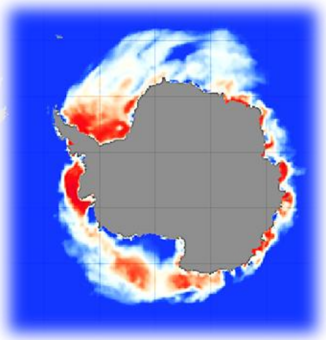
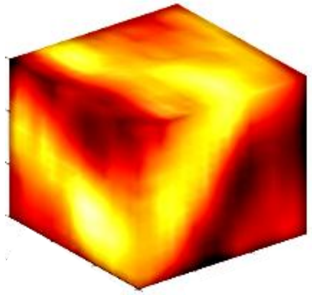

Verified Koopman Modes and an Example for Climate

Matthew Colbrook

02/07/2025

UNIVERSITY OF CAMBRIDGE

"To <u>classify</u> is to bring order into chaos." - **George Pólya**

My thanks to a cast of great collaborators!

Alex Townsend
(Cornell)

Igor Mezić
(UC Santa Barbara)

Alexei Stepanenko
(Cam. -> Industry)

Nicolas Boullé
(Imperial)

Gustav Conradie
(Cambridge)

- C., Townsend. *"Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems."* **Communications on Pure and Applied Mathematics,** 2024.
- C., Mezić, Stepanenko, *"Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning."* (winding its way through **Nature Communications**).
- Boullé, C., Conradie, *"Convergent Methods for Koopman Operators on Reproducing Kernel Hilbert Spaces."* (***SpecRKHS*** - **hot off the press: https://arxiv.org/abs/2506.15782**)

What is a Koopman operator?

- $\mathcal{X}$ – *the state space*
- $\mathcal{X} \ni x$ – *the state*

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

Henri Poincaré
(Sorbonne)

- Poincaré, *''Les méthodes nouvelles de la mécanique céleste,''* **Vol. 2. Gauthier-Villars et fils, imprimeurs-libraires**, 1893.

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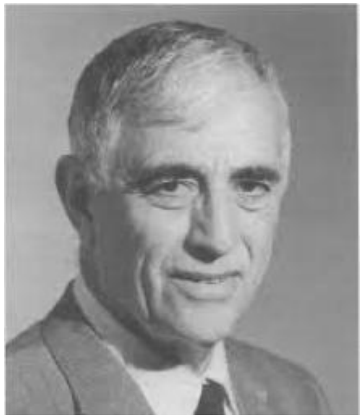
- Functions $g: \mathcal{X} \to \mathbb{C}$ a.k.a "observables"
- Koopman operator $\mathcal{K}_F$: $[\mathcal{K}_F g](x) = g(F(x))$

LINEAR!

Observe g one time step forward

Bernard Koopman
(Columbia)



John von Neumann
(IAS)

- Koopman, "*Hamiltonian systems and transformation in Hilbert space,*" **Proc. Natl. Acad. Sci. USA**, 1931.
- Koopman, v. Neumann, "*Dynamical systems of continuous spectra,*" **Proc. Natl. Acad. Sci. USA**, 1932.

What is a Koopman operator?

- $\mathcal{X}$ – *the state space*
- $\mathcal{X} \ni x$ – *the state*
- ***Unknown*** cts $F: \mathcal{X} \to \mathcal{X}$ – *the dynamics:* $x_{n+1} = F(x_n)$
- Functions $g: \mathcal{X} \to \mathbb{C}$ a.k.a "observables"
- Koopman operator $\mathcal{K}_F$: $[\mathcal{K}_F g](x) = g(F(x))$ LINEAR!
- ***Available*** snapshot data: $\left\{\left(x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right) : m = 1, \dots, M\right\}$

Can we compute spectral properties from trajectory data?

Why?

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

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

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

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

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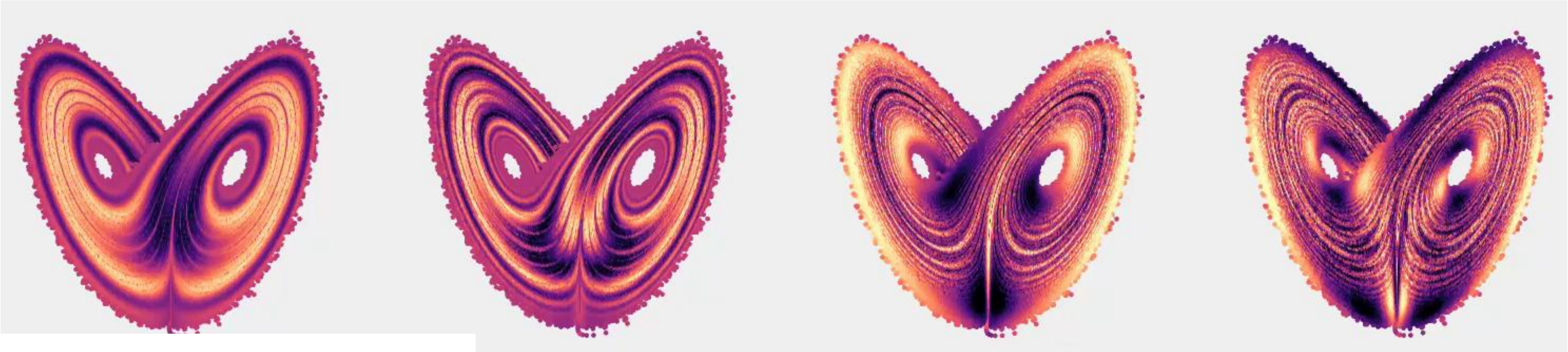

Coherent features!

Lorenz attractor

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

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

Why?

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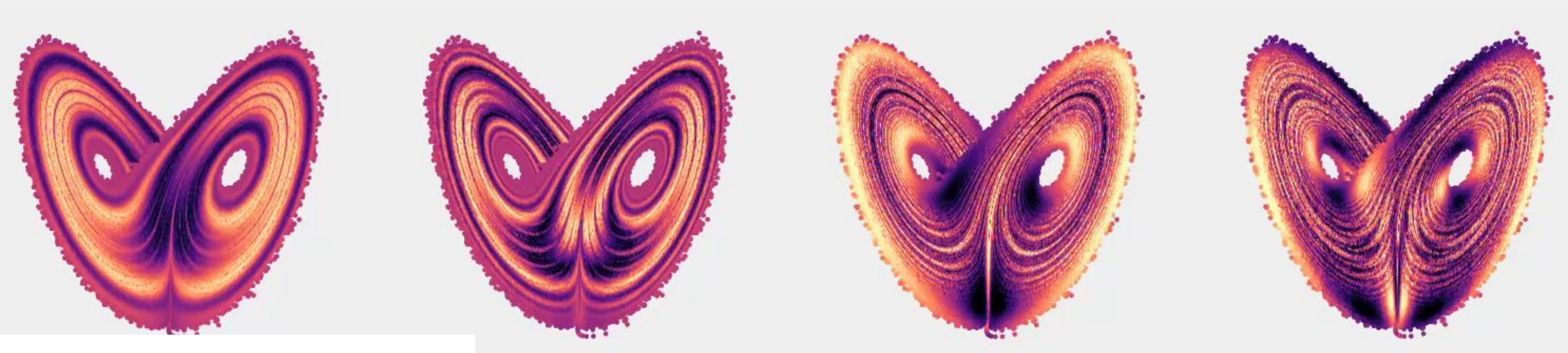


Coherent features!

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

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

Koopman Mode Decomposition

Verified Eigenfunctions

- Find (g_j, λ_j) with $\|\mathcal{K}g_j - \lambda_j g_j\| \leq \varepsilon$
- Expand state:

Koopman modes

$$x \approx \sum_j c_j g_j(x)$$

- Forecasts:

