

Navigating Limits in Learning Complex Systems

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

Data-driven dynamical systems

- 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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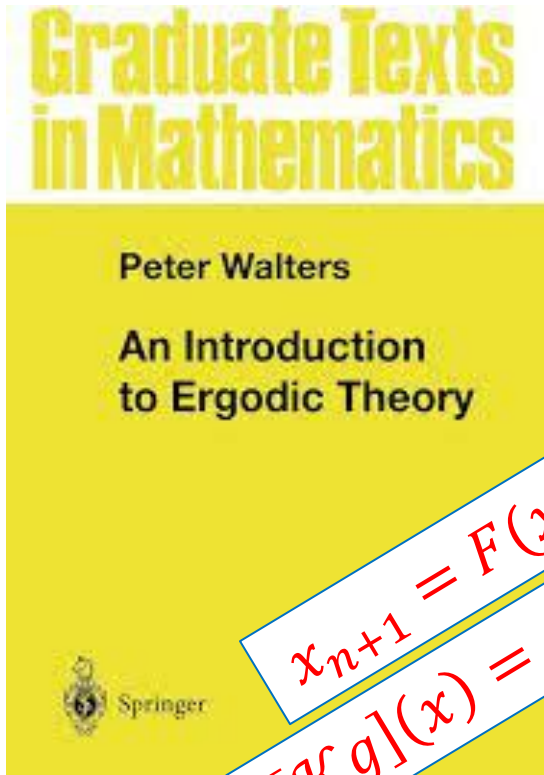
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19th century**
- Analysis
20th century**
- Data
21st century**

(DO NOT ASSUME MEASURE-PRESERVING)

Why you should care about Koopman

Fundamental in ergodic theory



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

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

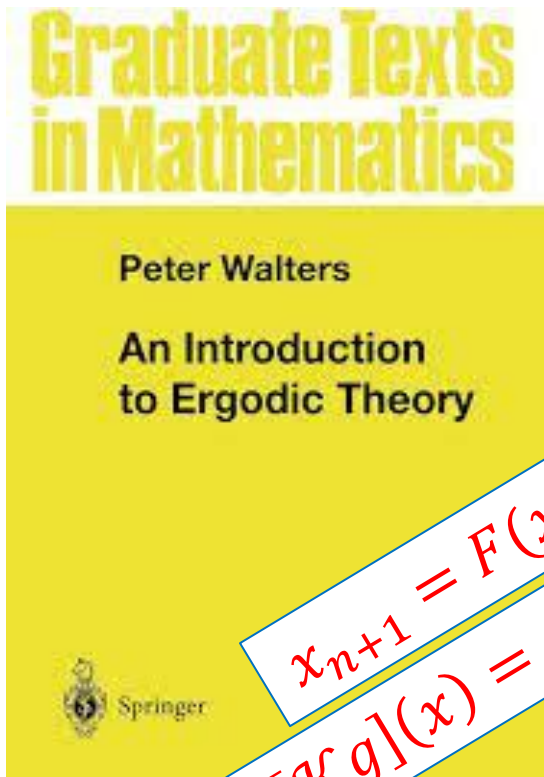
E.g., key to ergodic theorems of Birkhoff and von Neumann.

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

Why you should care about Koopman

Fundamental in ergodic theory

Can provide a *diagonalization* of a nonlinear system.



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

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

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

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

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

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

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

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

Why you should care about Koopman

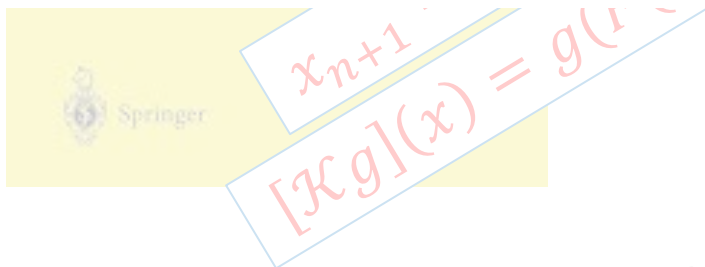
Fundamental in ergodic theory

Can provide a *diagonal*

Graduate Texts
in Mathematics

Peter Walters

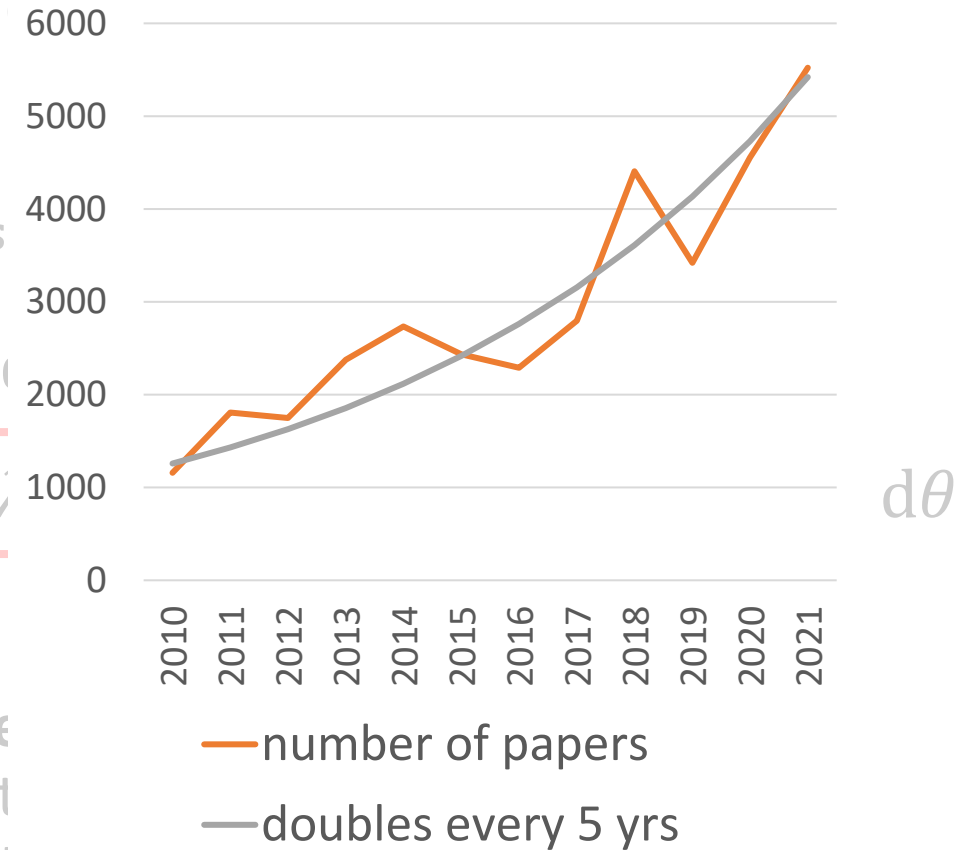
+ HUGE recent interest in their spectral properties!



