When Do Koopman Methods Work?

Spectra, Prediction, and Practical Limits

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Papers and talks:

http://www.damtp.cam.ac.uk/user/mjc249/home.html

Amazing collaborators and friends!

Nicolas Boullé (Imperial)

Steve Brunton (UW)

Gustav Conradie (Cambridge)

JC Loiseau (Arts et Métiers)

Igor Mezić (UC Santa Barbara)

Alexei Stepanenko (Industry)

Alex Townsend (Cornell)

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What is a Koopman operator?

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

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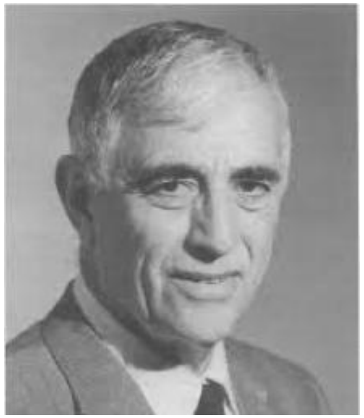
cts $F: \mathcal{X} \to \mathcal{X}$ – *the dynamics:* $x_{n+1} = F(x_n)$

- Functions $g: \mathcal{X} \to \mathbb{C}$ a.k.a "observables", $g \in L^2(\mathcal{X}, \omega)$
- 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?

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

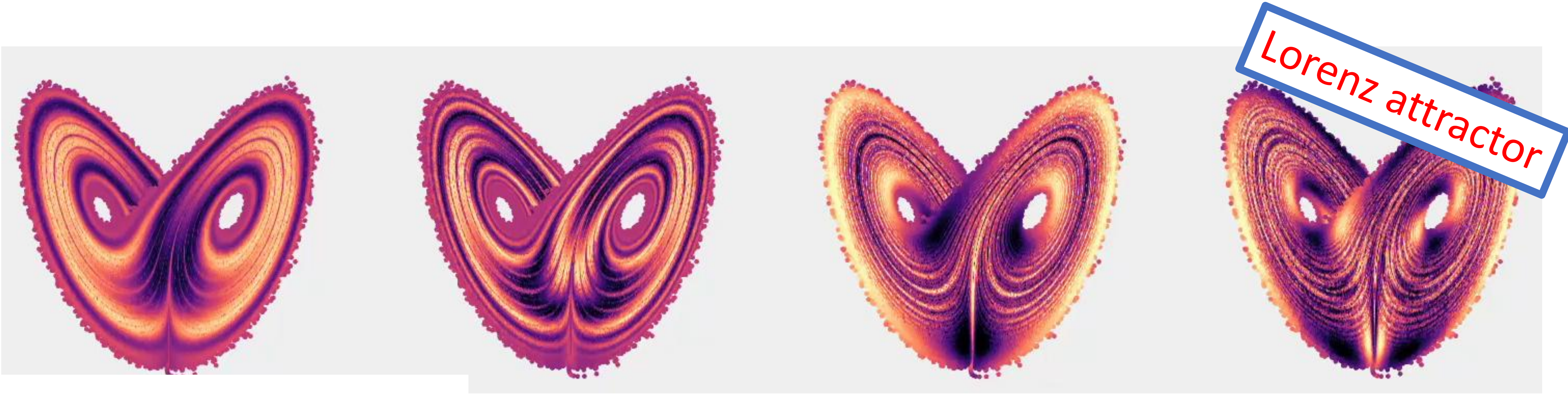
$$g(x_n) = [\mathcal{K}^n g](x_0)$$

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

Why?

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

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!

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

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 observable:

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

coefficients, called "Koopman modes"

- Forecasts:

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

Intuition: A nonlinear separation of variables through a linear operator!

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

$$\begin{pmatrix} \ddots & \ddots & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & 0 & 1 & \\ & & & & 0 & \ddots \\ & & & & & \ddots \end{pmatrix} \longrightarrow \begin{pmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in \mathbb{C}^{N \times N}$$

Two-way infinite

- 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!

Explicit example: Matrix approximation of $\mathcal{K}$ (EDMD)