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

$$x_n = \sum_j \lambda_j^n c_j g_j(x) + \mathcal{O}(n\varepsilon)$$

Building a matrix approximation of $\mathcal{K}$: EDMD

Observables $\psi_j : \mathcal{X} \to \mathbb{C}, j = 1, \ldots, N$

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

quadrature points

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

quadrature weights

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

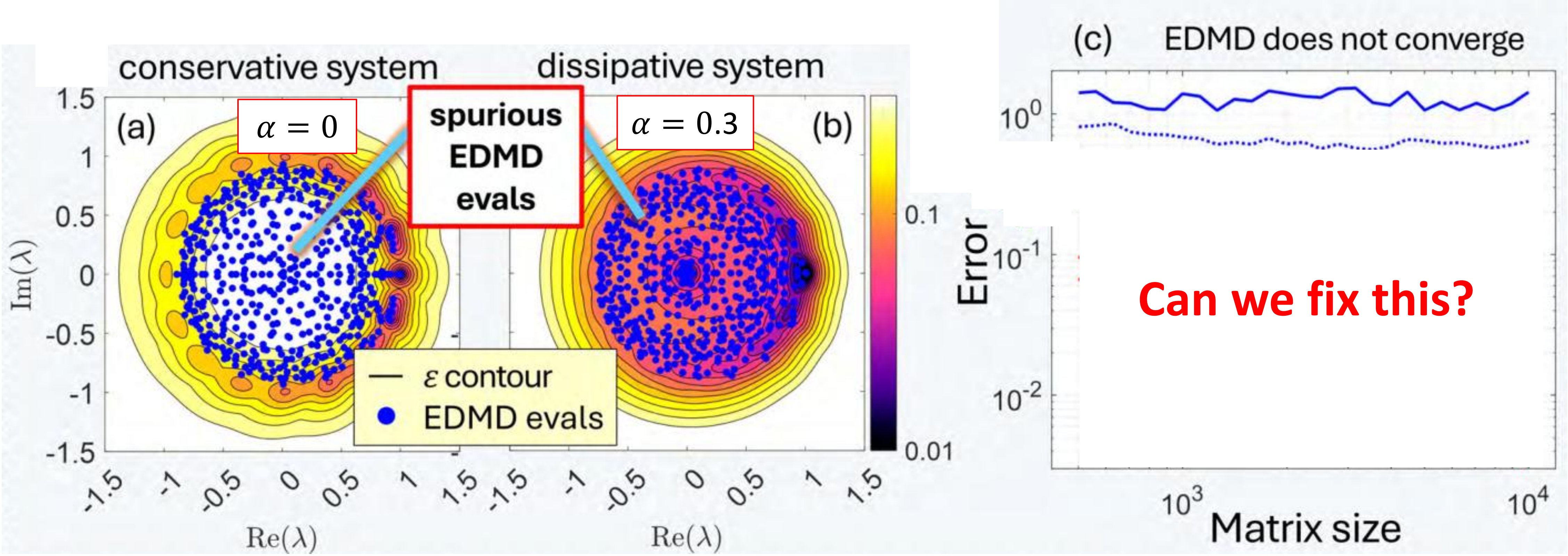
Galerkin Approximation

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

- 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.

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 ($M = 50000$)



The fix: Residual DMD (ResDMD)

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

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

- C., Townsend, "*Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*," **Commun. Pure Appl. Math.**, 2023.
- C., Ayton, Szőke, "*Residual Dynamic Mode Decomposition*," **J. Fluid Mech.**, 2023.
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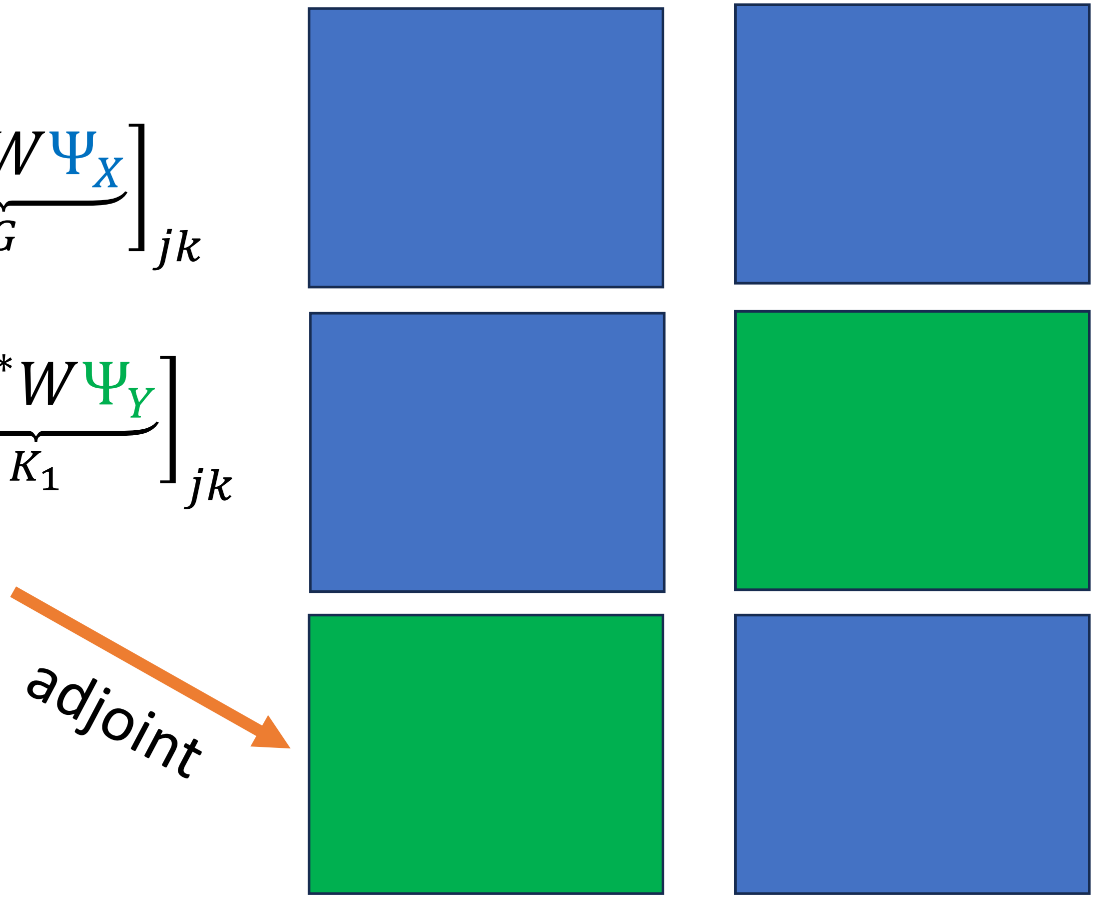

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Residuals: $g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j,\ \|\mathcal{K}g - \lambda g\|^2 = \langle \mathcal{K}g - \lambda g, \mathcal{K}g - \lambda g \rangle$

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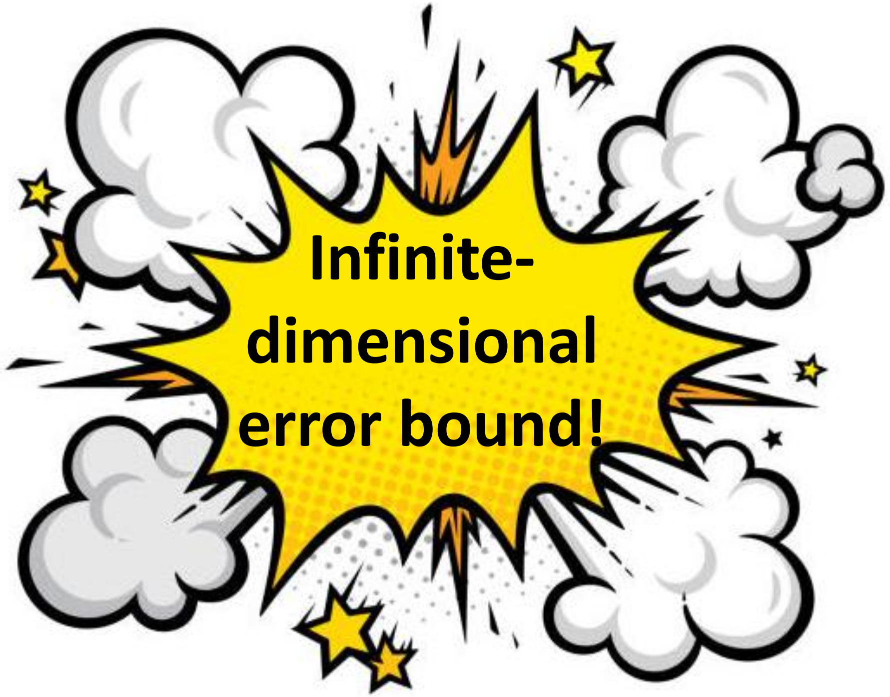

Residuals: $g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j$, $\|\mathcal{K}g - \lambda g\|^2 = \lim_{M\to\infty} \mathbf{g}^* [K_2 - \lambda K_1{}^* - \bar{\lambda} K_1 + |\lambda|^2 G]\mathbf{g}$

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ResDMD does converge!

