

What can we learn about a dynamical system from data?

Matthew Colbrook
University of Cambridge
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"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
$$F: \mathcal{X} \to \mathcal{X}$$
 – the dynamics: $x_{n+1} = F(x_n)$

Dynamics (geometry)
19th century

- Borel measure ω 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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Analysis 20th century

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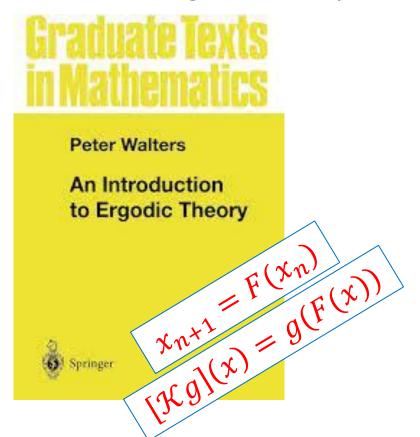
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Dynamics (geometry)
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Analysis 20th century

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.

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Why you should care about Koopman



Graduate Texts in Mathematics

Peter Walters

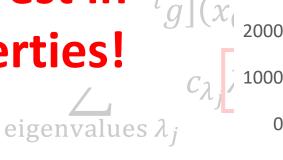
Can provide a diagon





+ HUGE recent interest in their spectral properties!

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







number of papersdoubles every 5 yrs

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

Perils of discretization: Warmup on $\ell^2(\mathbb{Z})$

- Spectrum is unit circle.
- Spectrum is stable.
- Continuous spectra.
- Unitary evolution.

- Spectrum is $\{0\}$.
- Spectrum is unstable.
- Discrete spectra.
- Nilpotent evolution.

Lots of Koopman operators are built up from operators like these!

Perils of discretization: Warmup on $\ell^2(\mathbb{Z})$



Issue: Many practitioners view Koopman as a magic bullet, but standard algorithms typically fail to converge! (Inf-dim spectral problems.)

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

- Spectrum is stable.
- Continuous spectra.
- Unitary evolution.

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- Nilpotent evolution.

Lots of Koopman operators are built up from operators like these!

Functions $\psi_i: \mathcal{X} \to \mathbb{C}$, j = 1, ..., 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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Functions
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quadrature points

$$\langle \psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \psi_k(x^{(m)}) = \begin{bmatrix} \left(\psi_1(x^{(1)}) & \cdots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_N(x^{(M)}) \end{pmatrix}^* \underbrace{\begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_M \end{pmatrix}}_{\hat{W}} \underbrace{\begin{pmatrix} \psi_1(x^{(1)}) & \cdots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_N(x^{(M)}) \end{pmatrix}}_{jk}$$
quadrature weights

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \underbrace{\begin{bmatrix} \left(\psi_1(x^{(1)}) & \cdots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \cdots & \psi_N(x^{(M)}) \\ \end{bmatrix}^*}_{\psi_X} \underbrace{\begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_M \end{pmatrix}}_{w} \underbrace{\begin{pmatrix} \psi_1(y^{(1)}) & \cdots & \psi_N(y^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(y^{(M)}) & \cdots & \psi_N(y^{(M)}) \\ \end{pmatrix}}_{jk}$$

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Galerkin Approximation

$$\mathcal{K} \longrightarrow \mathbb{K} = (\Psi_X^* W \Psi_X^*)^{-1} \Psi_X^* W \Psi_Y = (\sqrt{W} \Psi_X^*)^{\dagger} \sqrt{W} \Psi_Y \in \mathbb{C}^{N \times N}$$