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

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

quadrature points

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

quadrature weights

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

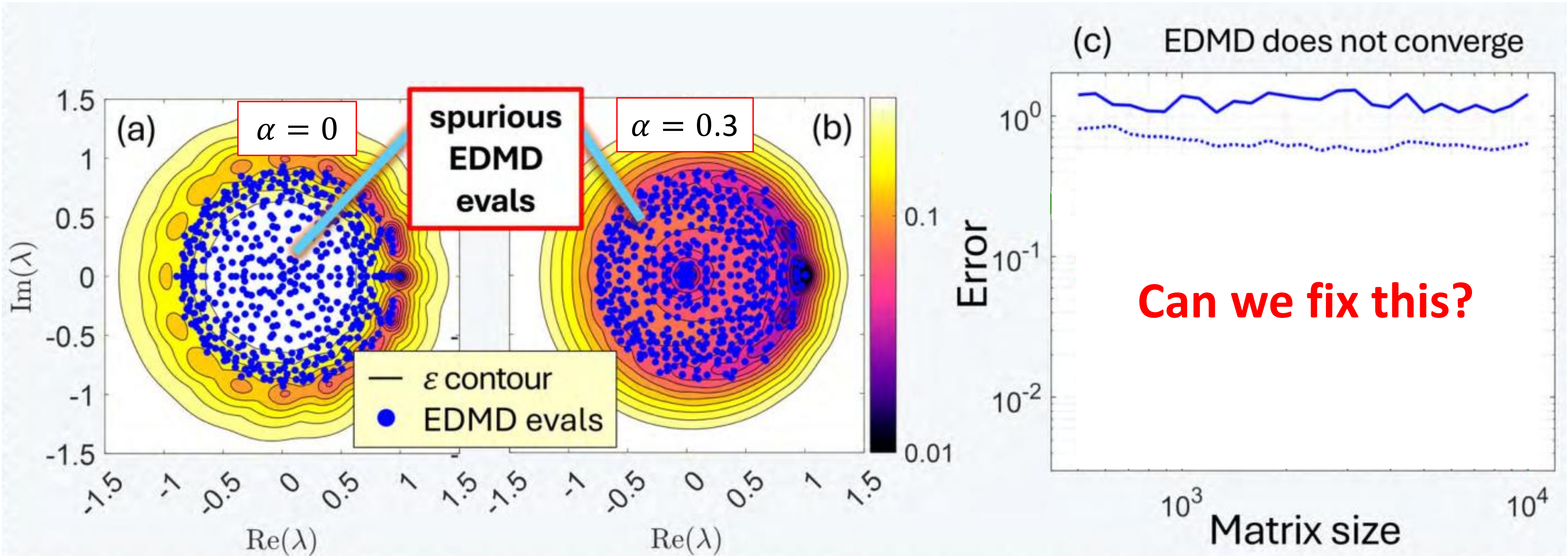
Galerkin Approximation

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

- 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)

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

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

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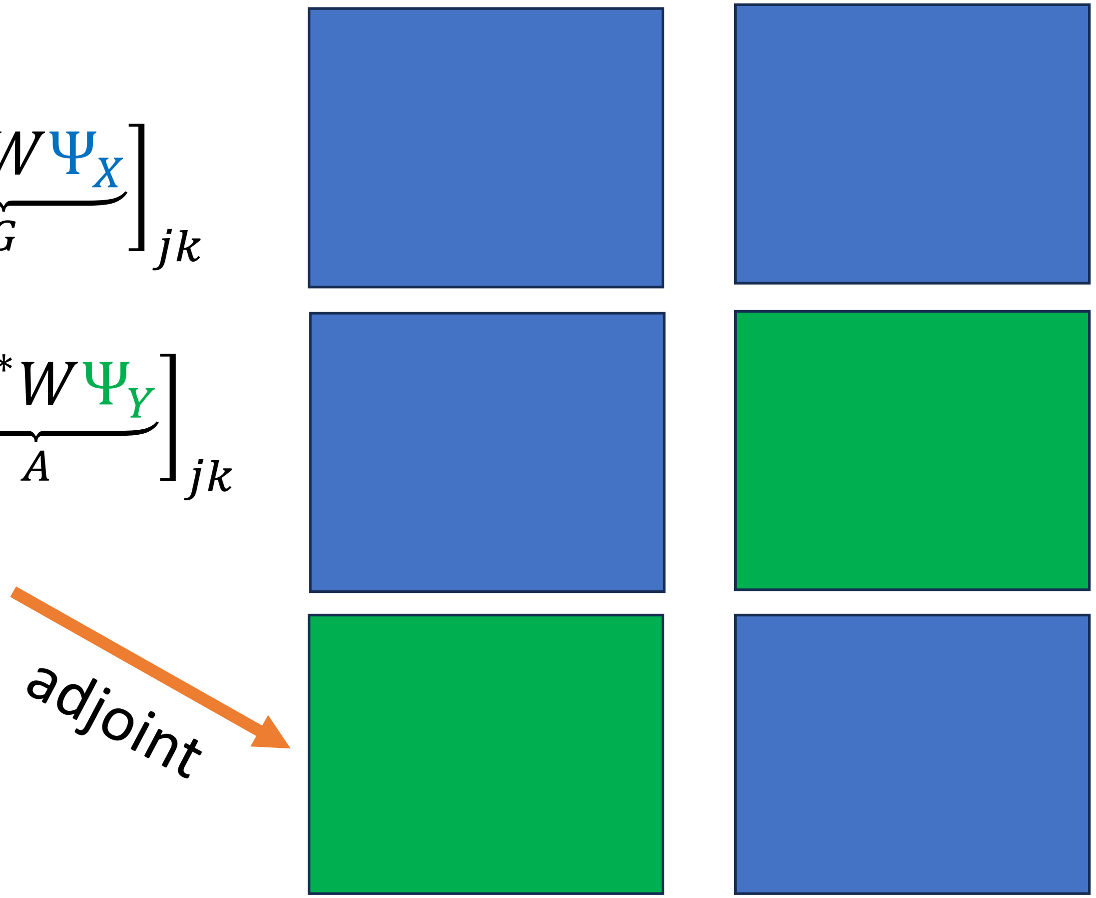