- Duffing oscillator: $\dot{x} = y, \dot{y} = -\alpha y + x(1 - x^2)$, sampled $\Delta t = 0.3$.
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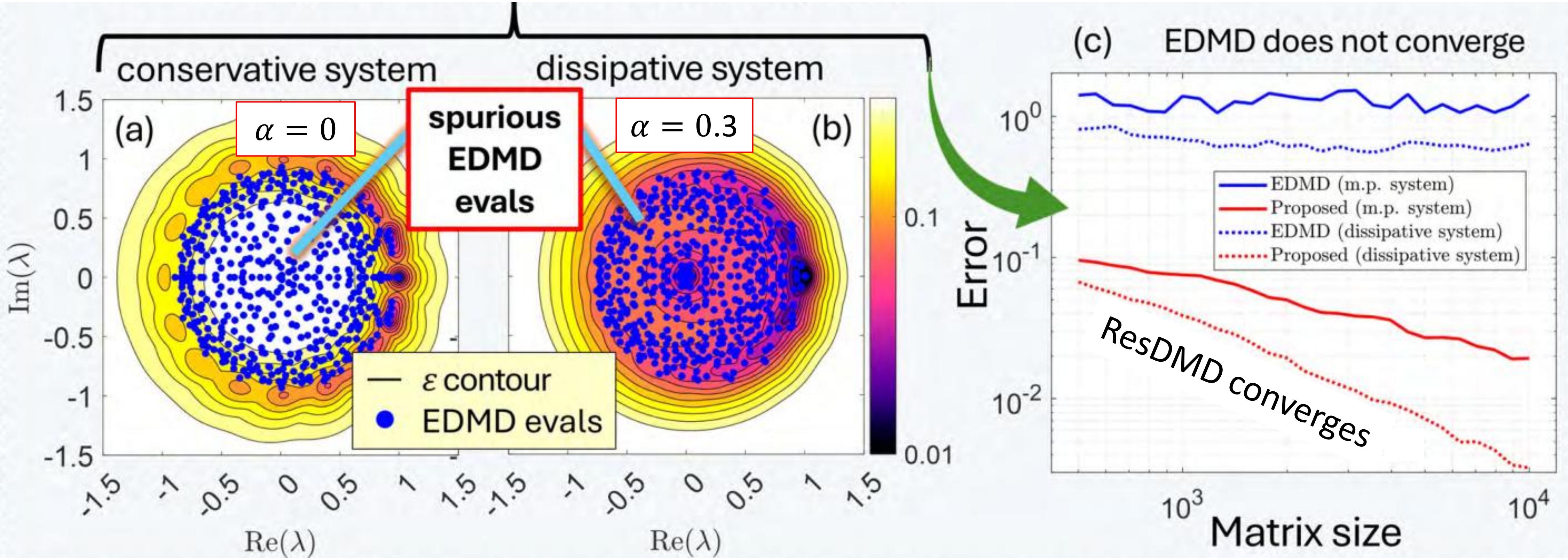
Compute $\mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K})$, local adaptive control on $\varepsilon \downarrow 0$



Can maths help guide the way?

Consider space of observables with finite energy: $L^2(\mathcal{X}, \omega)$

Theorem: There **exists** algorithms $\Gamma_{N,M}$ using snapshots such that

$$\lim_{N\to\infty}\lim_{M\to\infty}\Gamma_{N,M}(F) = \mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}_F)$$

for all systems.

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

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

- C., Mezić, Stepanenko, "Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning," **preprint**, 2025.

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

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for all systems.

Answer: *No! Even for smooth "nice" systems on a disc with unlimited data and accuracy, cannot converge in one limit by **any** algorithm with probability >1/2.*

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Peter Lax:

"The trick of the successful mathematician is to turn the question being asked into one he knows how to answer."

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"Mathematicians are like Frenchmen: whatever you say to them they translate into their own language and forthwith it is something entirely different."

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Let's perform this trick by changing the space…

Reproducing kernel Hilbert space (RKHS)

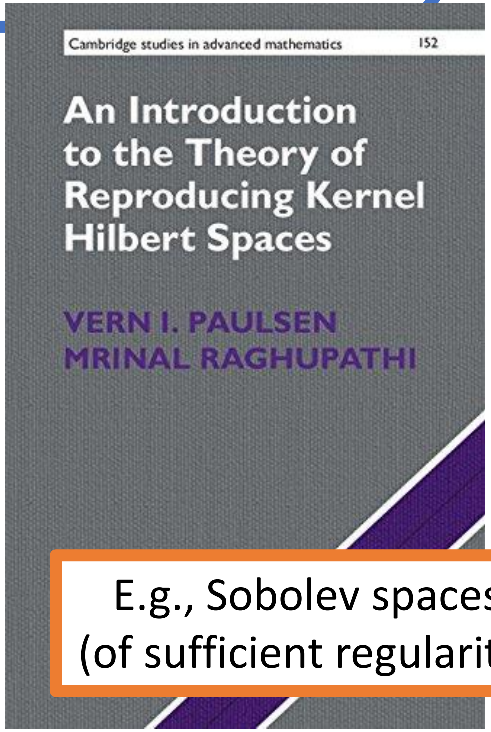
Hilbert space of functions on $\mathcal{X}$ s.t. $g \mapsto g(x)$ bounded $\forall x \in \mathcal{X}$.

Generated by a kernel $\mathfrak{K}: \mathcal{X} \times \mathcal{X} \to \mathbb{C}$

$$g(x) = \langle g, \mathfrak{K}_x \rangle, \qquad \mathfrak{K}(x,y) = \langle \mathfrak{K}_x, \mathfrak{K}_y \rangle = \mathfrak{K}_x(y)$$

Advantages over $L^2(\mathcal{X}, \omega)$:

- Forecasts: space bounds ⇒ pointwise bounds.
- High-dimensional systems practical through kernel trick.
- Fast methods for evaluating $\mathfrak{K}$.
- Different $\mathfrak{K}$ ⇒ different $\mathcal{K}$! Can be tailored to application. (This is where the community is currently heading.)
- Leads to fundamental "possibility" gains…



E.g., Sobolev spaces
(of sufficient regularity)

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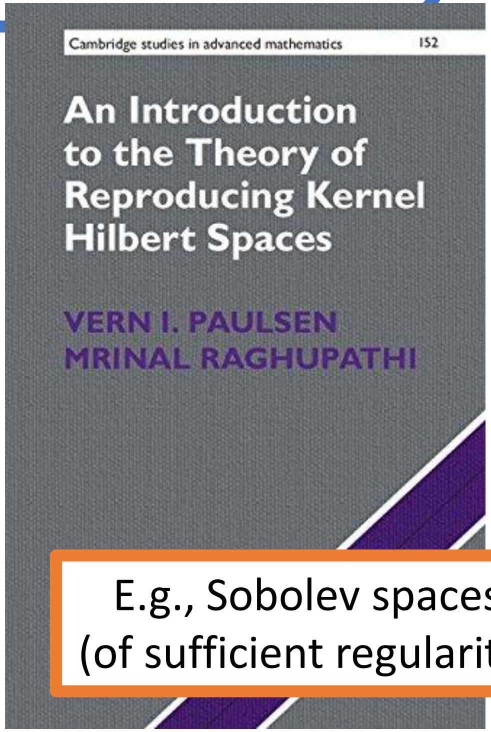


E.g., Sobolev spaces (of sufficient regularity)

SpecRKHS: Avoiding large data limit $M \to \infty$

Look at "Left eigenpairs" through $\mathcal{K}^*$: $\mathcal{K}^*\mathfrak{K}_x = \mathfrak{K}_{F(x)}$

Evolution of functionals.

$g(x) = \langle g, \mathfrak{K}_x \rangle_{\mathcal{H}}$

No quadrature needed:

$$G_{jk} = \langle \mathfrak{K}_{x^{(k)}}, \mathfrak{K}_{x^{(j)}} \rangle = \mathfrak{K}\left(x^{(k)}, x^{(j)}\right)$$

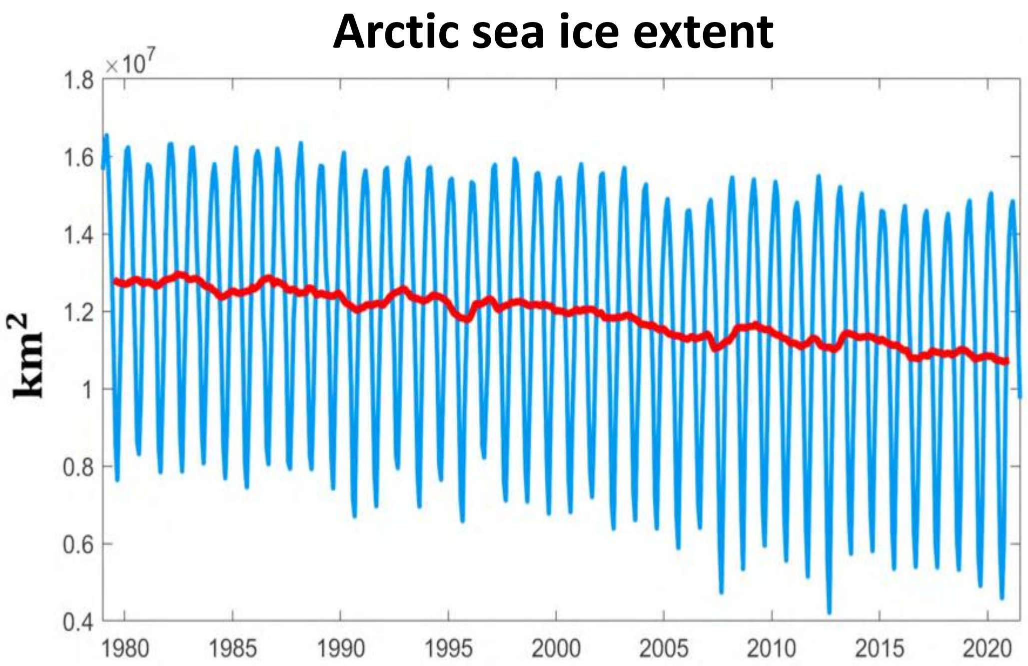
$$A_{jk} = \langle \mathcal{K}^*\mathfrak{K}_{x^{(k)}}, \mathfrak{K}_{x^{(j)}} \rangle = \left\langle \mathfrak{K}_{y^{(k)}}, \mathfrak{K}_{x^{(j)}} \right\rangle = \mathfrak{K}\left(y^{(k)}, x^{(j)}\right)$$

$$R_{jk} = \langle \mathcal{K}^*\mathfrak{K}_{x^{(k)}}, \mathcal{K}^*\mathfrak{K}_{x^{(j)}} \rangle = \left\langle \mathfrak{K}_{y^{(k)}}, \mathfrak{K}_{y^{(j)}} \right\rangle = \mathfrak{K}\left(y^{(k)}, y^{(j)}\right)$$

$$g = \sum_{m=1}^{M} \mathbf{g}_m \mathfrak{K}_{x^{(m)}}, \qquad \|\mathcal{K}^* g - \lambda g\|_{\mathcal{H}}^2 = \mathbf{g}^*(R - \lambda A^* - \bar{\lambda} A + G)\mathbf{g}$$

- Boullé, C., Conradie, *"Convergent Methods for Koopman Operators on Reproducing Kernel Hilbert Spaces,"* **preprint**, 2025.