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$$\langle \mathcal{K}\psi_{k},\psi_{j}\rangle \approx \sum_{m=1}^{M} w_{m}\overline{\psi_{j}(x^{(m)})}\underbrace{\psi_{k}(y^{(m)})}_{[\mathcal{K}\psi_{k}](x^{(m)})} = \underbrace{\begin{bmatrix} \left(\psi_{1}(x^{(1)}) & \cdots & \psi_{N}(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_{1}(x^{(M)}) & \cdots & \psi_{N}(x^{(M)}) \\ \end{bmatrix}^{*}}_{\psi_{X}} \underbrace{\begin{pmatrix} w_{1} & & & \\ & \ddots & & \\ & & w_{M} \end{pmatrix}}_{W} \underbrace{\begin{pmatrix} \psi_{1}(y^{(1)}) & \cdots & \psi_{N}(y^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_{1}(y^{(M)}) & \cdots & \psi_{N}(y^{(M)}) \\ \end{bmatrix}_{ik}$$

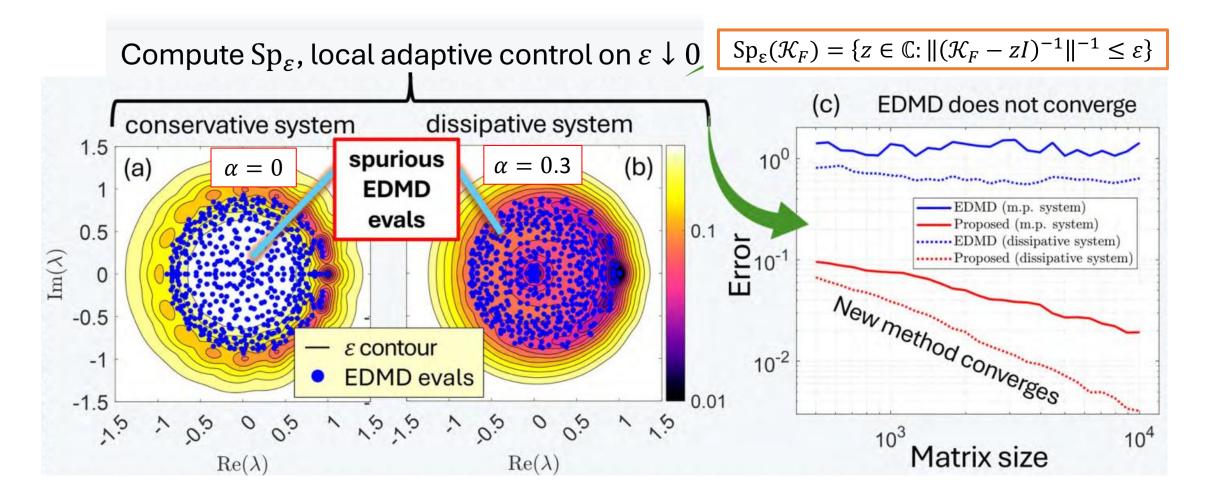


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Example: EDMD does NOT converge

- 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)



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

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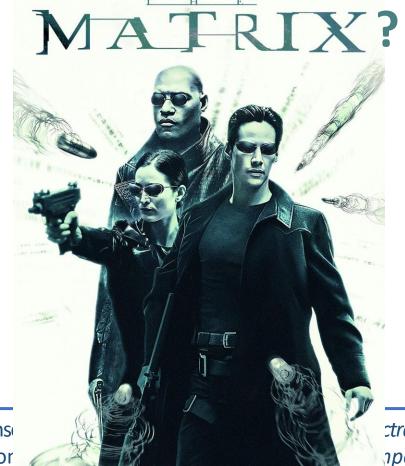
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$$\stackrel{\partial Q_{j_{0}j_{0}j_{0}}}{}_{jk}$$

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What's the missing



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

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

$$\stackrel{\partial Q_{joint}}{}$$

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C., Aytor

ctral properties of Koopman operators for dynamical systems," Commun. Pure Appl. Math., 2023. aposition," J. Fluid Mech., 2023.

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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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Bound projection errors!

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Proof sketch

Theorem A: There exists deterministic algorithms $\{\Gamma_{n_2,n_1}\}$ using snapshots such that $\lim_{n_2\to\infty} \lim_{n_1\to\infty} \Gamma_{n_2,n_1}(F) = \operatorname{Sp}(\mathcal{K}_F)$ for all measure-preserving systems.