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Residuals: $g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j, \ \|\mathcal{K}g - \lambda g\|^2 = \langle \mathcal{K}g - \lambda g, \mathcal{K}g - \lambda g \rangle$

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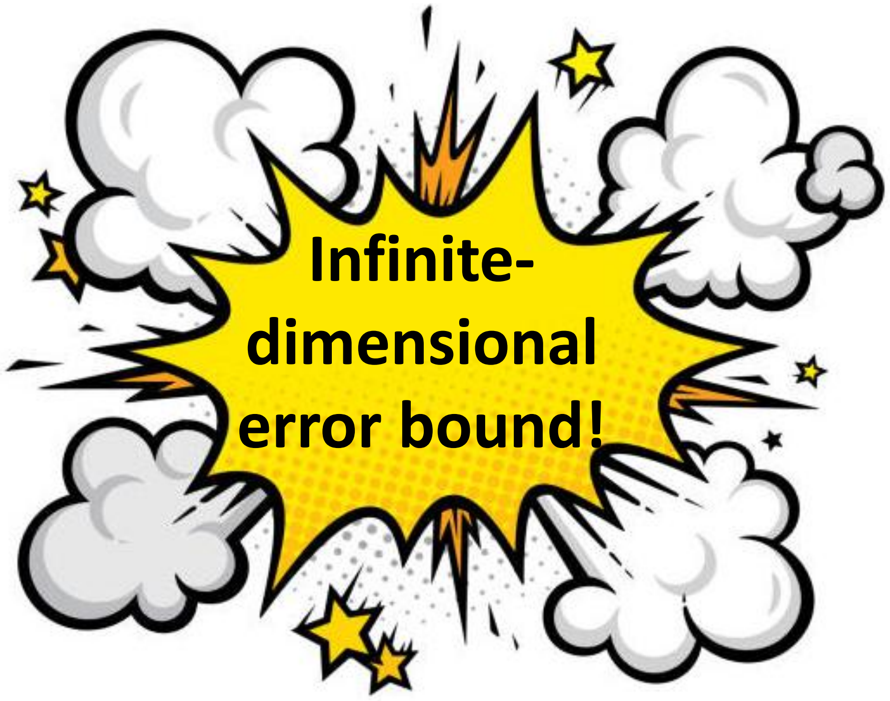

Residuals: $g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j,\ \|\mathcal{K}g - \lambda g\|^2 = \lim_{M\to\infty} \mathbf{g}^*[L - \lambda A^* - \bar{\lambda} A + |\lambda|^2 G]\mathbf{g}$

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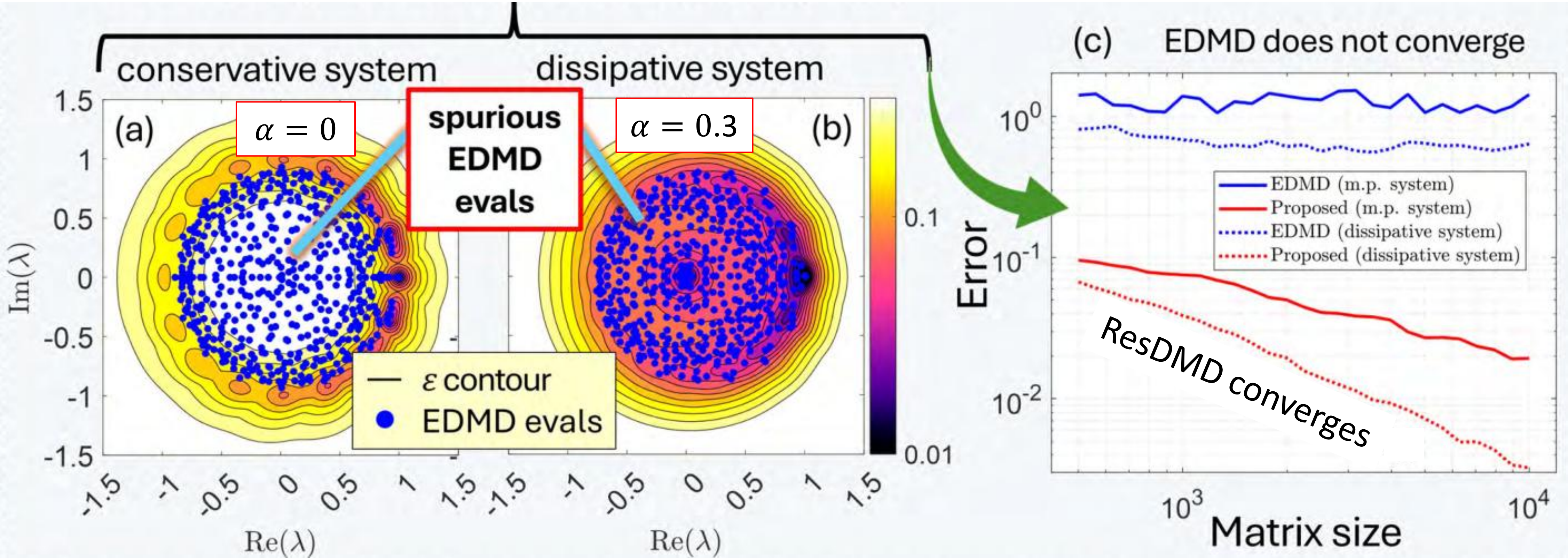
Compute $\mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K})$, local adaptive control on $\varepsilon \downarrow 0$