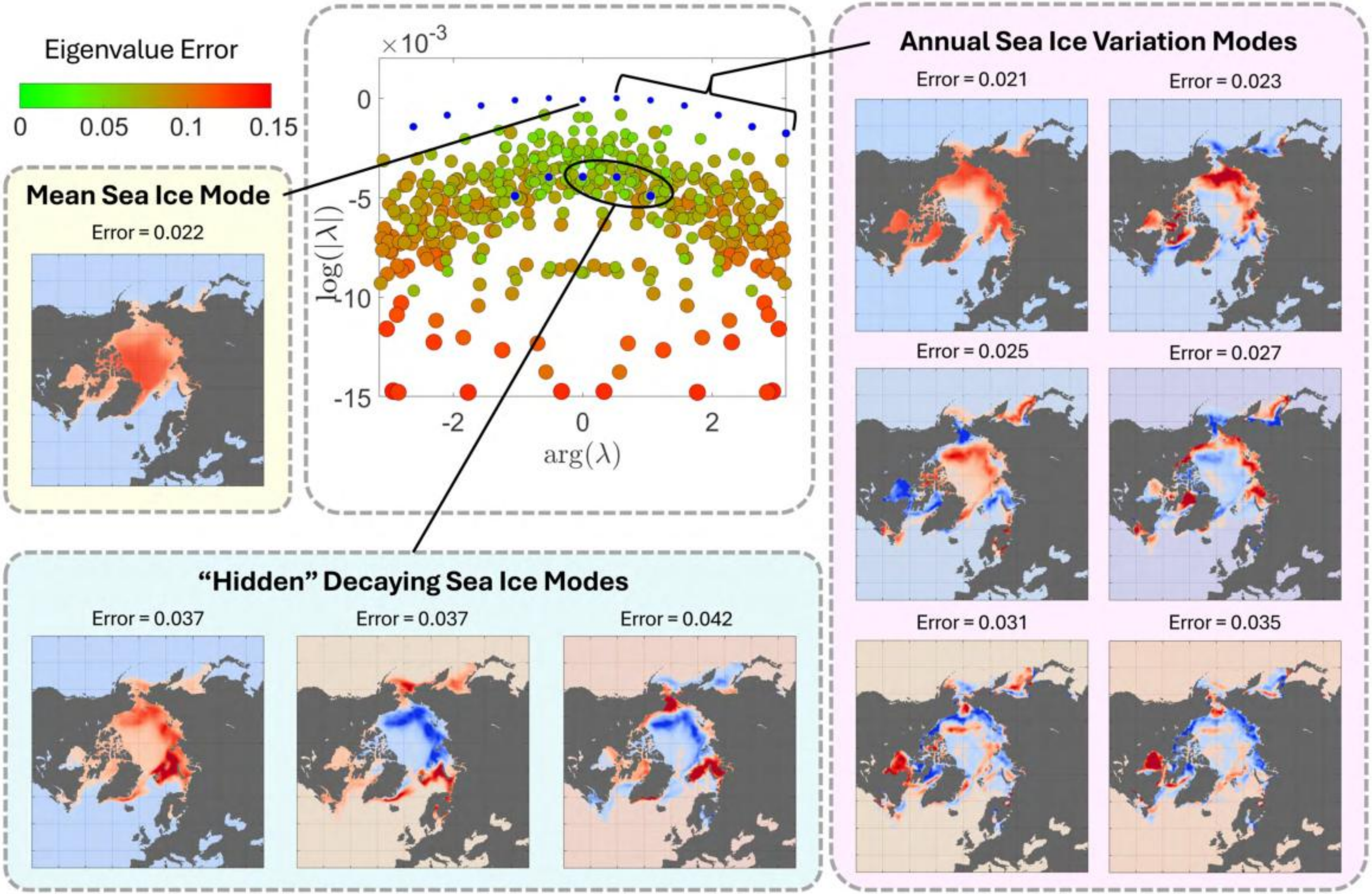
Practical gains: Sea ice forecasting



Monthly average from satellite passive microwave sensors.

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

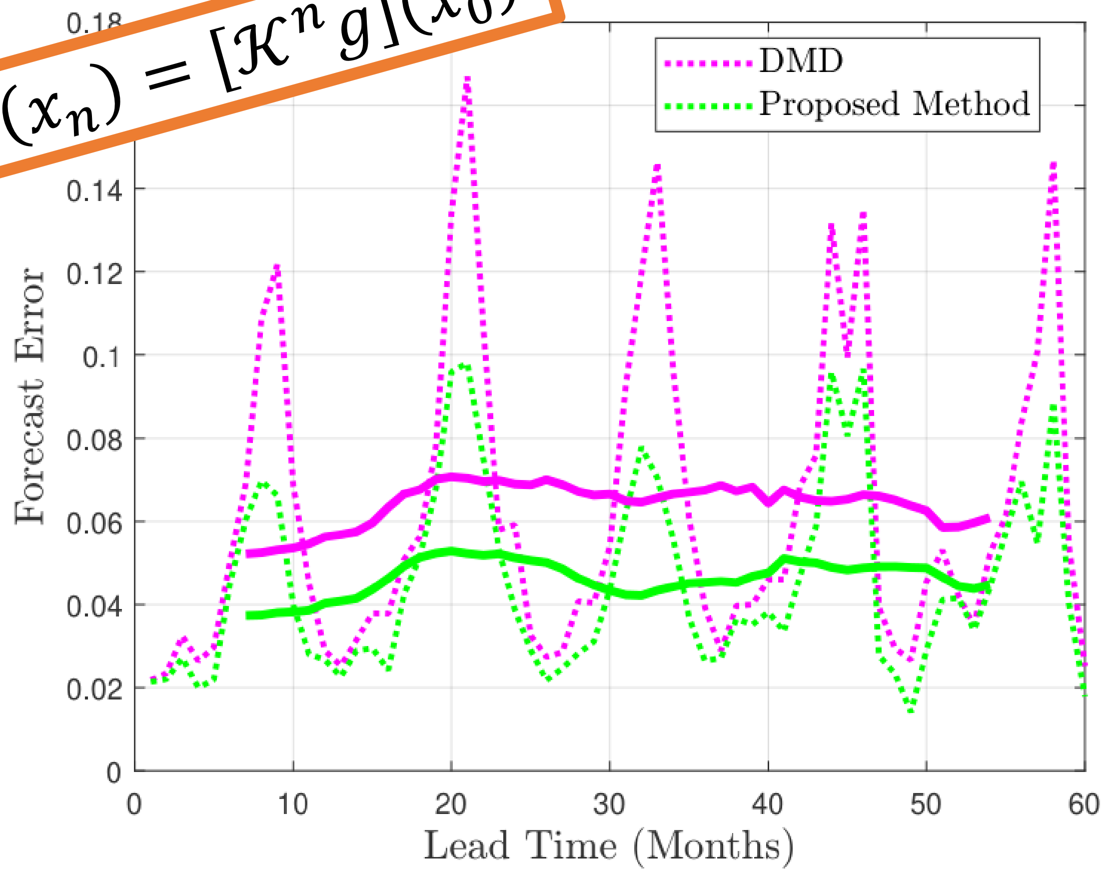
Problem: Very hard to predict more than two months in advance.