- Residuals $\to \lim_{N\to\infty} \lim_{M\to\infty} \gamma_{N,M}(z,F) = \|(\mathcal{K}_F zI)^{-1}\|^{-1}$. N = size of basis, M = amount of data (quadrature).
- Measure-preserving $\Rightarrow \|(\mathcal{K}_F zI)^{-1}\|^{-1} = \operatorname{dist}(z, \operatorname{Sp}(\mathcal{K}_F)).$
- Local N-adaptive minimisation of $\gamma_{N,M}(z,F)$ to approximate $\operatorname{Sp}(\mathcal{K}_F)$.

Proof sketch

Theorem A: There **exists** deterministic algorithms $\{\Gamma_{n_2,n_4}\}$ using snapshots such that $\lim_{n_2\to\infty}\lim_{n_1\to\infty}\Gamma_{n_2,n_1}(F)=\operatorname{Sp}(\mathcal{K}_F)$ for all measurepreserving systems.

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Double limit
$$\lim_{N\to\infty}\lim_{M\to\infty}$$
 Can we do better?

Theorem B (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 B: 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.

Double limit is necessary!

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

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 data $(x_j \rightarrow y_j)$ 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.

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...

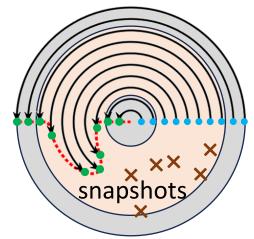
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Build an adversarial F...

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

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



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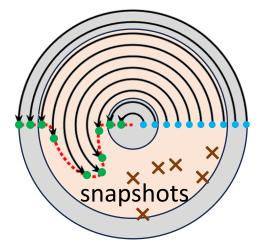
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 $\lim_{n\to\infty}\Gamma_n\big(\widetilde{F_1}\big)=\operatorname{Sp}(\mathcal{K}_{\widetilde{F_1}})\Rightarrow \exists n_1 \text{ s.t. } \operatorname{dist}(i,\Gamma_{n_1}\big(\widetilde{F_1}\big))\leq 1.$

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



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).

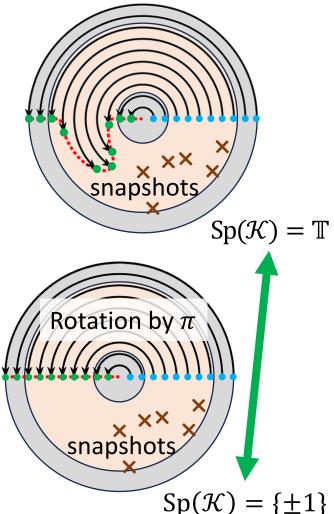
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BUT Γ_{n_1} uses finite amount of info to output $\Gamma_{n_1}(\widetilde{F_1})$. Let X, Y correspond to these snapshots.

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

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

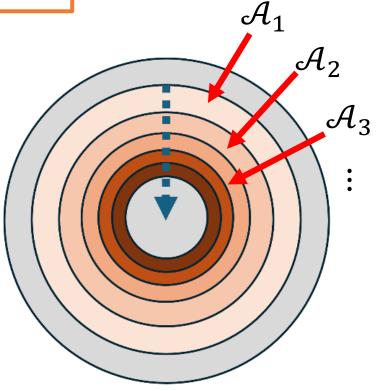
BUT Sp
$$(\mathcal{K}_{F_1}) = \operatorname{Sp}(\bar{\mathcal{K}}_{F_0}) = \{\pm 1\}$$