What can we do?

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)

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

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

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

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

Adversaries: Double limit is necessary!

Implies $\mathcal{K}$ is unitary

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

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

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

NB:

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

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

Proof idea: Constructing an adversary

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

Phase transition lemma: Let $X = \{x_1, \dots, x_N\}, Y = \{y_1, \dots, y_N\}$ be distinct points in annulus $\mathcal{A} = \{x \in \mathbb{D} | 0 < R < \|x\| < r < 1\}$ with $X \cap Y = \emptyset$. There exists a measure-preserving homeomorphism H such that H acts as the identity on $\mathbb{D} \backslash \mathcal{A}$ and $H(y_j) = F_0(H(x_j)), j = 1, \dots, N$.

Conjugacy of <u>data</u> ($x_j \to y_j$) with F_0

Idea: Use lemma to trick any algorithm into oscillating between spectra.

- Brown and Halperin. *"On certain area-preserving maps,"* **Annals of Mathematics**, 1935.

Proof idea: Constructing an adversary

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

Build an adversarial F…

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

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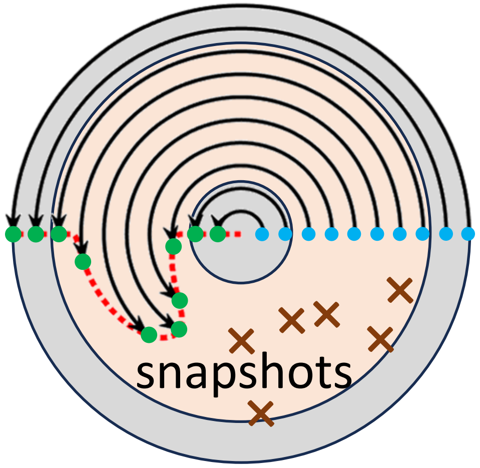

$\widetilde{F_1}(r,\theta) = \big(r, \theta + \pi + \phi(r)\big)$, $\mathrm{supp}(\phi) \subset$ [1/4, 3/4]
$\mathrm{Sp}(\mathcal{K}_{\widetilde{F_1}}) = \mathbb{T}$ (unit circle).

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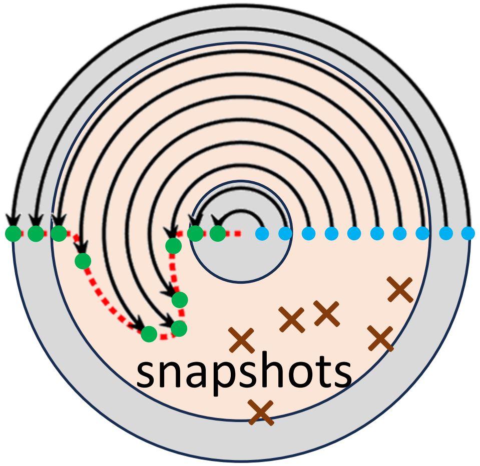

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$\lim_{n\to\infty} \Gamma_n(\widetilde{F_1}) = \mathrm{Sp}(\mathcal{K}_{\widetilde{F_1}}) \Rightarrow \exists n_1$ s.t. $\mathrm{dist}(i, \Gamma_{n_1}(\widetilde{F_1})) \leq 1$.

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

Let X, Y correspond to these snapshots.

