



# Towards a classification theory for data-driven dynamical systems

Matthew Colbrook
University of Cambridge
28/10/2024

"To classify is to bring order into chaos." - George Pólya

C., Mezić, Stepanenko "Limits and Powers of Koopman Learning," arxiv preprint, 2024.

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

### Data-driven dynamical systems

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

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

Dynamics (geometry)
19th century

- Borel measure  $\omega$  on X
- Function space  $L^2 = L^2(\mathcal{X}, \omega)$  (elements g called "observables")
- Koopman operator  $\mathcal{K}_F:L^2\to L^2$ ;  $[\mathcal{K}_Fg](x)=g(F(x))$
- <u>Available</u> snapshot data:  $\{(x^{(m)}, y^{(m)} = F(x^{(m)})) : m = 1, ..., M\}$

**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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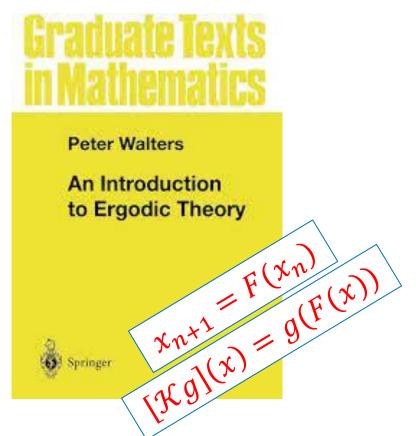
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Dynamics (geometry)
19th century

Analysis 20<sup>th</sup> century

### Why you should care about Koopman

Fundamental in ergodic theory



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

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

continuous

## Why you should care about Koopman

Fundamental in ergodic theory

Peter Walters An Introduction to Ergodic Theory

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

Can provide a diagonalization of a nonlinear system.

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

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

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

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

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

continuous

### Why you should care about Koopman

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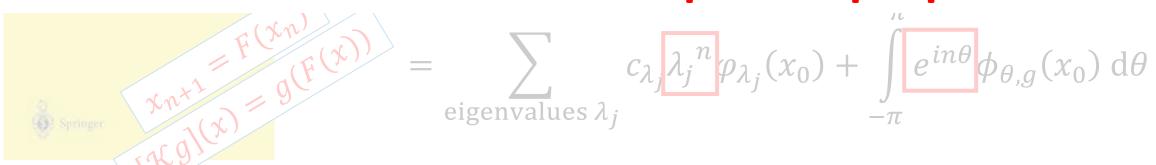
Can provide a diagonalization of a nonlinear system.



eigenfunction of 
$$\mathcal{K}$$

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

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



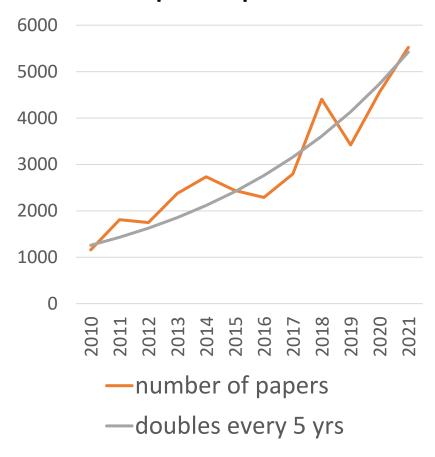
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#### New Papers on "Koopman Operators"

#### Central in data-driven era



Loads of applications!!!

#### **New Papers on** "Koopman Operators"

#### Central in data-driven era



—number of papers

—doubles every 5 yrs

#### Loads of applications!!!

2012

CHAOS 22, 047510 (2012)



#### Applied Koopmanisma)

Marko Budišić, Ryan Mohr, and Igor Mezić Department of Mechanical Engineering, University of California, Sante Bankara California 02106 5070 115 A

(Received 11 June 2012; accepted 30 November 2012; publishe

A majority of methods from dynamical system analysis, espec on Poincaré's geometric picture that focuses on "dynamics of st our field for a century, it has shown difficulties in handling h uncertain systems, which are more and more common in engine "big data" measurements. This overview article presents an alsystems, based on the "dynamics of observables" picture. To operator: an infinite-dimensional, linear operator that is noneth nonlinear dynamics. The first goal of this paper is to make it c different papers and contexts all relate to each other through s operator. The second goal is to present these methods in a conc framework accessible to researchers who would like to apply tl them. Finally, we aim to provide a road map through the litera described in detail. We describe three main concepts: Ko eigenquotients, and continuous indicators of ergodicity. For eaof theoretical concepts required to define and study them, n developed for their analysis, and, when possible, application Koopman framework is showing potential for crossing over fre industrial practice. Therefore, the paper highlights its strengths Additionally, we point out areas where an additional research pu adopted as an off-the-shelf framework for analysis and desi Physics. [http://dx.doi.org/10.1063/1.4772195]