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

Spectral properties of invariant measures, their behavior, coherent structures, quasiperiodicity, etc.

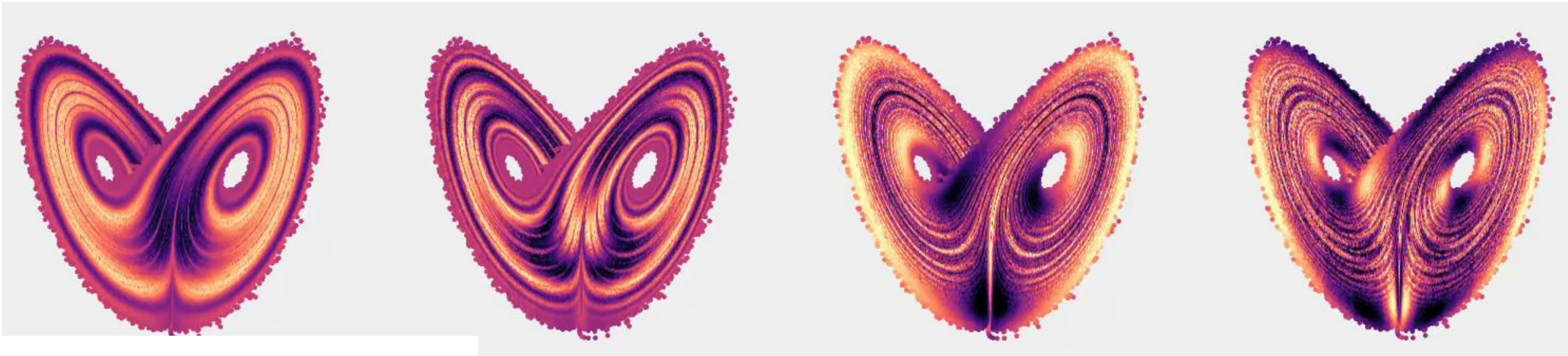
New Papers on
"Koopman Operators"



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

Example

If $\|\mathcal{K}g - \lambda g\| \leq \varepsilon$, then $g(x_n) = [\mathcal{K}^n g](x_0) = \lambda^n g(x_0) + \mathcal{O}(n\varepsilon)$



Coherent features!

$$\text{Sp}_{\text{ap},\varepsilon}(\mathcal{K}) = \{z \in \mathbb{C} : \exists g, \|g\| = 1, \|\mathcal{K}g - zg\| \leq \varepsilon\}$$

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

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

$$\begin{pmatrix} \ddots & & & & \\ & \ddots & & & \\ & 0 & 1 & & \\ & & 0 & 1 & \\ & & & 0 & 1 \\ & & & & 0 & \ddots \end{pmatrix} \xrightarrow{\text{Two-way infinite}} \begin{pmatrix} 0 & 1 & & & \\ & \ddots & \ddots & & \\ & & \ddots & 1 & \\ & & & \ddots & 0 \end{pmatrix} \in \mathbb{C}^{N \times N}$$

- 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!

Extended Dynamic Mode Decomposition (EDMD)

Functions $\psi_j: \mathcal{X} \rightarrow \mathbb{C}, j = 1, \dots, N$

$$\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^M$$

quadrature points

$$\langle \psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \psi_k(x^{(m)}) = \left[\underbrace{\begin{pmatrix} \psi_1(x^{(1)}) & \dots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \dots & \psi_N(x^{(M)}) \end{pmatrix}}_{\Psi_X} \right]^* \underbrace{\begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_M \end{pmatrix}}_W \underbrace{\begin{pmatrix} \psi_1(x^{(1)}) & \dots & \psi_N(x^{(1)}) \\ \vdots & \ddots & \vdots \\ \psi_1(x^{(M)}) & \dots & \psi_N(x^{(M)}) \end{pmatrix}}_{\Psi_X} \right]_{jk}$$

quadrature weights

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

Galerkin
Approximation

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

- Schmid, "Dynamic mode decomposition of numerical and experimental data," **J. Fluid Mech.**, 2010.
- Rowley, Mezić, Bagheri, Schlatter, Henningson, "Spectral analysis of nonlinear flows," **J. Fluid Mech.**, 2009.
- Williams, Kevrekidis, Rowley "A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition," **J. Nonlinear Sci.**, 2015.

Residual DMD (ResDMD)

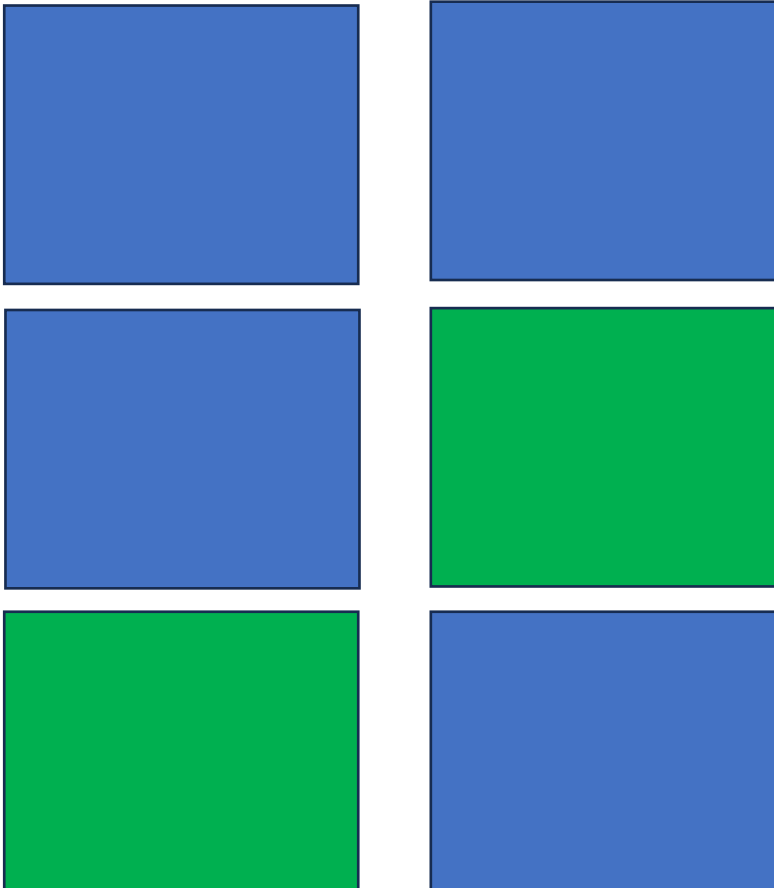
$$\langle \psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \psi_k(x^{(m)}) = \left[\underbrace{\Psi_X^* W \Psi_X}_G \right]_{jk}$$