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

Proof idea: Constructing an adversary

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

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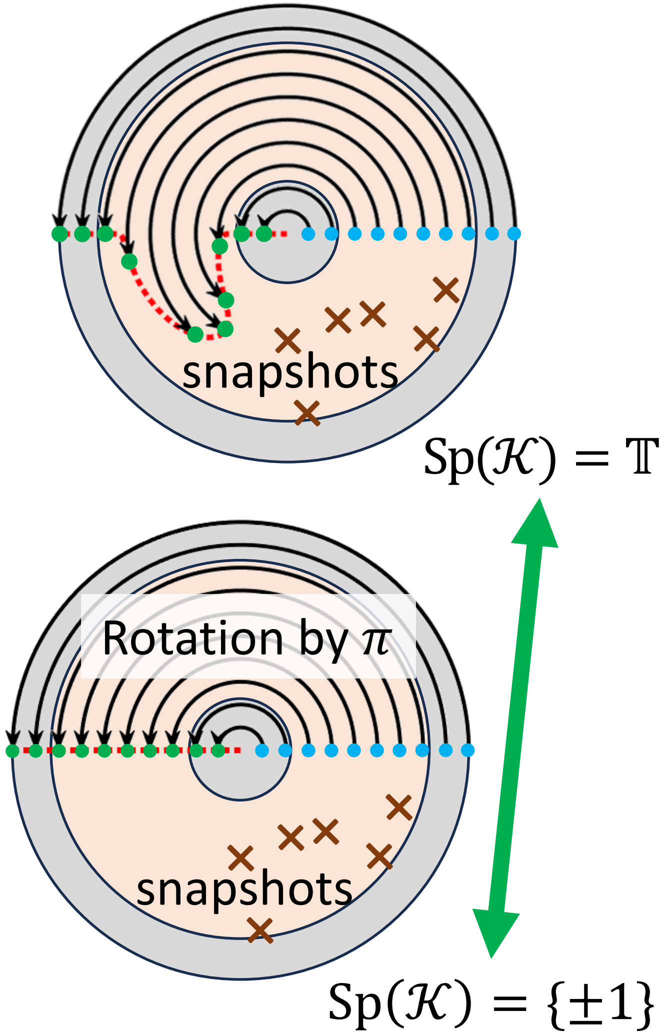


Lemma: $F_1 = H_1^{-1} \circ F_0 \circ H_1$ on annulus $\mathcal{A}_1$.
Consistent data $\Rightarrow \Gamma_{n_1}(F_1) = \Gamma_{n_1}(\widetilde{F_1})$, $\mathrm{dist}(i, \Gamma_{n_1}(F_1)) \leq 1$
BUT $\mathrm{Sp}(\mathcal{K}_{F_1}) = \mathrm{Sp}(\mathcal{K}_{F_0}) = \{\pm 1\}$