A majority of methods from dynamical systems 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

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#### **Modern Koopman Theory for Dynamical Systems\***

Steven L. Brunton<sup>†</sup> Marko Budišić1 Eurika Kaiser<sup>†</sup> J. Nathan Kutz§

Abstract. The field of dynamical systems is being transformed by the mathematical tools and al-

gorithms emerging from modern computing and da and asymptotic reductions are giving way to data-d in operator-theoretic or probabilistic frameworks. as a dominant perspective over the past decade, sented in terms of an infinite-dimensional linear ope measurement functions of the system. This linear has tremendous potential to enable the prediction systems with standard textbook methods develope ing finite-dimensional coordinate systems and emb approximately linear remains a central open challe is due primarily to three key factors: (1) there exis sical geometric approaches for dynamical systems; of measurements, making it ideal for leveraging big and (3) simple, yet powerful numerical algorithms sition (DMD), have been developed and extended in real-world applications. In this review, we pro operator theory, describing recent theoretical and a ing these methods with a diverse range of applicat challenges in the rapidly growing field of machine developments and significantly transform the theorem

Key words. dynamical systems, Koopman operator, data-dri theory, operator theory, dynamic mode decompos

AMS subject classifications. 34A34, 37A30, 37C10, 37M10, 3

The multiverse of dynamic mode decomposition algorithms 2024

#### Matthew J. Colbrook

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ckward dynamic

quares dynamic

dynamic mode

155

157 158

160

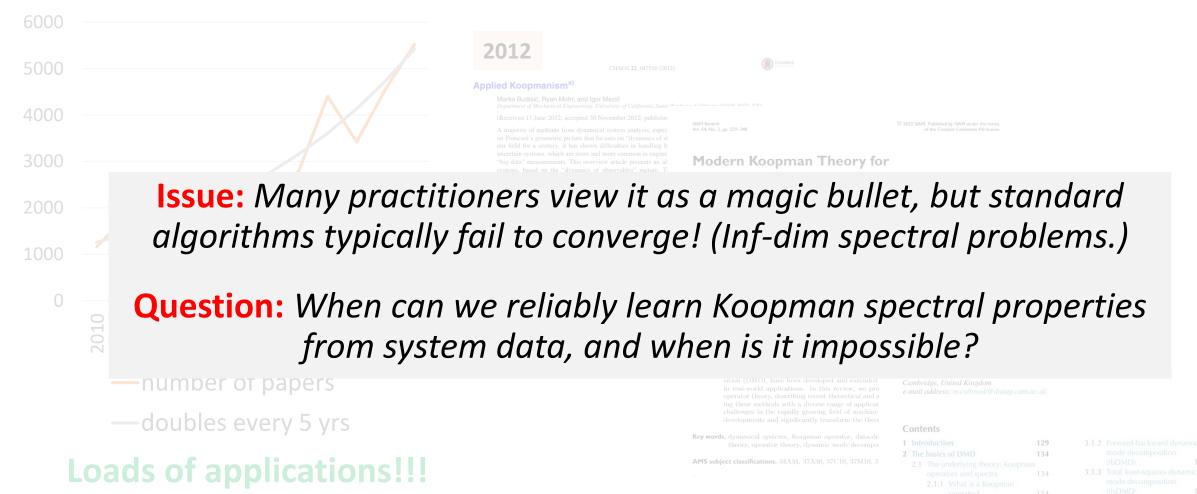
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New Papers on "Koopman Operators"

#### Central in data-driven era



#### Outline

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

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

# Theorem A (impossibility)

Implies  ${\mathcal K}$  is unitary

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

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

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

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

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

**Phase transition lemma:** Let  $X = \{x_1, ..., x_N\}, Y = \{y_1, ..., y_N\}$  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  $\mathbb{D} \setminus \mathcal{A}$  and  $H(y_j) = F_0(H(x_j)), j = 1, ..., N$ .