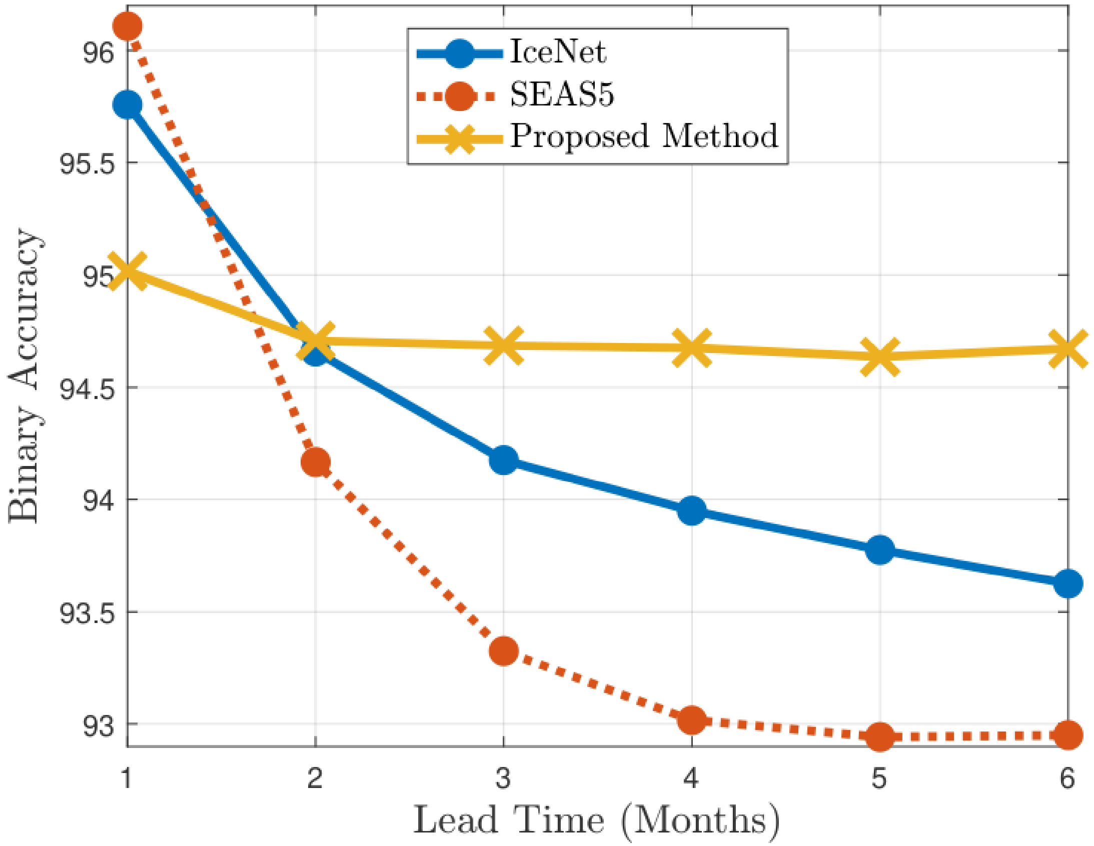
- C., Mezić, Stepanenko, "Adversarial Dynamical Systems Reveal Limits and Rules for Trustworthy Data-Driven Learning," **preprint**, 2025.

Arctic case: Avoiding spurious eigenvalues helps!

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



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.)*

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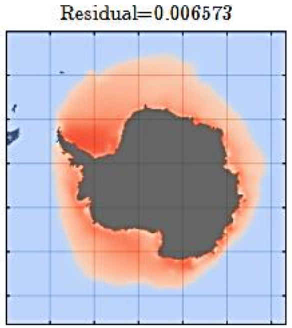
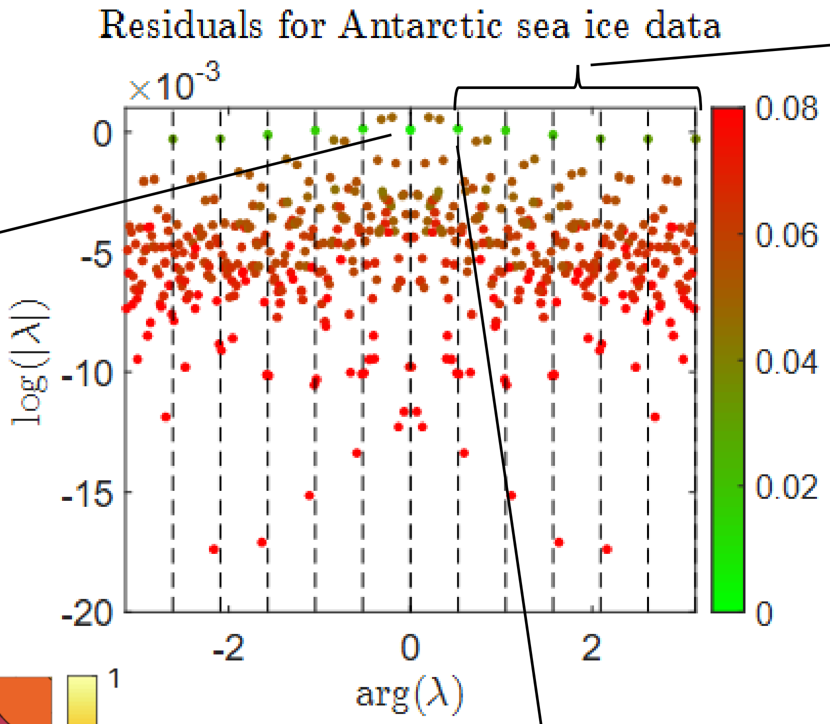
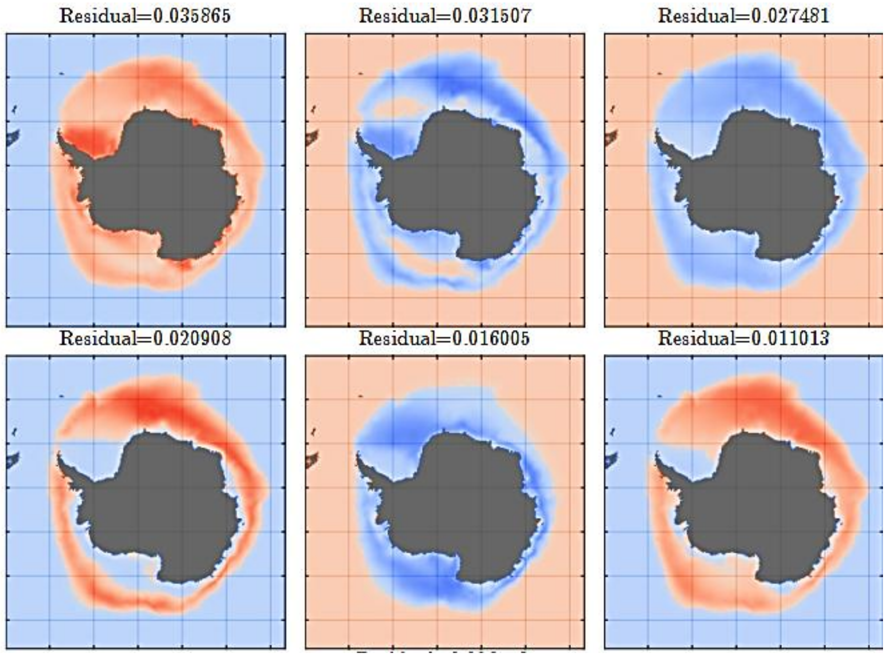
Antarctic case