$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})} = \left[\underbrace{\Psi_X^* W \Psi_Y}_{K_1} \right]_{jk}$$

- C., Townsend, “Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems,” **Commun. Pure Appl. Math.**, 2023.
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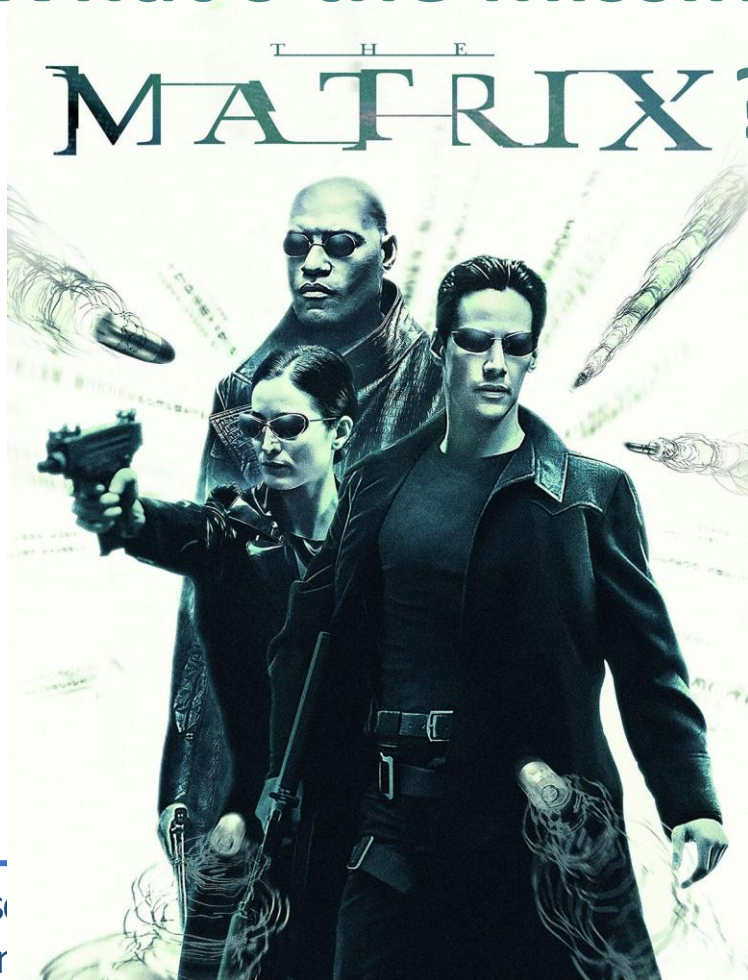
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The diagram illustrates the relationship between the Gram matrix G and the cross-covariance matrix K_1 . G is represented by a blue square, and K_1 is represented by a green square. An orange arrow labeled "adjoint" points from K_1 to G , indicating that G is the adjoint of K_1 .

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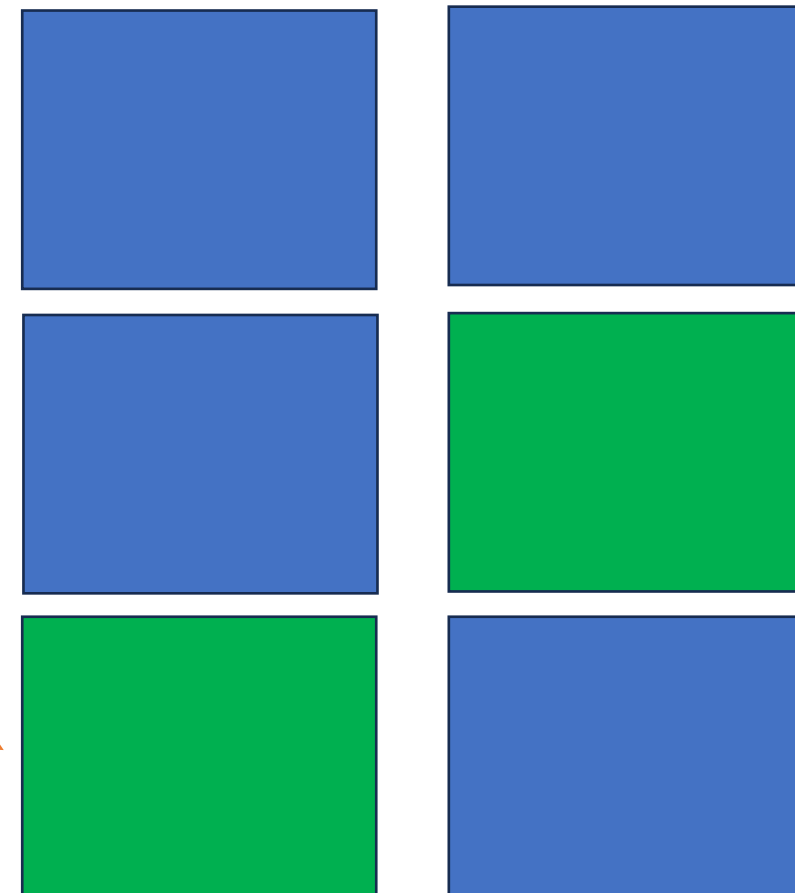
What's the missing