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

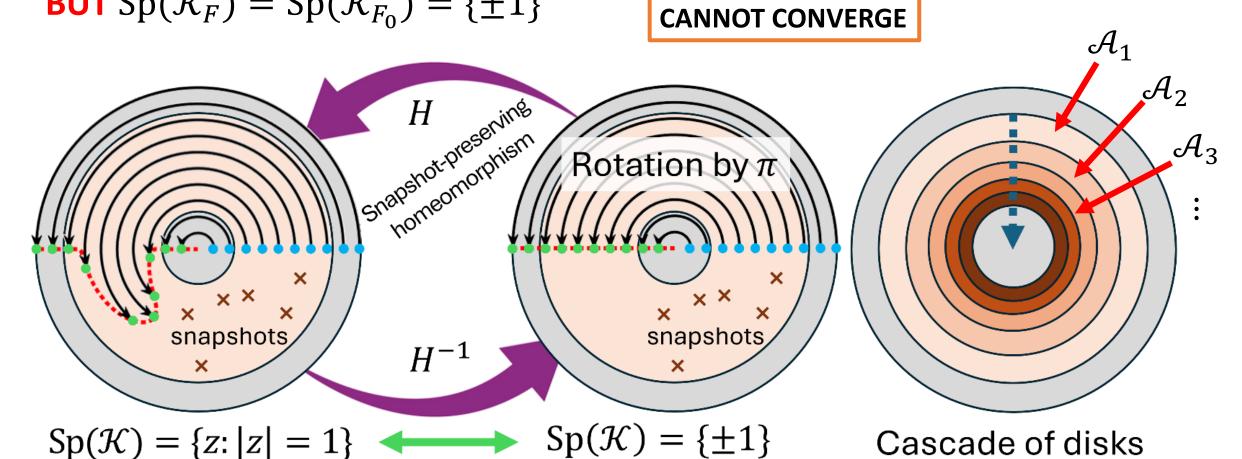


Cascade of disks

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

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}

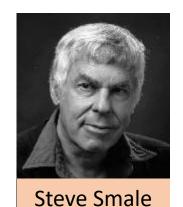


Successive limits seems unavoidable!?!?

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.
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Classifications: Solvability Complexity Index (SCI)

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

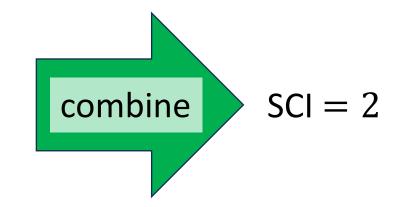
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Theorem A: $SCI \leq 2$

Theorem B: SCI > 1



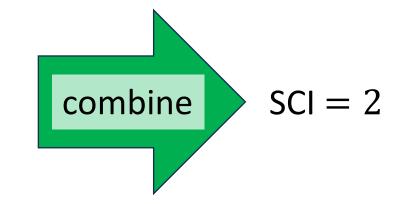
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So far literature has only proven upper bounds, that need not be sharp...

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Are these sharp?

Koopman literature has tonnes of upper bounds!

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

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	$SCI \le 2^*$	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 ∇F (otherwise additional limit)	$SCI \le 2$	N/C	$SCI \le 2$ (see [89])	n/a
Compactification [42]	ctstime, m.p. ergodic systems	$SCI \le 4$	N/C	$SCI \le 4$	n/a
Resolvent compactification [43]	ctstime, m.p. ergodic systems	$SCI \leq 5$	N/C	$SCI \leq 5$	n/a
Diffusion maps [90] (see also [10])	ctstime, m.p. ergodic systems	$SCI \leq 3$	n/a	n/a [

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., $d(\Gamma_n(F), \operatorname{Sp}(\mathcal{K}_F)) \leq 2^{-n}$.
- Δ_{m+1} : $SCI \leq m$.
- Σ_m : SCI $\leq m$, final limit from below.

E.g.,
$$\Sigma_1$$
: $\sup_{z \in \Gamma_n(F)} \operatorname{dist}(z, \operatorname{Sp}(\mathcal{K}_F)) \leq 2^{-n}$.

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

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$$\Pi_1$$
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E.g.,
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•
$$\Pi_m$$
: $\mathrm{SCl} \leq m$, final limit from above.
E.g., Π_1 : $\sup_{z \in \mathrm{Sp}(\mathcal{H}_F)} \mathrm{dist}(z, \Gamma_n(F)) \leq 2^{-n}$.