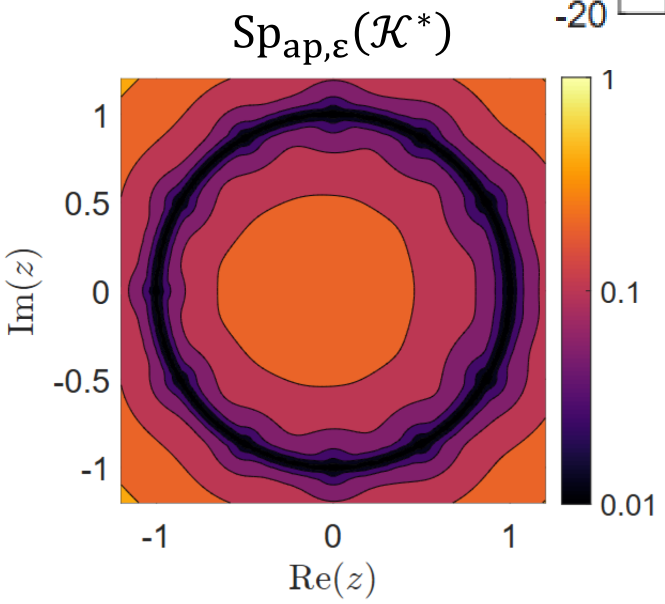
Mean Sea Ice Mode

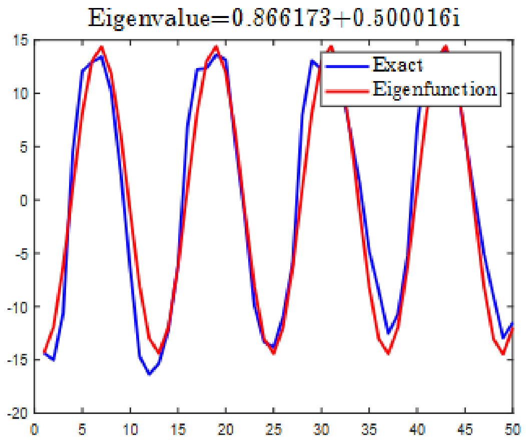




Annual Sea Ice Variation Modes







State space dimension: 82907

$N = M = 550$

RKHS: Sobolev space $H^{41454}(\mathbb{R}^{82907})$

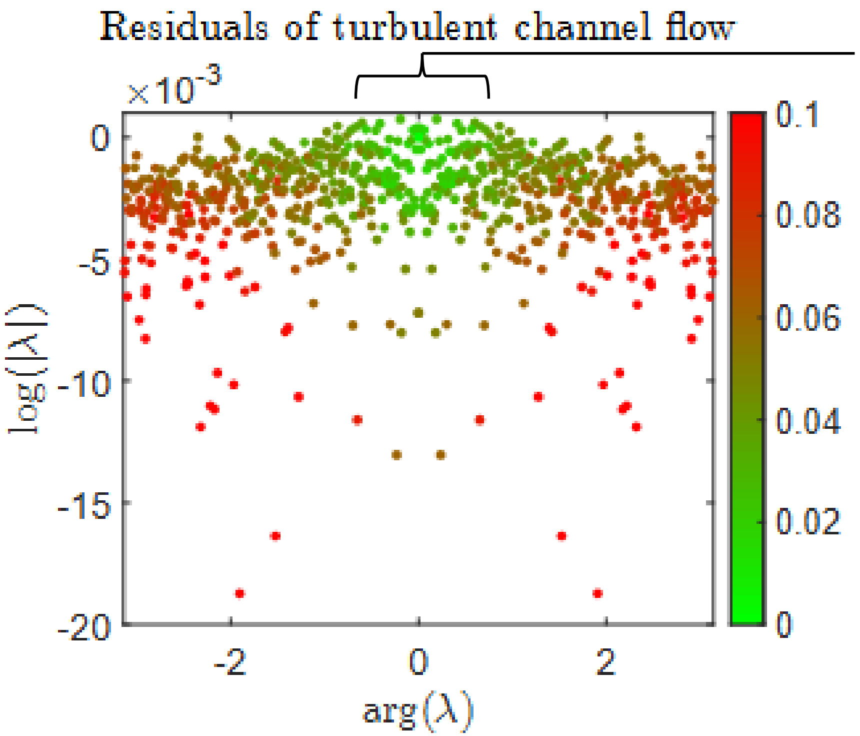
Matérn kernel

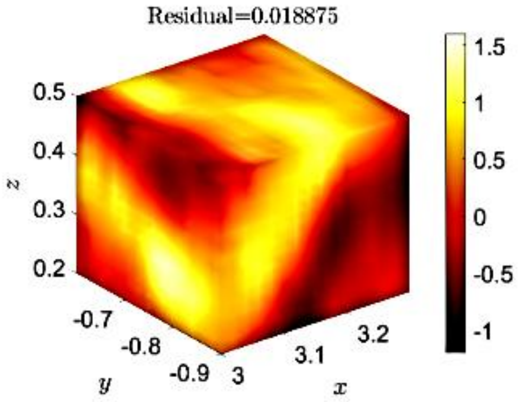
$$\propto (\sigma\|x-y\|_2)^{1/2} K_{-1/2}(\sigma\|x-y\|_2)$$

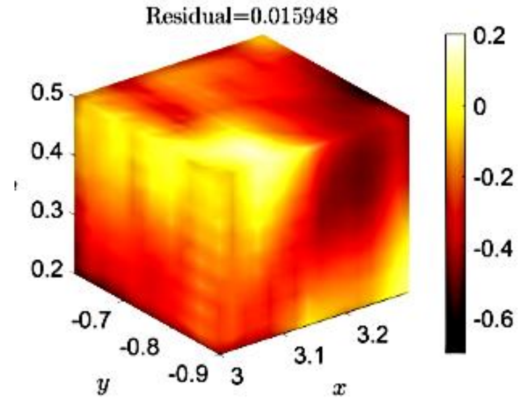
Modified Bessel function of second kind of order -1/2

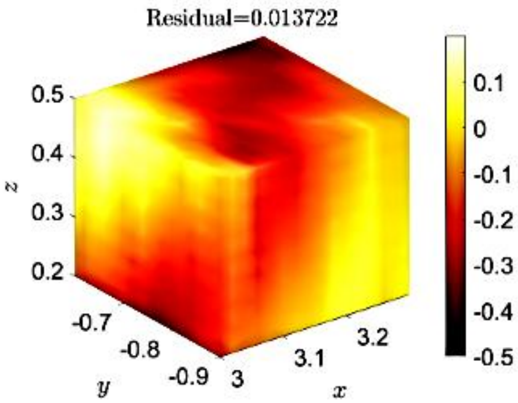
scaling parameter

3D turbulence ($Re \approx 1000$)



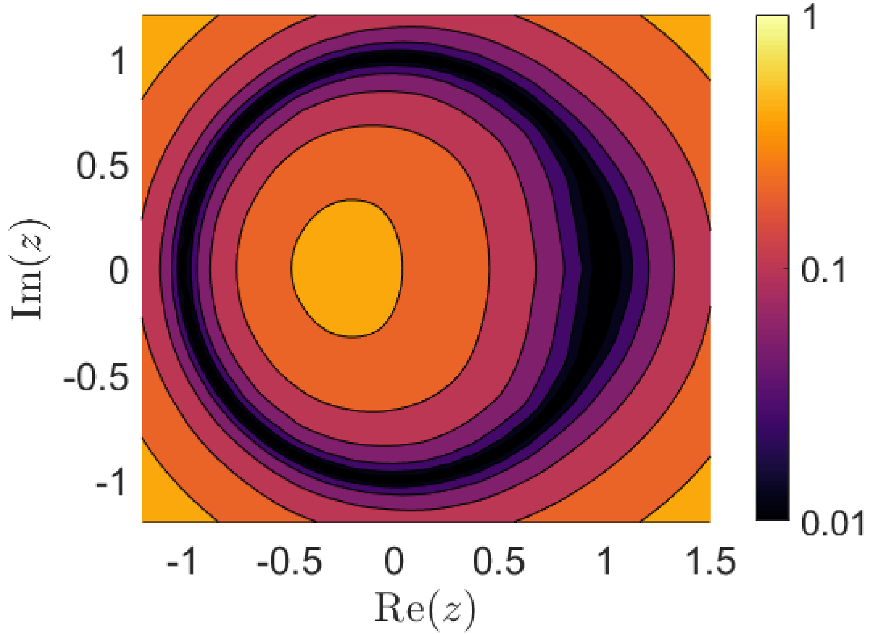






Can handle very non-normal systems!

$\mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}^*)$



State space dimension: 4096

$N = M = 800$

RKHS: Sobolev space $H^{2049}(\mathbb{R}^{4096})$

Matérn kernel

$$\propto (\sigma\|x-y\|_2)K_{-1}(\sigma\|x-y\|_2)$$

Classifications: *Solvability Complexity Index (SCI)*

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

- Δ_1: One limit, error control. Know how far answer is from true answer.
- Δ_{m+1}: SCI $\leq m$.
- Σ_m: SCI $\leq m$, final limit from below.
- Π_m: SCI $\leq m$, final limit from above.

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

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			
		KMD	*Spectrum*	*Spectral Measure (if m.p.)*	*Spectral Type (if m.p.)*
Extended DMD [47]	general L^2 spaces	$\mathrm{SCI} \leq 2^*$	N/C	N/C	n/a
Residual DMD [44]	general L^2 spaces	$\mathrm{SCI} \leq 2^*$	$\mathrm{SCI} \leq 3^*$	$\mathrm{SCI} \leq 2^*$	varies, see [84] e.g., a.c. density: $\mathrm{SCI} \leq 2^*$
Measure-preserving EDMD [45]	m.p. systems	$\mathrm{SCI} \leq 1$	N/C	$\mathrm{SCI} \leq 2^*$ (general) $\mathrm{SCI} \leq 1$ (delay-embedding)	n/a
Hankel DMD [85]	m.p. ergodic systems	$\mathrm{SCI} \leq 2^*$	N/C	N/C	n/a
Periodic approximations [86]	m.p. + ω a.c.	$\mathrm{SCI} \leq 2$	N/C	$\mathrm{SCI} \leq 2$ (see [87])	a.c. density: $\mathrm{SCI} \leq 3$
Christoffel–Darboux kernel [40]	m.p. ergodic systems	$\mathrm{SCI} \leq 3$	n/a	$\mathrm{SCI} \leq 2$	e.g., a.c. density: $\mathrm{SCI} \leq 2$
Generator EDMD [88]	cts.-time, samples ∇F (otherwise additional limit)	$\mathrm{SCI} \leq 2$	N/C	$\mathrm{SCI} \leq 2$ (see [89])	n/a
Compactification [42]	cts.-time, m.p. ergodic systems	$\mathrm{SCI} \leq 4$	N/C	$\mathrm{SCI} \leq 4$	n/a
Resolvent compactification [43]	cts.-time, m.p. ergodic systems	$\mathrm{SCI} \leq 5$	N/C	$\mathrm{SCI} \leq 5$	n/a
Diffusion maps [90] (see also [10])	cts.-time, m.p. ergodic systems	$\mathrm{SCI} \leq 3$	n/a	n/a	