Conjugacy of <u>data</u>  $(x_i \rightarrow y_i)$  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.

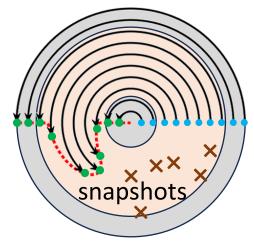
Suppose (for contradiction)  $\{\Gamma_n\}$  uses  $\mathcal{T}_F$ ,  $\lim_{n\to\infty}\Gamma_n(F)=\operatorname{Sp}(\mathcal{K}_F)\ \forall F\in\Omega_{\mathbb{D}}$ . Build an adversarial F...

$$T_F = \{(x, y_m) \mid ||F(x) - y_m|| \le 2^{-m}\}$$

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

Build an adversarial F...

$$\widetilde{F_1}(r,\theta) = (r,\theta + \pi + \phi(r)), \operatorname{supp}(\phi) \subset [1/4, 3/4]$$
  
 $\operatorname{Sp}(\mathcal{K}_{\widetilde{F_1}}) = \mathbb{T}$  (unit circle).



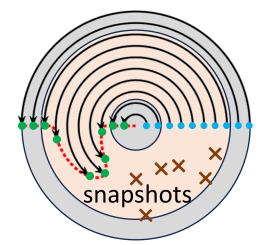
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 $\lim_{n\to\infty}\Gamma_n\big(\widetilde{F_1}\big)=\operatorname{Sp}(\mathcal{K}_{\widetilde{F_1}})\Rightarrow \exists n_1 \text{ s.t. } \operatorname{dist}(i,\Gamma_{n_1}\big(\widetilde{F_1}\big))\leq 1.$ 

**BUT**  $\Gamma_{n_1}$  uses finite amount of info to output  $\Gamma_{n_1}(\widetilde{F_1})$ . Let X, Y correspond to these snapshots.



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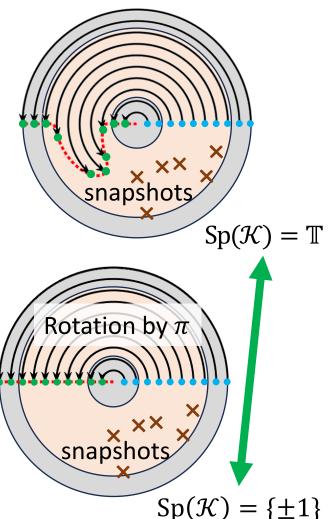
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**BUT**  $\Gamma_{n_1}$  uses finite amount of info to output  $\Gamma_{n_1}(\widetilde{F_1})$ . Let X, Y correspond to these snapshots.

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

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

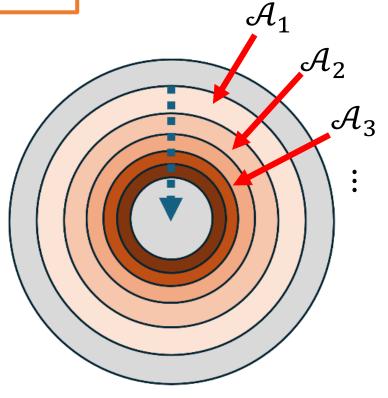
**BUT** Sp $(\mathcal{K}_{F_1}) = \operatorname{Sp}(\bar{\mathcal{K}}_{F_0}) = \{\pm 1\}$ 