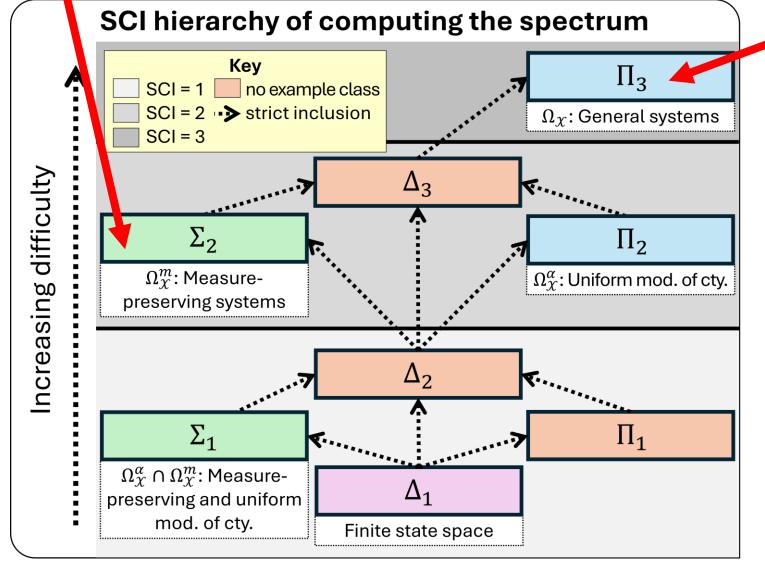
covers spectrum

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Theorems A + B

Classification for Koopman I

3 limits needed in general!



Different classes:

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

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

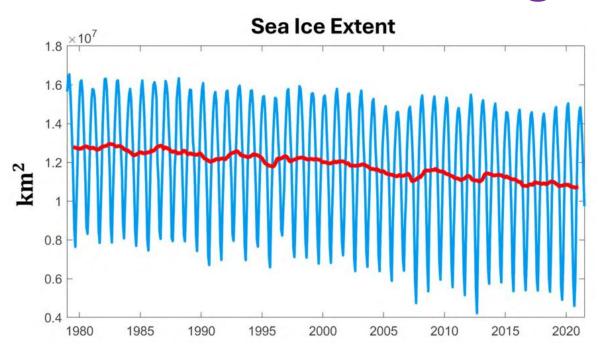
$$\Omega_{\mathcal{X}}^{\alpha} = \{F: \mathcal{X} \to \mathcal{X} \mid F \text{ mod. cty. } \alpha\}$$

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

Optimal algorithms and classifications of dynamical systems.