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

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

adjoint



- C., Towns
 - C., Aytor
 - Code: <https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition>
- central properties of Koopman operators for dynamical systems," *Commun. Pure Appl. Math.*, 2023.
- composition," *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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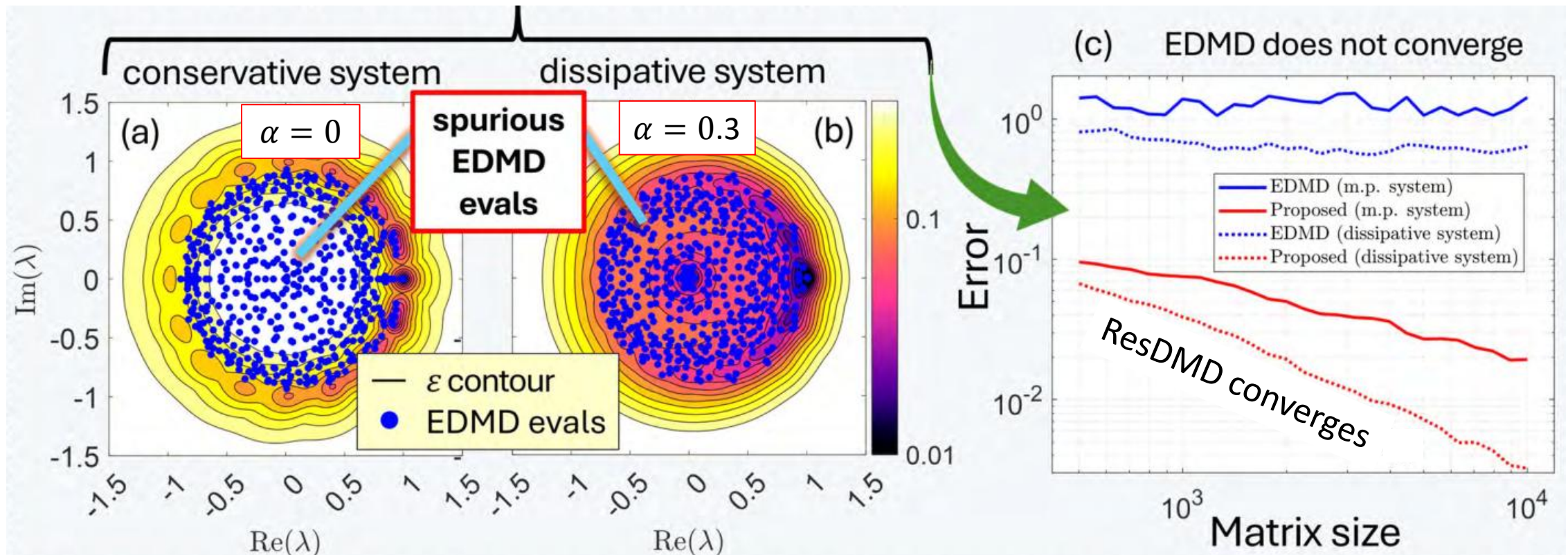
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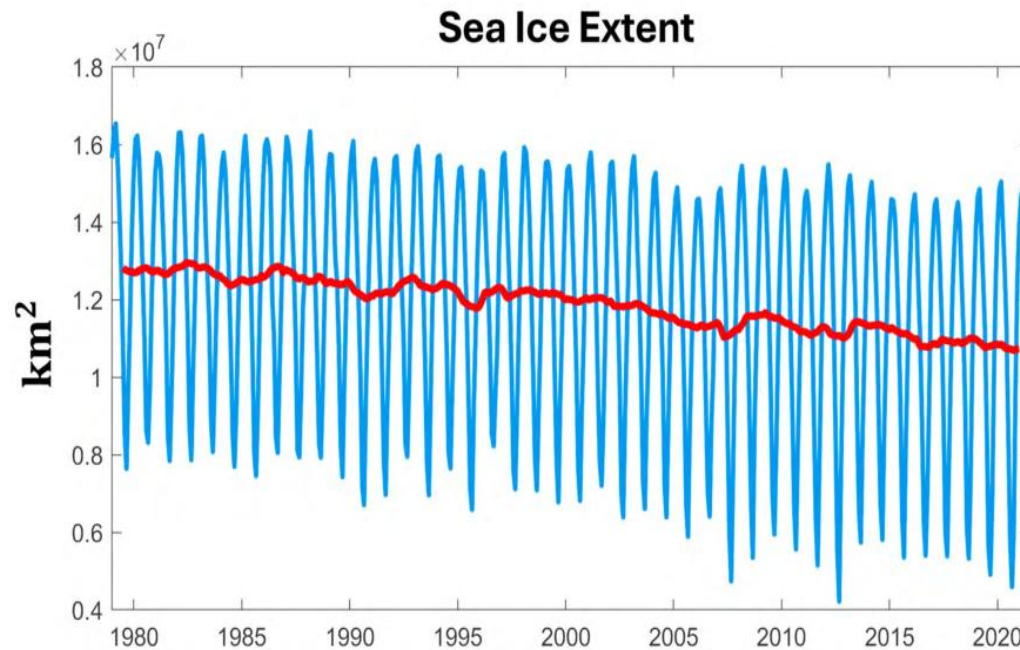
Example: EDMD doesn't converge

- 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 ($M = 50000$)

Compute $\text{Sp}_{\text{ap},\varepsilon}(\mathcal{K})$, local adaptive control on $\varepsilon \downarrow 0$