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

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

**CANNOT CONVERGE** 



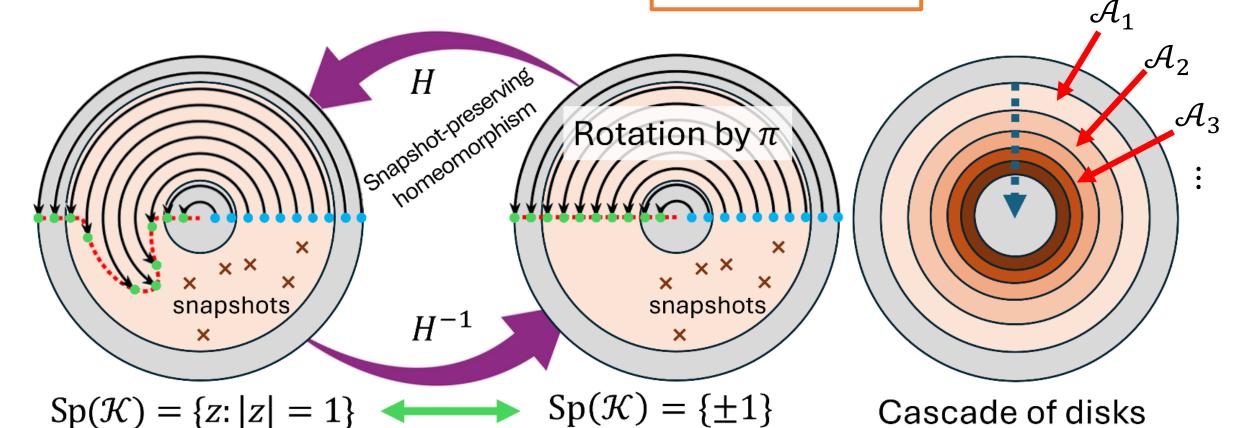
Cascade of disks

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

**CANNOT CONVERGE** 

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

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



# Theorem B (possibility)

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

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

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

**Double** limit 
$$\lim_{n_2 \to \infty} \lim_{n_1 \to \infty}$$

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

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

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

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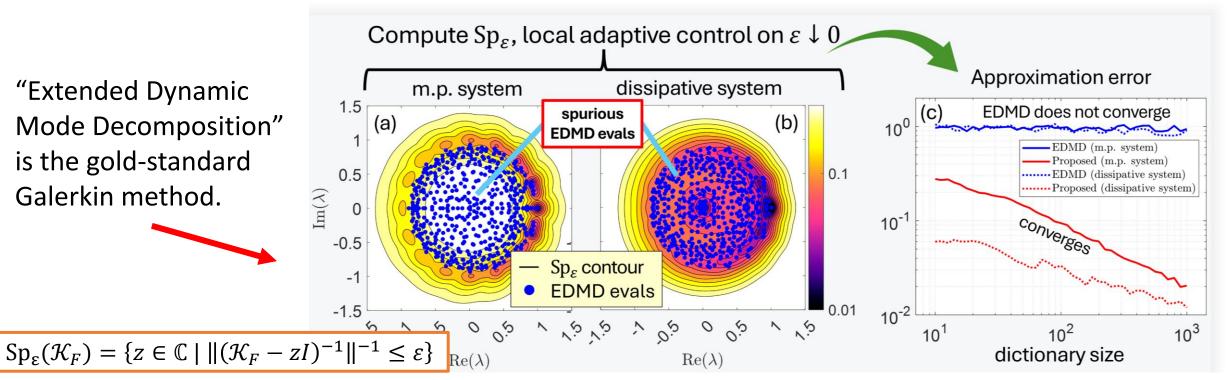
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- Local N-adaptive minimisation of  $\gamma_{N,M}(F,z)$  to approximate  $\operatorname{Sp}(\mathcal{K}_F)$

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"Extended Dynamic Mode Decomposition" is the gold-standard Galerkin method.

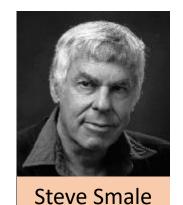


# Limits of limits: Towers of algorithms

**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.** 

First appeared in dynamical systems theory:

algorithms



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



"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.

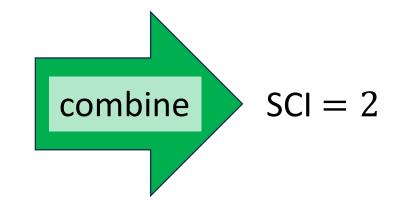
SCI: Fewest number of limits needed to solve a computational problem.

- 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.
- C., Hansen, "The foundations of spectral computations via the solvability complexity index hierarchy," J. Eur. Math. Soc., 2022.
- C., Antun, Hansen, "The difficulty of computing stable and accurate neural networks," Proc. Natl. Acad. Sci. USA, 2022.
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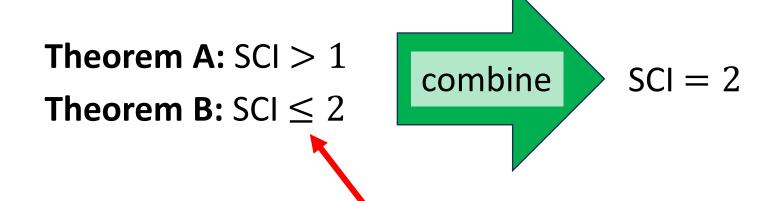
Theorem A: SCI > 1