Practical Gains: Arctic Sea Ice Forecasting

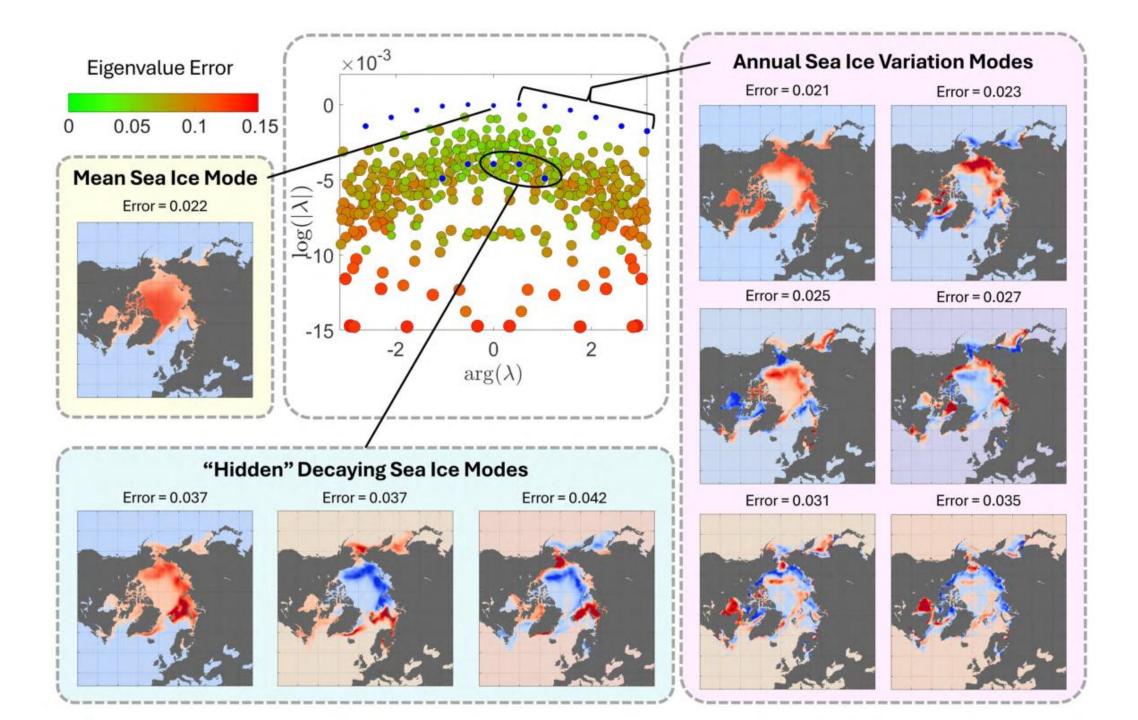
Monthly average from satellite passive microwave sensors. Data from the European Organisation for the Exploitation of Meteorological Satellites' (EUMETSAT) Ocean and Sea Ice Satellite Application Facilities (OSI-SAF) data record, comprising retrieval algorithms OSI-450 (1979–2015) and OSI-430-b (2016 onwards).



Motivation: Arctic amplification, polar bears, local communities, effect on extreme weather in Northern hemisphere,...

Problems:

- Very hard to predict more than two months in advance.
- Which geographical regions are significant?



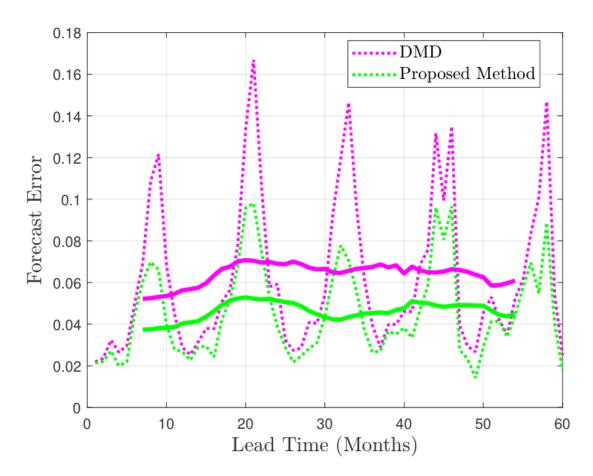


Figure 4: Forecast error for entire sea ice concentration. The relative mean squared error of forecasts over five years. The solid lines show the moving 12-month mean. In each case, the model is built using the data from the years 2005–2015, and then tested on 2016-2020. The proposed method consistently outperforms DMD.