Practical Gains: Arctic Sea Ice Forecasting

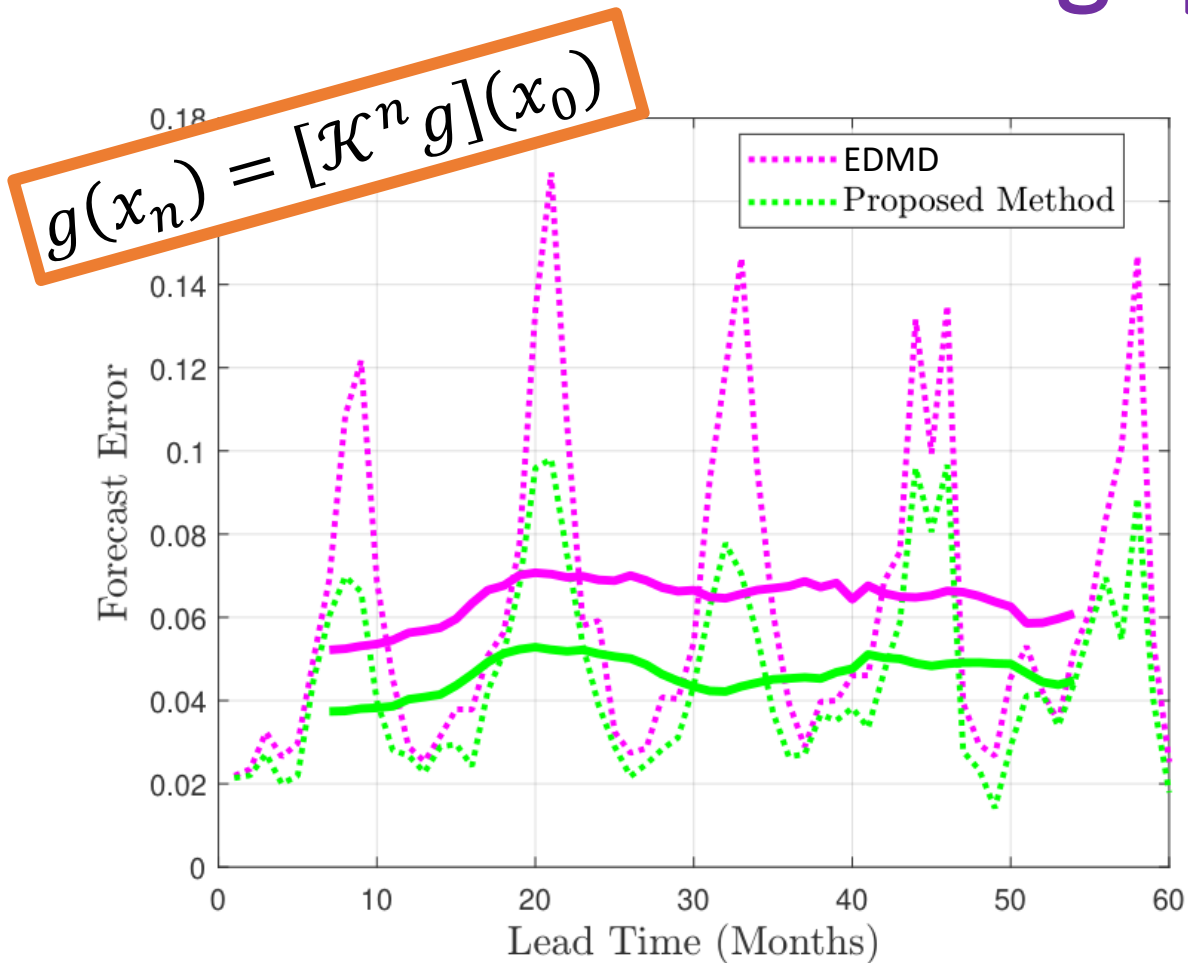


Monthly average from
satellite passive
microwave sensors.

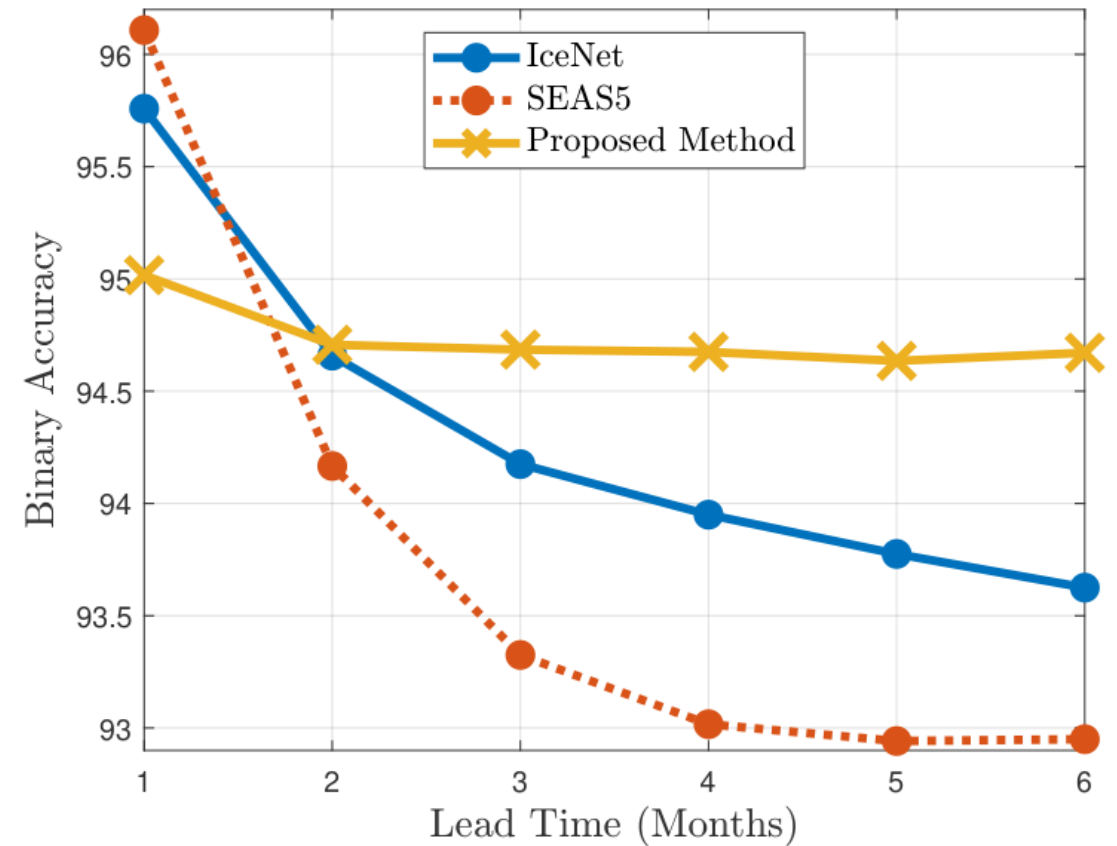
Motivation: Arctic amplification, polar bears, local communities, effect on extreme weather in Northern hemisphere,...