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



- Hansen, "On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators." J. Am. Math. Soc., 2011.
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- 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					
Algorithm		KMD	Spectrum	Spectral Measure (if m.p.)	Spectral Type (if m.p.)		
Extended DMD [47]	general $L^2$ spaces	$SCI \le 2^*$	N/C	N/C	n/a		
Residual DMD [44]	general $L^2$ spaces	$SCI \le 2^*$	$SCI \le 3^*$	$SCI \le 2^*$	varies, see [84] e.g., a.c. density: $SCI \le 2^*$		
Measure-preserving EDMD [45]	m.p. systems	$SCI \le 1$	N/C	$SCI \le 2^*$ (general) $SCI \le 1$ (delay-embedding)	n/a		
Hankel DMD [85]	m.p. ergodic systems	$SCI \le 2^*$	N/C	N/C	n/a		
Periodic approximations [86]	m.p. $+\omega$ a.c.	$SCI \leq 2$	N/C	$SCI \le 2$ (see [87])	a.c. density: $SCI \leq 3$		
Christoffel–Darboux kernel [40]	m.p. ergodic systems	$SCI \leq 3$	n/a	$SCI \leq 2$	e.g., a.c. density: $SCI \leq 2$		
Generator EDMD [88]	ctstime, samples $\nabla F$ (otherwise additional limit)	$SCI \le 2$	N/C	$SCI \leq 2$ (see [89])	n/a		
Compactification [42]	ctstime, m.p. ergodic systems	$SCI \le 4$	N/C	$SCI \leq 4$	n/a		
	ctstime, m.p. ergodic systems			$SCI \leq 5$	n/a		
Diffusion maps [90] (see also [10])	4		4	n/a			
Provious tachniques n		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,...

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

- $\Delta_1$ : One limit, full error control. E.g.,  $d(\Gamma_n(F), \operatorname{Sp}(\mathcal{K}_F)) \leq 2^{-n}$ .
- $\Delta_{m+1}$ :  $SCI \leq m$ .
- $\Sigma_m$ : SCI  $\leq m$ , final limit from below.

E.g., 
$$\Sigma_1$$
:  $\Gamma_n(F) \subset \operatorname{Sp}(\mathcal{K}_F) + B_2^{-n}(0)$ .

•  $\Pi_m$ : SCI  $\leq m$ , final limit from above.

E.g., 
$$\Pi_1$$
: Sp( $\mathcal{K}_F$ )  $\subset \Gamma_n(F) + B_2^{-n}(0)$ .

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verification

# Classifications: Solvability Complexity Index (SCI)

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

- $\Delta_1$ : One limit, full error control. E.g.,  $d(\Gamma_n(F), \operatorname{Sp}(\mathcal{K}_F)) \leq 2^{-n}$ .
- $\Delta_{m+1}$ :  $SCI \leq m$ .
- $\Sigma_m$ : SCI  $\leq m$ , final limit from below.

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

•  $\Pi_m$ :  $\operatorname{SCI} \leq m$ , final limit from above.

E.g., 
$$\Pi_1$$
: Sp( $\mathcal{K}_F$ )  $\subseteq \Gamma_n(F) + B_2^{-n}(0)$ .