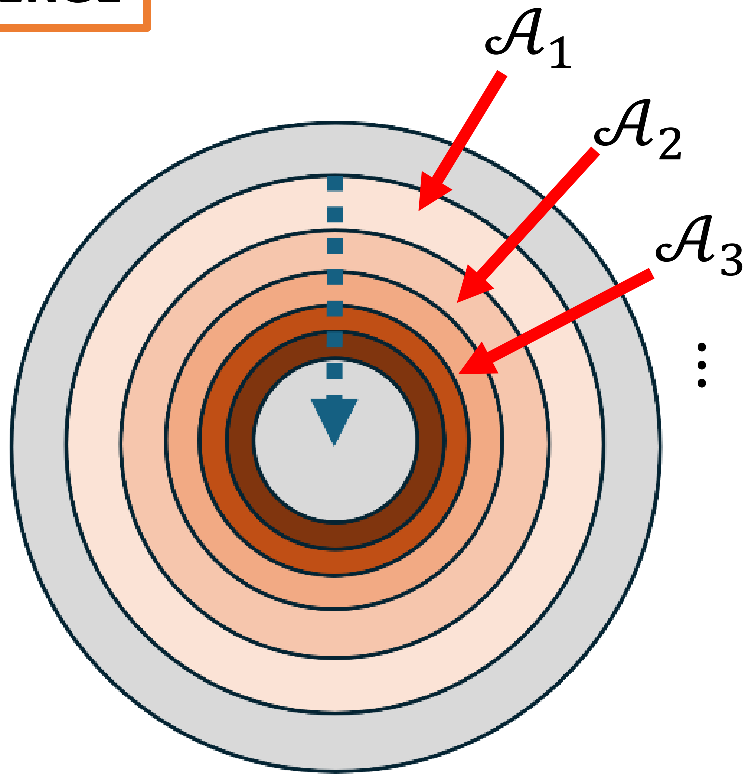
Proof idea: Constructing an adversary

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

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

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

CANNOT CONVERGE



Cascade of disks

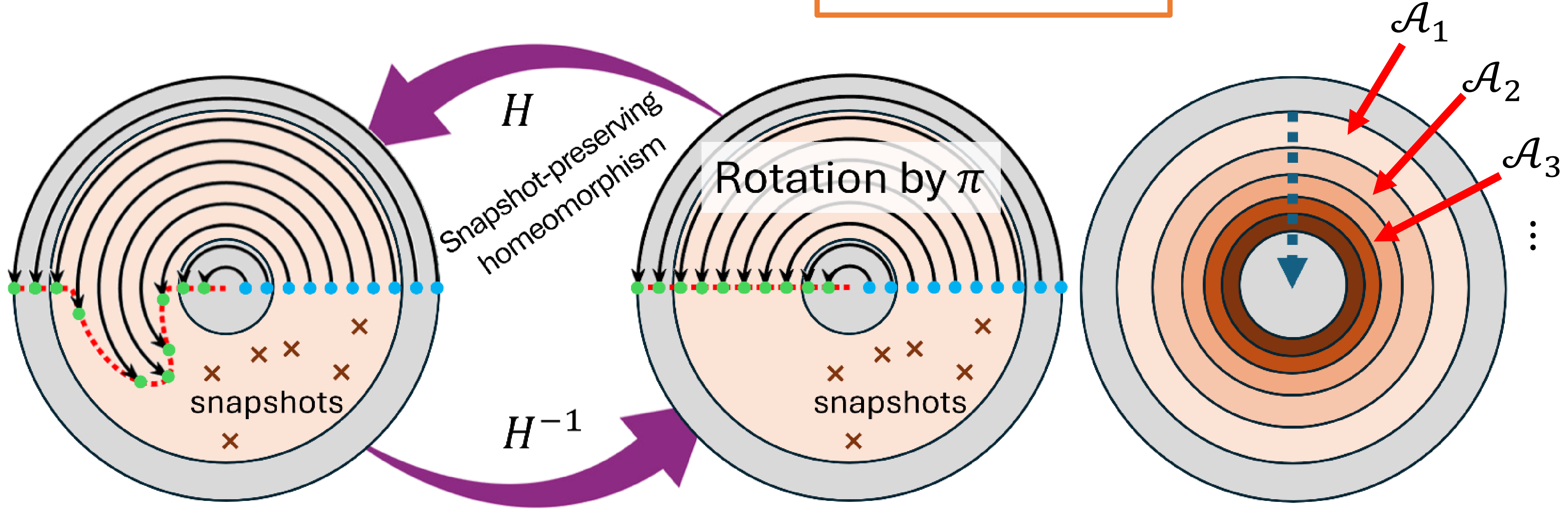
Proof idea: Constructing an adversary

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

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

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

CANNOT CONVERGE



$\mathrm{Sp}(\mathcal{K}) = \{z : |z| = 1\}$ ⟷ $\mathrm{Sp}(\mathcal{K}) = \{\pm 1\}$

Cascade of disks

Classifications: *Solvability Complexity Index (SCI)*

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

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

trust output → E.g., Σ_1: $\sup_{z\in\Gamma_n(F)} \mathrm{dist}(z, \mathrm{Sp}(\mathcal{K}_F)) \leq 2^{-n}$.

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

E.g., Π_1: $\sup_{z\in\mathrm{Sp}(\mathcal{K}_F)} \mathrm{dist}\big(z, \Gamma_n(F)\big) \leq 2^{-n}$. ← **covers spectrum**