Problem: Very hard to predict more than two months in advance.

Arctic case: Avoiding spurious eigenvalues helps!



Relative mean squared error over 2016-2020. Model built from 2005-2015 data. (Solid lines moving 12-month mean.)



Mean binary accuracy over test years 2012-2020. (*IceNet: Andersson et al, "Seasonal Arctic sea ice forecasting with probabilistic deep learning." Nature Communications, 2021.*)

Good news!

Theorem A: There **exists** *deterministic* algorithms $\{\Gamma_{N,M}\}$ using snapshots such that $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} \Gamma_{N,M}(F) = \text{Sp}_{\text{ap},\varepsilon}(\mathcal{K}_F)$ for all systems.

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

Question?

Theorem A: There **exists** *deterministic* algorithms $\{\Gamma_{N,M}\}$ using snapshots such that $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty} \Gamma_{N,M}(F) = \text{Sp}_{\text{ap},\varepsilon}(\mathcal{K}_F)$ for all systems.

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

Double limit $\lim_{N \rightarrow \infty} \lim_{M \rightarrow \infty}$

Can we do better?

Adversaries: Double limit is necessary!

Implies \mathcal{K} is unitary

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

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

Theorem B: There **does not exist** any sequence of deterministic algorithms $\{\Gamma_n\}$ using \mathcal{T}_F such that $\lim_{n \rightarrow \infty} \Gamma_n(F) = \text{Sp}_{\text{ap}, \varepsilon}(\mathcal{K}_F) \forall F \in \Omega_{\mathbb{D}}.$

NB:

- n can index anything.
- Universal - any type of algorithm or computational model.
- Similarly, no random algorithms converging with probability $> 1/2$.

Adversaries occur with high probability.

Proof idea: Constructing an adversary

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

Phase transition lemma: Let $X = \{x_1, \dots, x_N\}, Y = \{y_1, \dots, y_N\}$ be distinct points in annulus $\mathcal{A} = \{x \in \mathbb{D} \mid 0 < R < \|x\| < r < 1\}$ 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: Constructing an adversary

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 ...

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

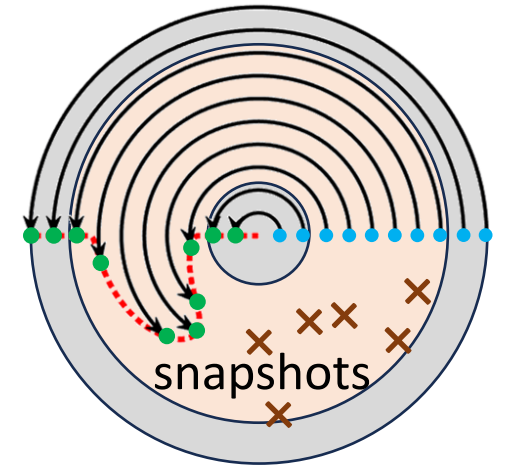
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Build an **adversarial** F ...

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

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



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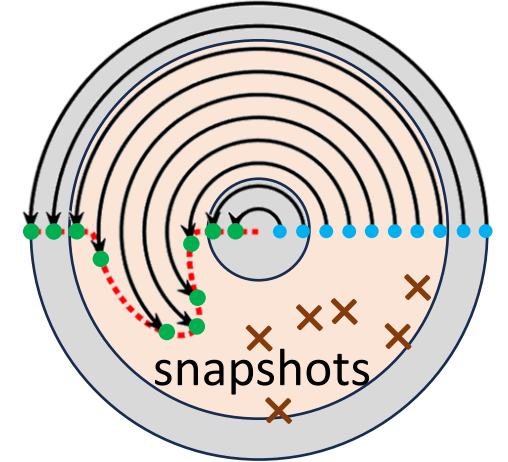
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$$\lim_{n \rightarrow \infty} \Gamma_n(\widetilde{F}_1) = \text{Sp}(\mathcal{K}_{\widetilde{F}_1}) \Rightarrow \exists n_1 \text{ s.t. } \text{dist}(i, \Gamma_{n_1}(\widetilde{F}_1)) \leq 1.$$

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

Let X, Y correspond to these snapshots.



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

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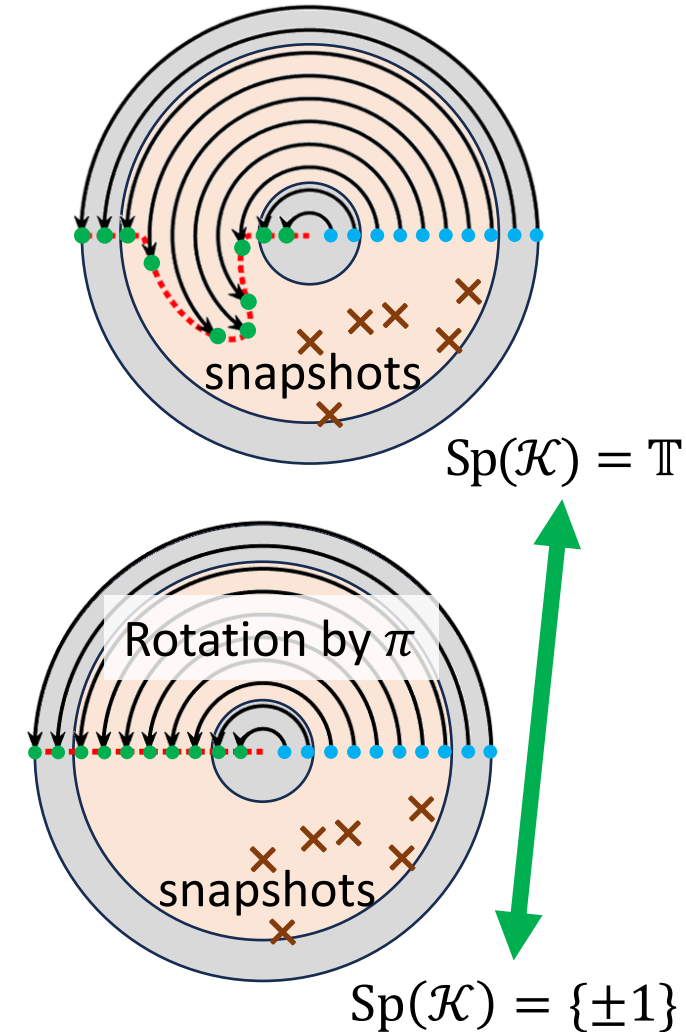
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Let X, Y correspond to these snapshots.