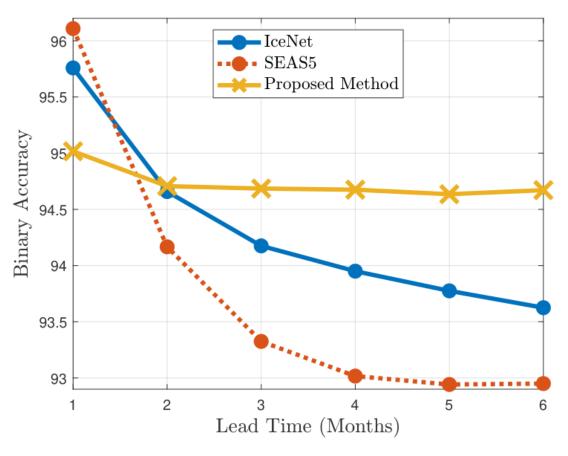
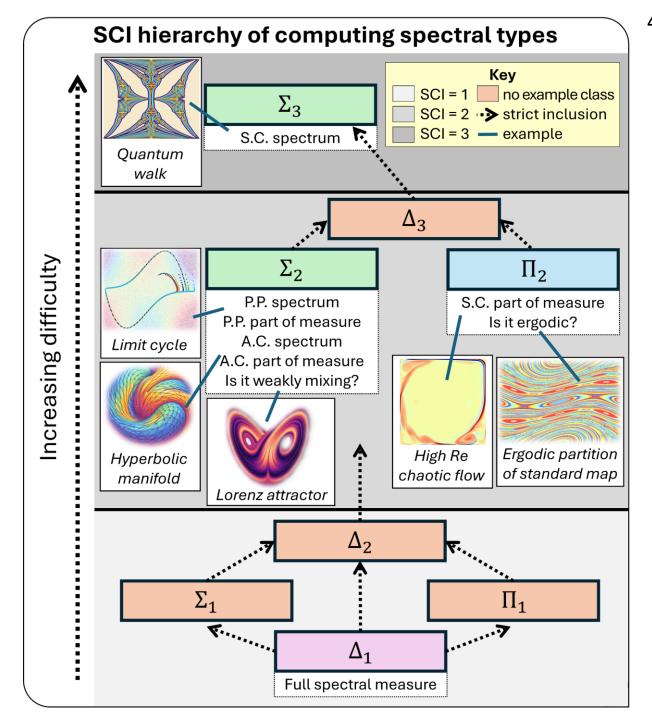


Figure 5: Comparison with machine learning and statistical prediction benchmarks. Mean binary accuracy over the test years 2012–2020, shown for IceNet, SEAS5, and our proposed method that avoids spurious Koopman eigenvalues. Our proposed method achieves better accuracy for lead times greater than one month, with very little increase of errors at larger lead times.

• Andersson et al, "Seasonal Arctic sea ice forecasting with probabilistic deep learning." **Nature Communications**, 2021.

Classification for Koopman II

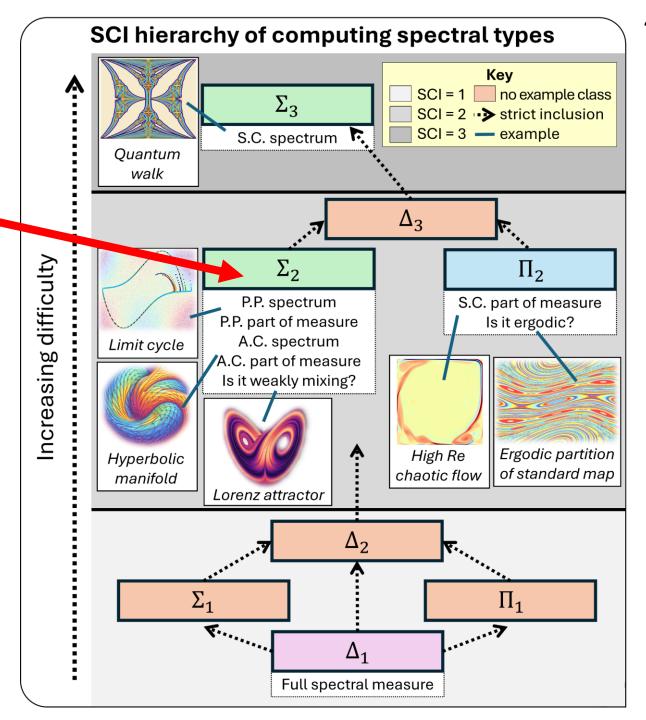


Classification for Koopman II

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)

- Brunton, Proctor, Kutz, "Discovering governing equations from data by sparse identification of nonlinear dynamical systems," **Proc. Natl.** Acad. Sci. USA, 2016.
- Karniadakis, Kevrekidis, Lu, Perdikaris, Wang, Yang, "Physics-informed machine learning," Nature Reviews Physics, 2021.
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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.
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Where does your problem/method fit into the SCI hierarchy? Is it optimal?

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