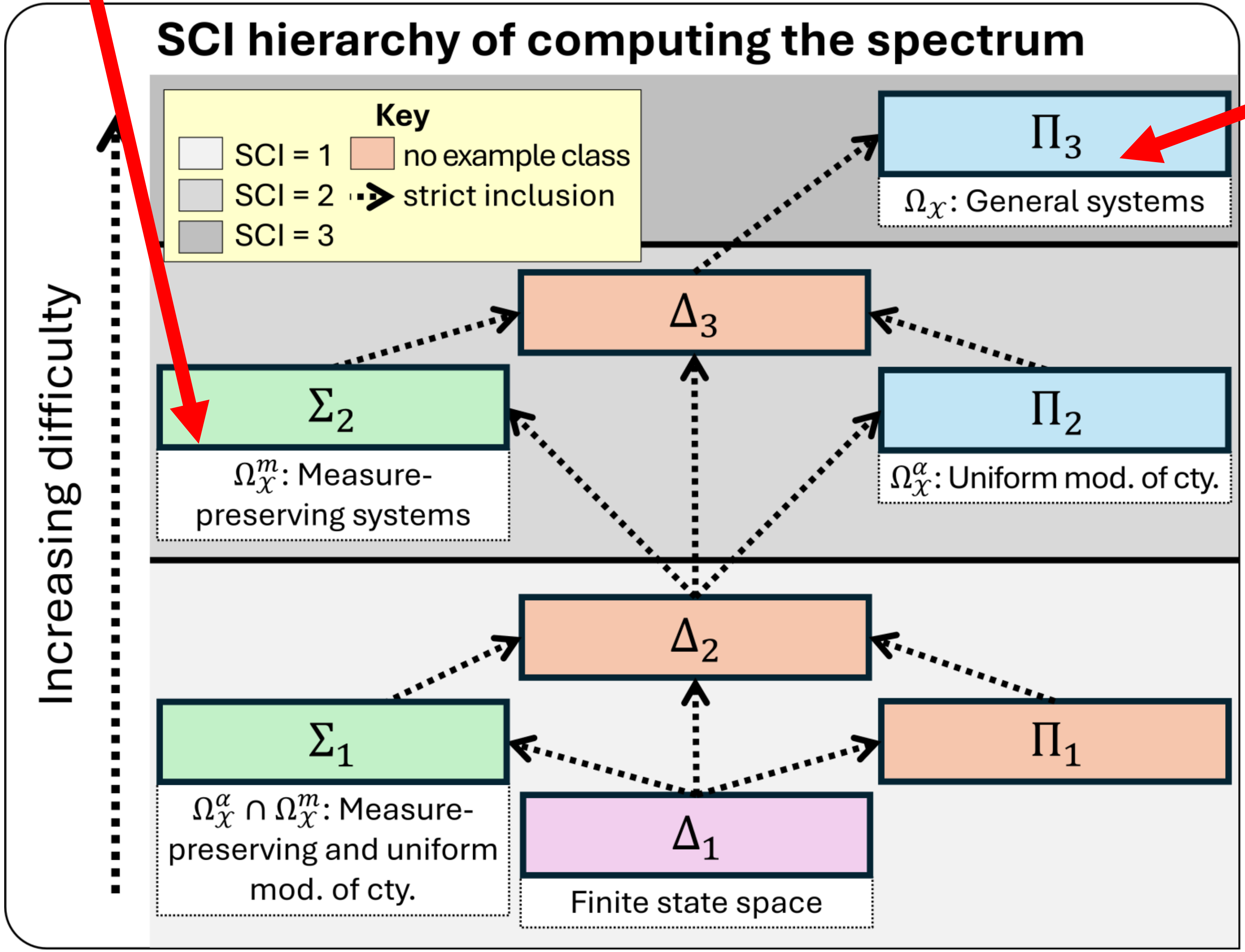
(both examples: **verification**)

- 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.

Classification for Koopman

Lower + upper bounds

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.

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

Johann Wolfgang von Goethe:

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

Let's change the space…

Reproducing kernel Hilbert space (RKHS)

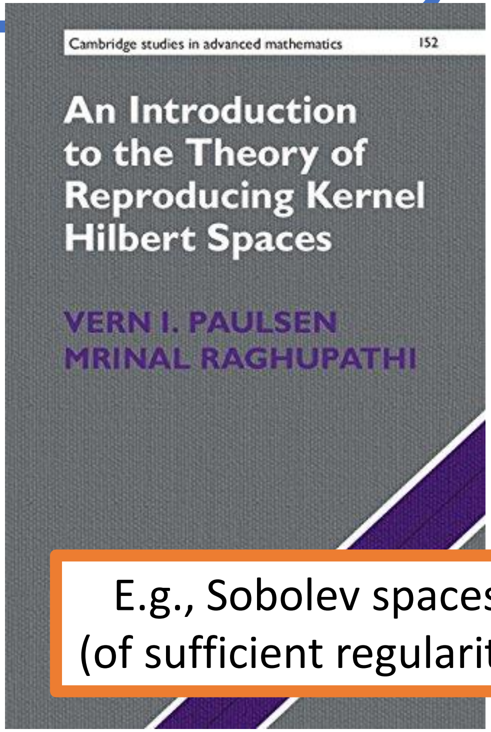
Hilbert space of functions on $\mathcal{X}$ s.t. $g \mapsto g(x)$ bounded $\forall x \in \mathcal{X}$.

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.)
- Couples M and N…



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:

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

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

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

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

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

SpecRKHS: Example algorithm

$$\mathrm{res}^*(\lambda,\mathbf{g})^2=\frac{\|\mathcal{K}^*g-\lambda g\|_{\mathcal{H}}^2}{\|g\|_{\mathcal{H}}^2}=\frac{\mathbf{g}^*\left[L-\lambda A^*-\bar{\lambda}A+|\lambda|^2G\right]\mathbf{g}}{\mathbf{g}^*G\mathbf{g}}$$

1. Compute $G,A,L\in\mathbb{C}^{N\times N}$ $(N=M)$
2. For z_k in grid, compute $\tau_k=\min_{g=\sum_{m=1}^{N}\mathbf{g}_m\mathfrak{K}_{x^{(m)}},}\mathrm{res}^*(z_k,\mathbf{g})$, corresponding g_k (gen. SVD).
3. **Output:** $\{z_k:\tau_k<\varepsilon\},\{g_k:\tau_k<\varepsilon\}$ (ε-pseudoeigenfunctions).