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

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

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



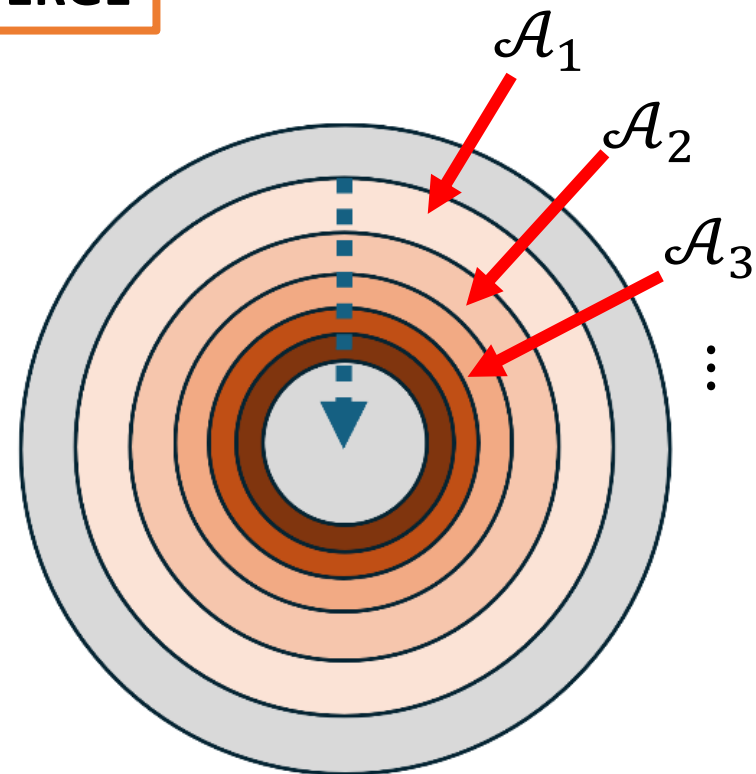
Proof idea: Constructing an adversary

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

CANNOT CONVERGE



Cascade of disks

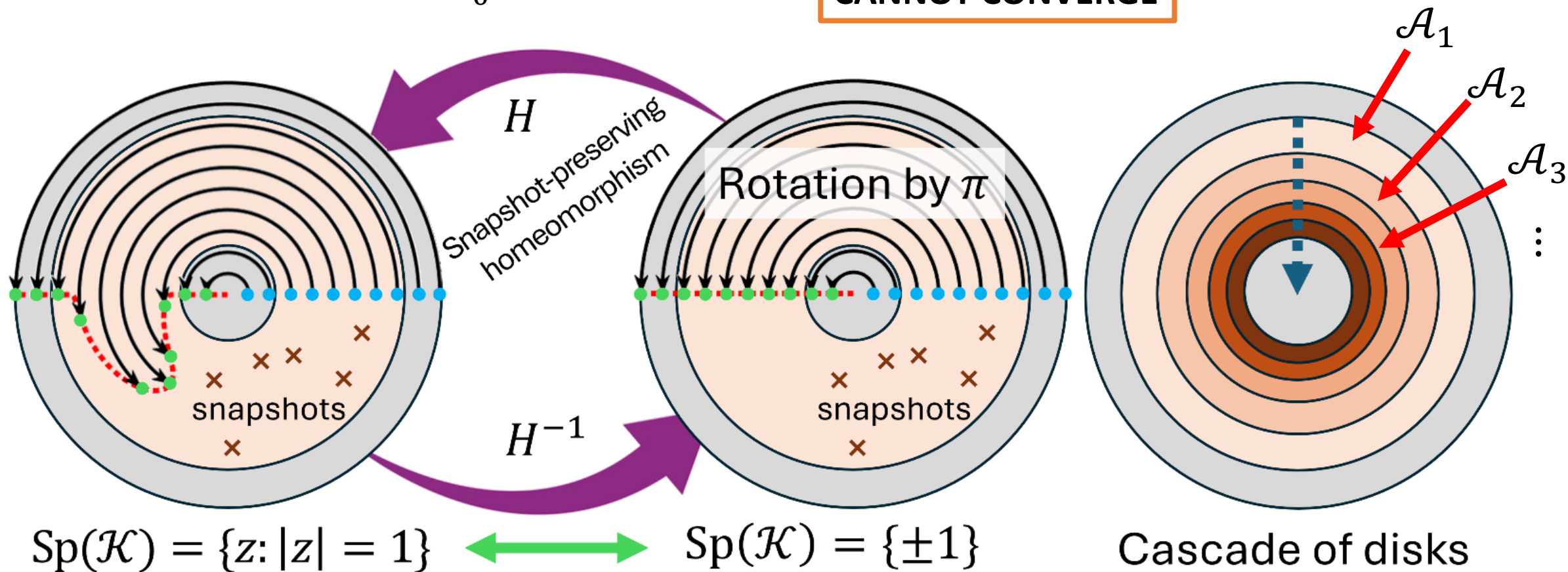
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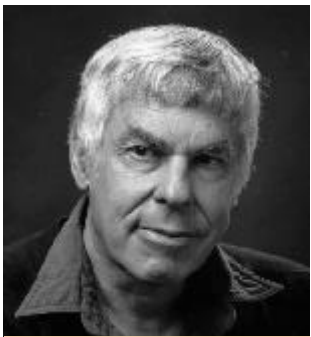
CANNOT CONVERGE



Successive limits seems unavoidable!?!?

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: algorithms



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.