trust output

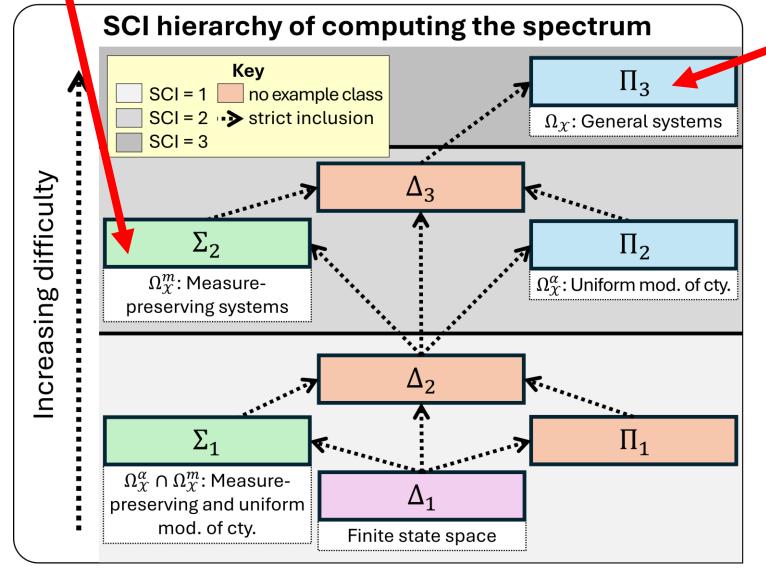
#### covers spectrum

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#### Theorems A + B

# Classification for Koopman I

3 limits needed in general!



#### **Different classes:**

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

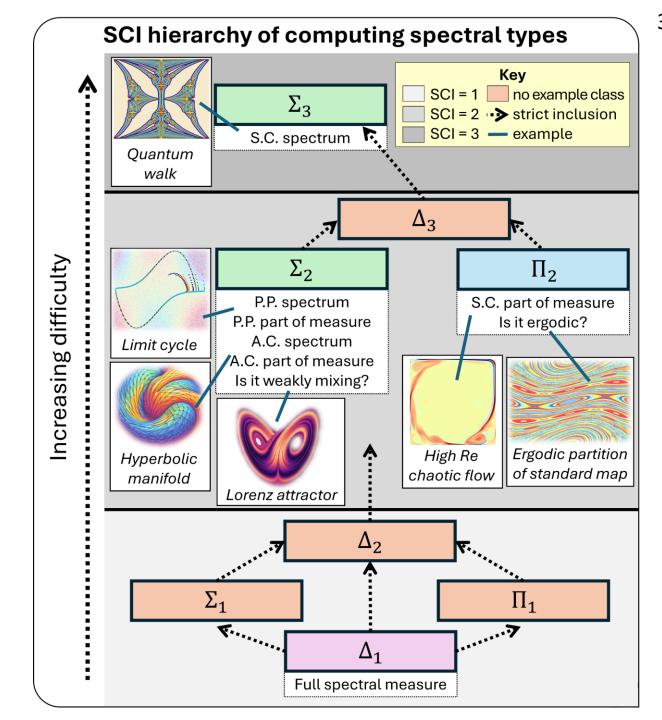
$$\Omega_{\mathcal{X}}^{m} = \{F: \mathcal{X} \to \mathcal{X} \mid F \text{ cts, m. p.}\}$$

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

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

Optimal algorithms and classifications of dynamical systems.

# Classification for Koopman II

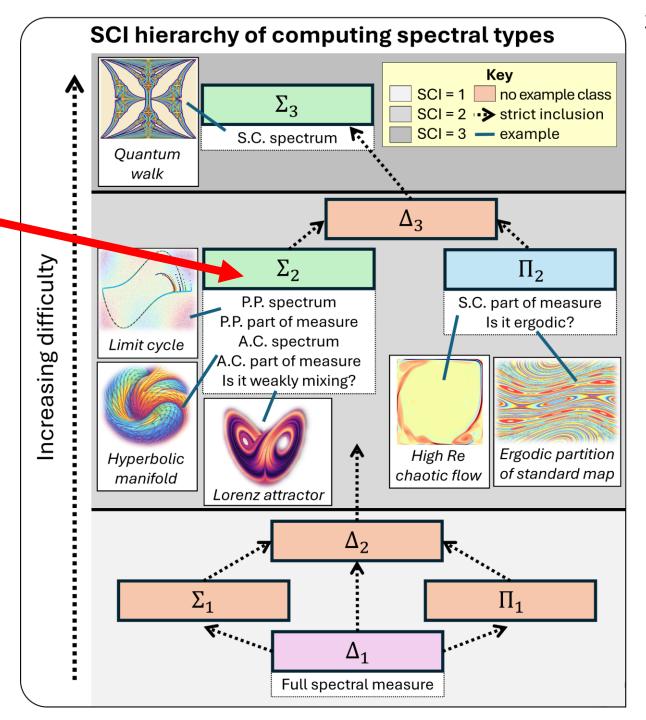


# Classification for Koopman II

**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)
  - $\Rightarrow$  classify difficulty of problems + prove optimality of algorithms.
- Ergodic theory + approximation theory + computational analysis
   ⇒ started to map out this terrain.

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

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

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