshots
snapshots
$\mathrm{Sp}(\mathcal{K}) = \{z : |z| = 1\}$
$\mathrm{Sp}(\mathcal{K}) = \{\pm 1\}$
Cascade of disks
Sp for Lipschitz F
Fractal Curve
intervals
F
F'
α_1
α_2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

Two definitions

Computational problem: $\Xi: \Omega \to \mathcal{M}$

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

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

Don't need this slide