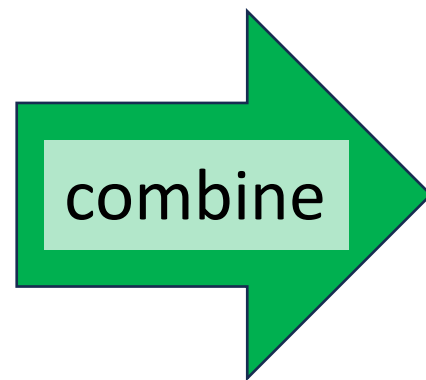
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Theorem A: $\text{SCI} \leq 2$

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



$\text{SCI} = 2$

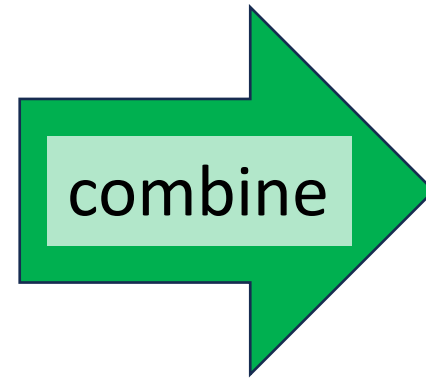
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$\text{SCI} = 2$

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

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Lots of SCI upper bounds lurking in Koopman literature!

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,...

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

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

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trust output

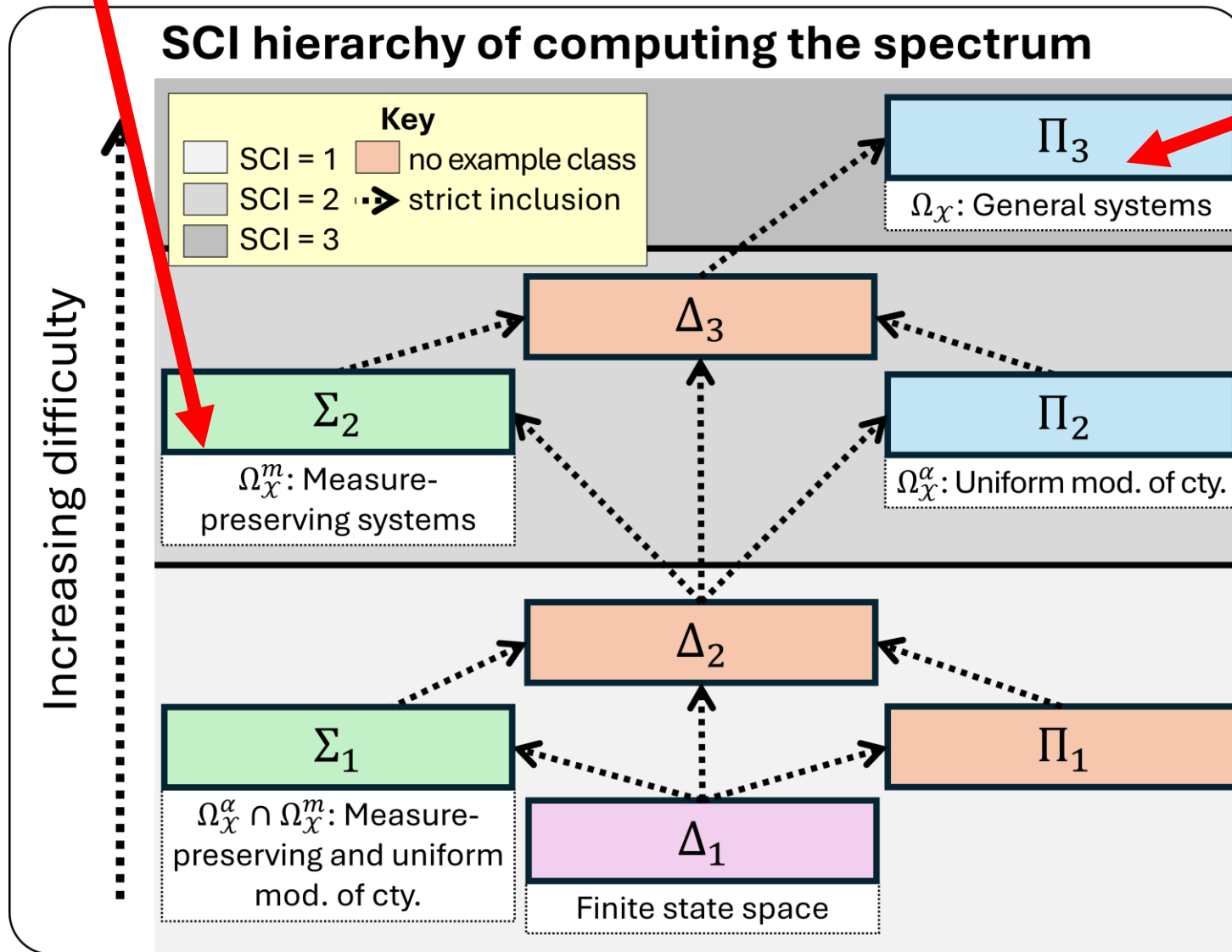
verification

covers spectrum

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Classification for Koopman

3 limits needed in general!



Different classes:

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

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

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

$$[d_X(F(x), F(y)) \leq \alpha(d_X(x, y))]$$

Optimal algorithms and classifications of dynamical systems.

Conclusion: FOUNDATIONS \leftrightarrow METHODS

- Data-driven spectral problems for Koopman operators are hugely popular.

BUT: Standard truncation methods often fail.

- *SCI hierarchy* classifies computational problems:

Lower bounds through method of adversarial dynamics.

Upper bounds \Rightarrow new “inf.-dim.” algorithms. Rigorous, optimal, practical.

(spectra, pseudospectra, spectral measures etc.)

E.g., Verification of approximate eigenfunctions leads to practical gains.

\rightarrow **We now have a near complete picture for Koopman on $L^2(\mathcal{X}, \omega)$!**

NB: *Similar story for spectral measures, dealing with continuous spectra (versus eigenvalues) and spectral type (different flavors of dynamics).*

Shameless final plug...

Upcoming book with CUP:

INFINITE-DIMENSIONAL SPECTRAL COMPUTATIONS

Foundations, Algorithms, and Modern Applications

100s of: classifications, algorithms,
examples (including full code), figures,
exercises (including full solutions).

****Out this (2025) holiday season
(hopefully!)...****

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*If something interests you,
please speak to me after.*

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