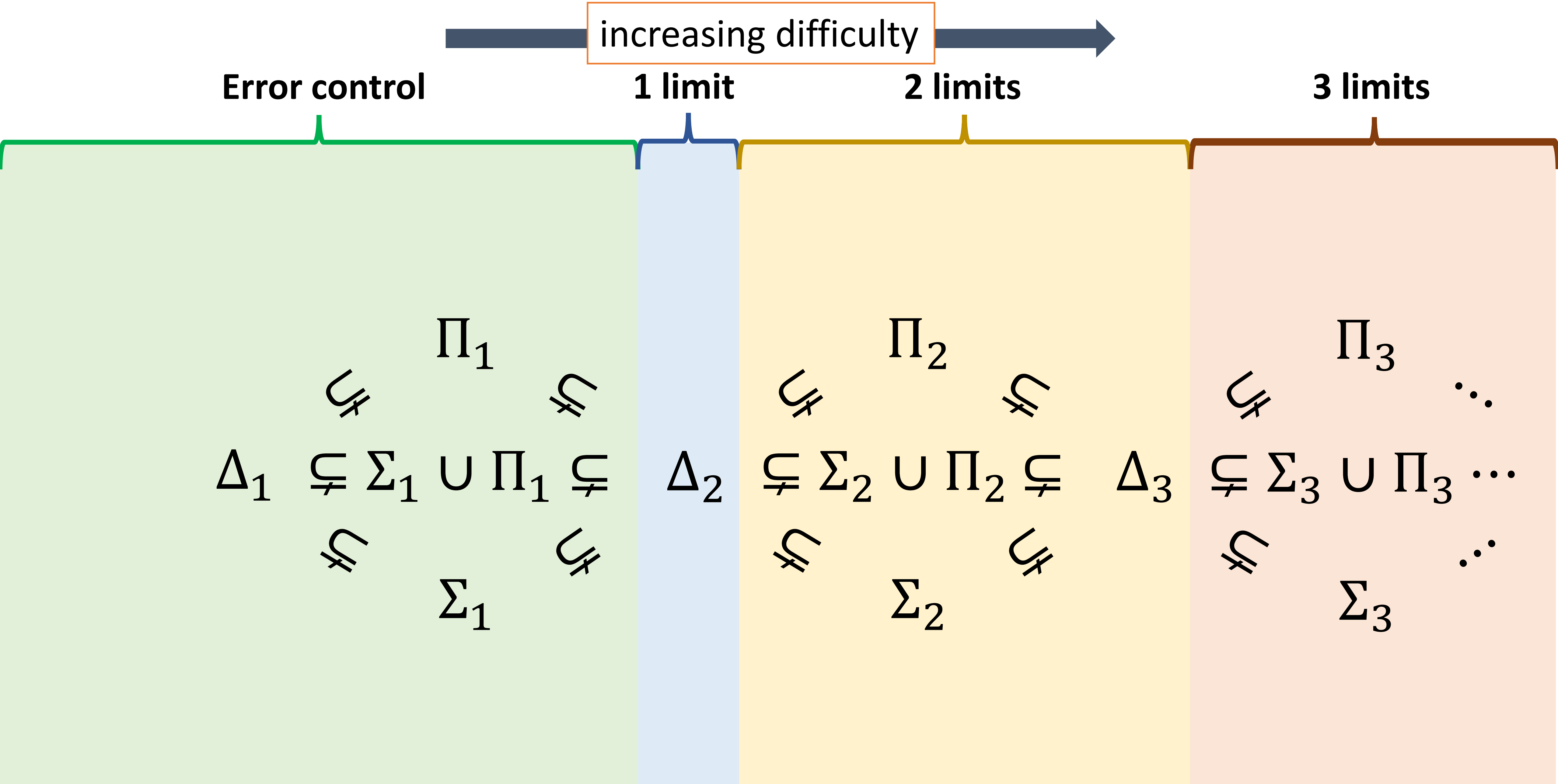
Are these sharp?

Previous techniques prove upper bounds on SCI.

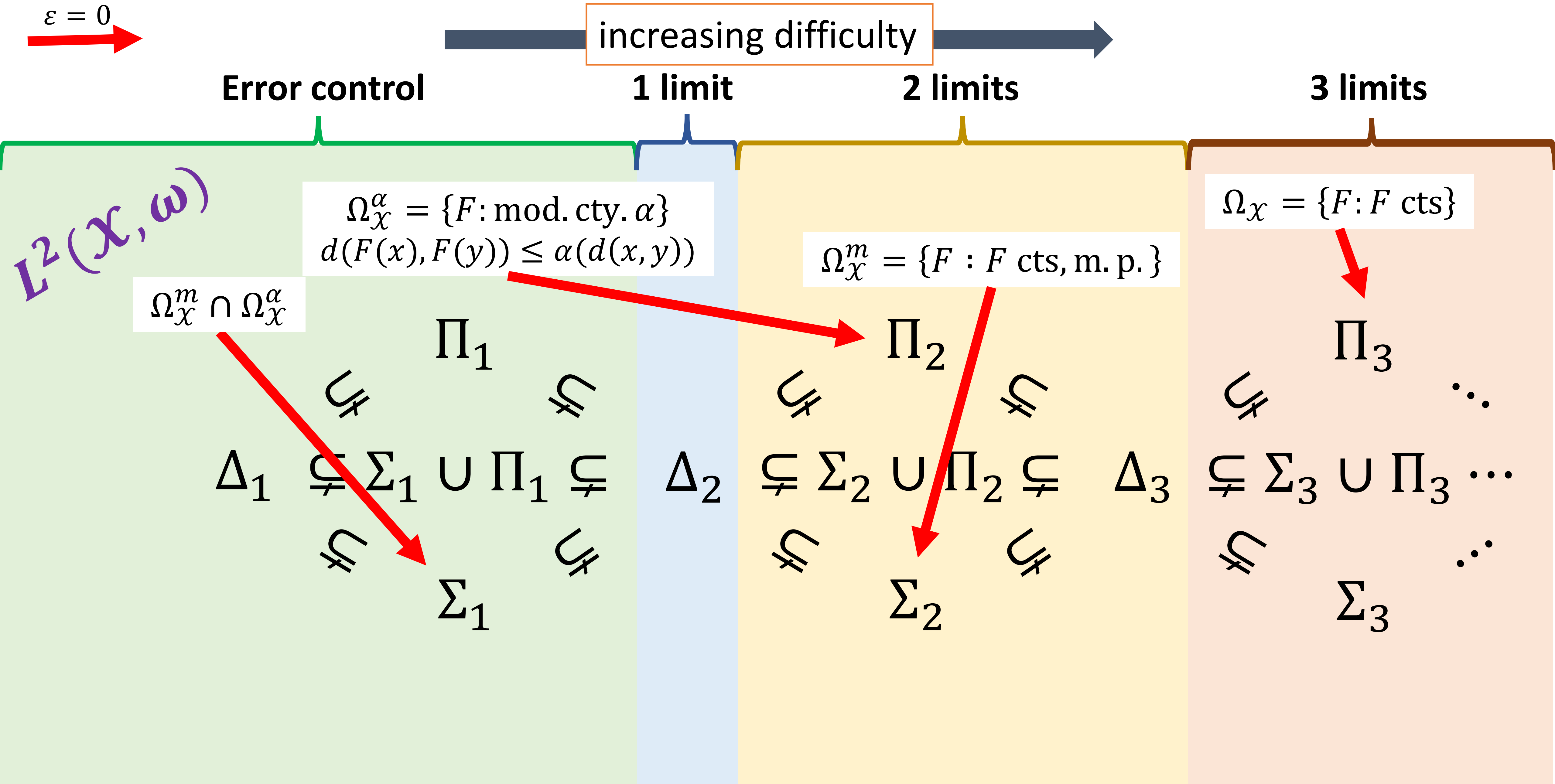
"N/C": method need not converge. "n/a": algorithm not applicable to problem.

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

Optimal algorithms and classifications of systems



Optimal algorithms and classifications of systems



Optimal algorithms and classifications of systems

$\varepsilon = 0$

increasing difficulty

Error control | **1 limit** | **2 limits** | **3 limits**

$L^2(\mathcal{X},\omega)$

$\Omega_{\mathcal{X}}^{\alpha} = \{F\colon \text{mod. cty. } \alpha\}$
$d(F(x),F(y)) \leq \alpha(d(x,y))$

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

$\Omega_{\mathcal{X}} = \{F\colon F \text{ cts}\}$

$\Omega_{\mathcal{X}}^{m} \cap \Omega_{\mathcal{X}}^{\alpha}$

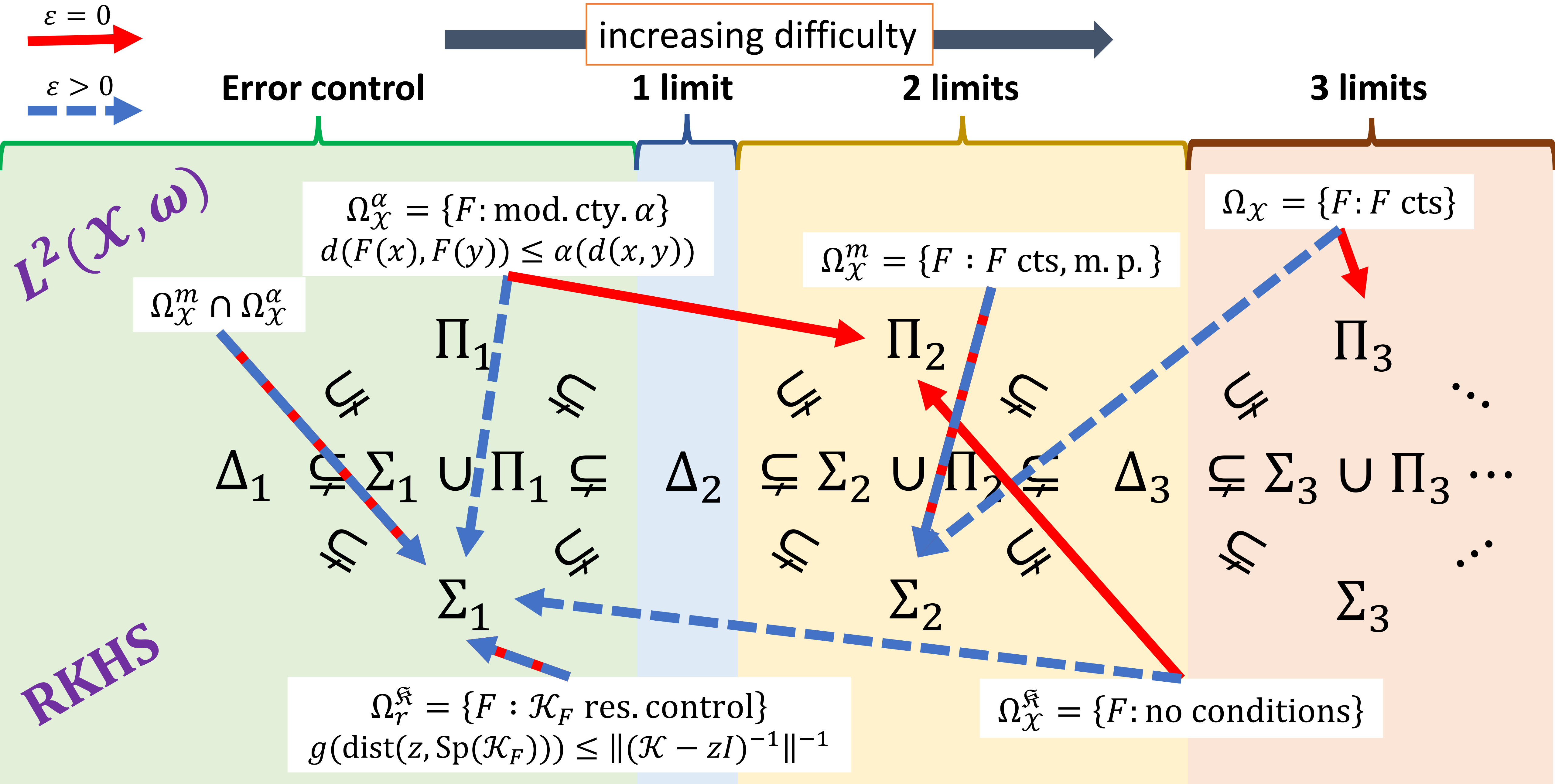
$$\begin{array}{ccccccccccc} & \Pi_1 & & & & \Pi_2 & & & & \Pi_3 & \\ \subsetneq & & \subsetneq & & \subsetneq & & \subsetneq & & \subsetneq & & \cdots \\ \Delta_1 \subsetneq & \Sigma_1 \cup \Pi_1 & \subsetneq & \Delta_2 & \subsetneq & \Sigma_2 \cup \Pi_2 & \subsetneq & \Delta_3 & \subsetneq & \Sigma_3 \cup \Pi_3 & \cdots \\ \subsetneq & & \subsetneq & & \subsetneq & & \subsetneq & & \subsetneq & & \cdots \\ & \Sigma_1 & & & & \Sigma_2 & & & & \Sigma_3 & \end{array}$$

RKHS

$\Omega_{r}^{\mathfrak{K}} = \{F : \mathcal{K}_F \text{ res. control}\}$
$g(\text{dist}(z, \text{Sp}(\mathcal{K}_F))) \leq \|(\mathcal{K} - zI)^{-1}\|^{-1}$

$\Omega_{\mathcal{X}}^{\mathfrak{K}} = \{F\colon \text{no conditions}\}$

Optimal algorithms and classifications of systems



Conclusion: **MATHS** $\longleftrightarrow$ **METHODS**

1. Data-driven spectral problems for Koopman operators are hugely popular.
   BUT: Standard truncation methods often fail.

2. **General method with convergence for spectral properties**
   (spectra, pseudospectra, spectral measures etc.) of K. operators on RKHS!

$\mathcal{K}^*\mathfrak{K}_x = \mathfrak{K}_{F(x)}$ *E.g., Verification of approximate eigenfunctions leads to practical gains.*

3. ***SCI hierarchy*** classifies computational problems:

   Lower bounds through method of *adversarial dynamics*.

   Upper bounds $\Longrightarrow$ new "inf.-dim." algorithms. *Rigorous, optimal, practical.*

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

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

References

[1] Colbrook, Matthew J., and Alex Townsend. "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems." Communications on Pure and Applied Mathematics 77.1 (2024): 221-283.

[2] Colbrook, Matthew J., Lorna J. Ayton, and Máté Szőke. "Residual dynamic mode decomposition: robust and verified Koopmanism." Journal of Fluid Mechanics 955 (2023): A21.

[3] Colbrook, M. J., Li, Q., Raut, R. V., & Townsend, A. "Beyond expectations: residual dynamic mode decomposition and variance for stochastic dynamical systems." Nonlinear Dynamics 112.3 (2024): 2037-2061.

[4] Colbrook, Matthew J. "The Multiverse of Dynamic Mode Decomposition Algorithms." Handbook of Numerical Analysis, vol. 25, pp. 127-230. Elsevier, 2024..

[5] Colbrook, Matthew J. "The mpEDMD algorithm for data-driven computations of measure-preserving dynamical systems." SIAM Journal on Numerical Analysis 61.3 (2023): 1585-1608.

[6] Colbrook, Matthew J., Catherine Drysdale, and Andrew Horning. "Rigged Dynamic Mode Decomposition: Data-Driven Generalized Eigenfunction Decompositions for Koopman Operators." SIAM Journal on Applied Dynamical Systems 24, no. 2 (2025): 1150-1190.

[7] Boullé, Nicolas, and Matthew J. Colbrook. "Multiplicative Dynamic Mode Decomposition." SIAM Journal on Applied Dynamical Systems 24, no. 2 (2025): 1945-1968.

[8] Boullé, Nicolas and Matthew J. Colbrook, "On the Convergence of Hermitian Dynamic Mode Decomposition" Physica D: Nonlinear Phenomena, 472 (2025).

[9] Colbrook, Matthew J., Andrew Horning, and Tianyiwa Xie. "Computing Generalized Eigenfunctions in Rigged Hilbert Spaces." arXiv preprint arXiv:2410.08343 (2024).

[10] Zagli, Niccolò, et al. "Bridging the Gap between Koopmanism and Response Theory: Using Natural Variability to Predict Forced Response." arXiv preprint arXiv:2410.01622 (2024).

[11] Colbrook, Matthew J. "Another look at Residual Dynamic Mode Decomposition in the regime of fewer Snapshots than Dictionary Size." Physica D: Nonlinear Phenomena 469 (2024).

[12] Colbrook, Matthew. "The foundations of infinite-dimensional spectral computations." Diss. University of Cambridge, 2020.

[13] Ben-Artzi, J., Colbrook, M. J., Hansen, A. C., Nevanlinna, O., & Seidel, M. (2020). "Computing Spectra--On the Solvability Complexity Index Hierarchy and Towers of Algorithms." arXiv preprint arXiv:1508.03280.

[14] Colbrook, Matthew J., Vegard Antun, and Anders C. Hansen. "The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem." Proceedings of the National Academy of Sciences 119.12 (2022): e2107151119.

[15] Colbrook, Matthew, Andrew Horning, and Alex Townsend. "Computing spectral measures of self-adjoint operators." SIAM review 63.3 (2021): 489-524.

[16] Colbrook, Matthew J., Bogdan Roman, and Anders C. Hansen. "How to compute spectra with error control." Physical Review Letters 122.25 (2019): 250201.

[17] Colbrook, Matthew J., and Anders C. Hansen. "The foundations of spectral computations via the solvability complexity index hierarchy." Journal of the European Mathematical Society (2022).

[18] Colbrook, Matthew J. "Computing spectral measures and spectral types." Communications in Mathematical Physics 384 (2021): 433-501.

[19] Colbrook, Matthew J., and Anders C. Hansen. "On the infinite-dimensional QR algorithm." Numerische Mathematik 143 (2019): 17-83.

[20] Colbrook, Matthew J. "On the computation of geometric features of spectra of linear operators on Hilbert spaces." Foundations of Computational Mathematics (2022): 1-82.

[21] Brunton, Steven L., and Matthew J. Colbrook. "Resilient Data-driven Dynamical Systems with Koopman: An Infinite-dimensional Numerical Analysis Perspective."

[22] Colbrook, Matthew J., Igor Mezić, and Alexei Stepanenko. "Limits and Powers of Koopman Learning." arXiv preprint arxiv:2407.06312 (2024).

[23] Herwig, April, Matthew J. Colbrook, Oliver Junge, Péter Koltai, and Julia Slipantschuk. "Avoiding spectral pollution for transfer operators using residuals." arXiv preprint arXiv:2507.16915 (2025).

[24] Boullé, Nicolas, Matthew J. Colbrook, and Gustav Conradie. "Convergent Methods for Koopman Operators on Reproducing Kernel Hilbert Spaces." arXiv preprint arXiv:2506.15782 (2025).