Theorem:
- **Error control:** $\{z_k:\tau_k<\varepsilon\}\subseteq\mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}^*)$
- **Convergence:** Converges locally uniformly to $\mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}^*)$ (as $N\to\infty$)

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

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

Optimal algorithms and classifications of systems

increasing difficulty →

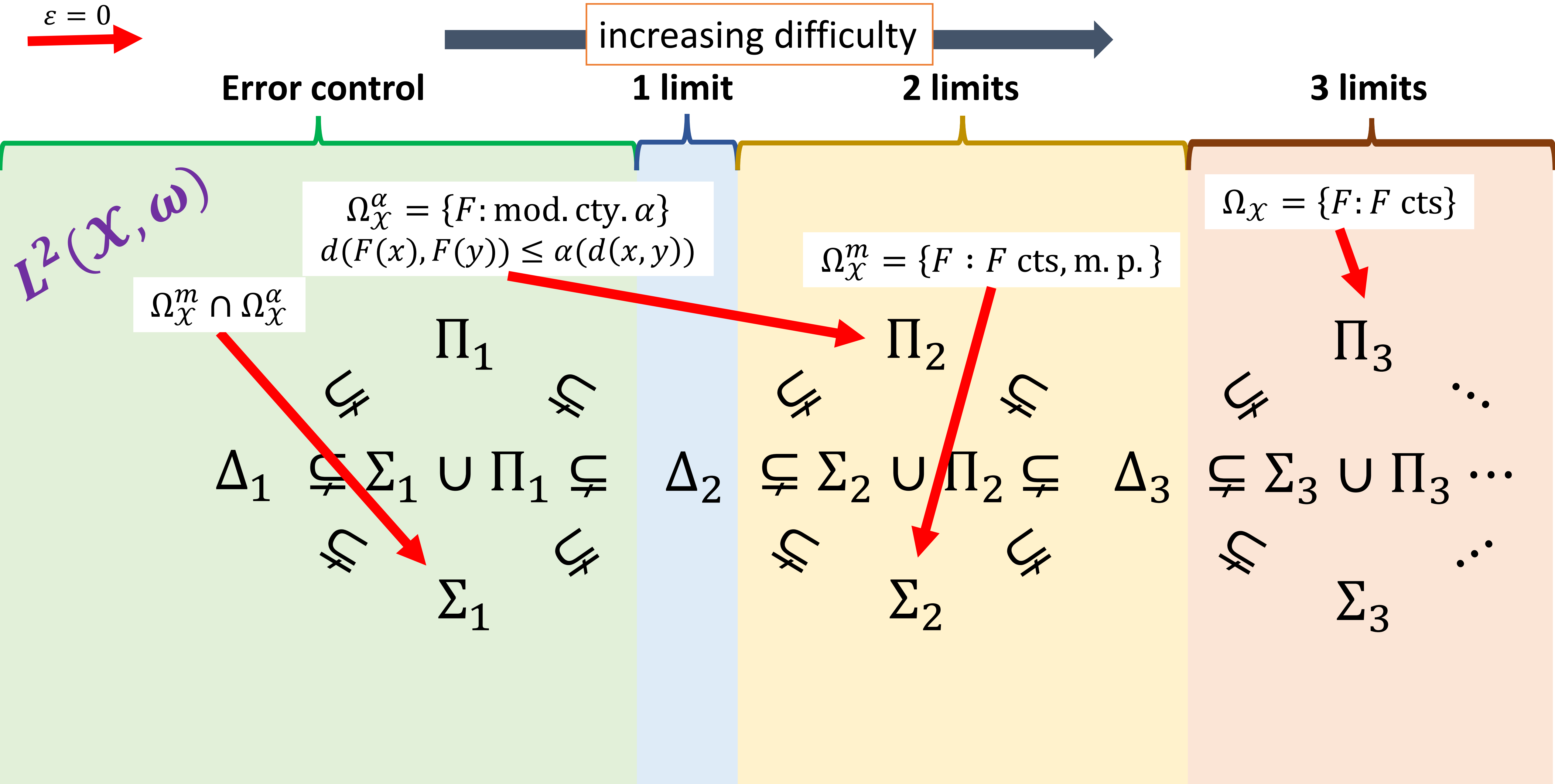
Error control | **1 limit** | **2 limits** | **3 limits**

$$\Pi_1 \qquad \Pi_2 \qquad \Pi_3$$

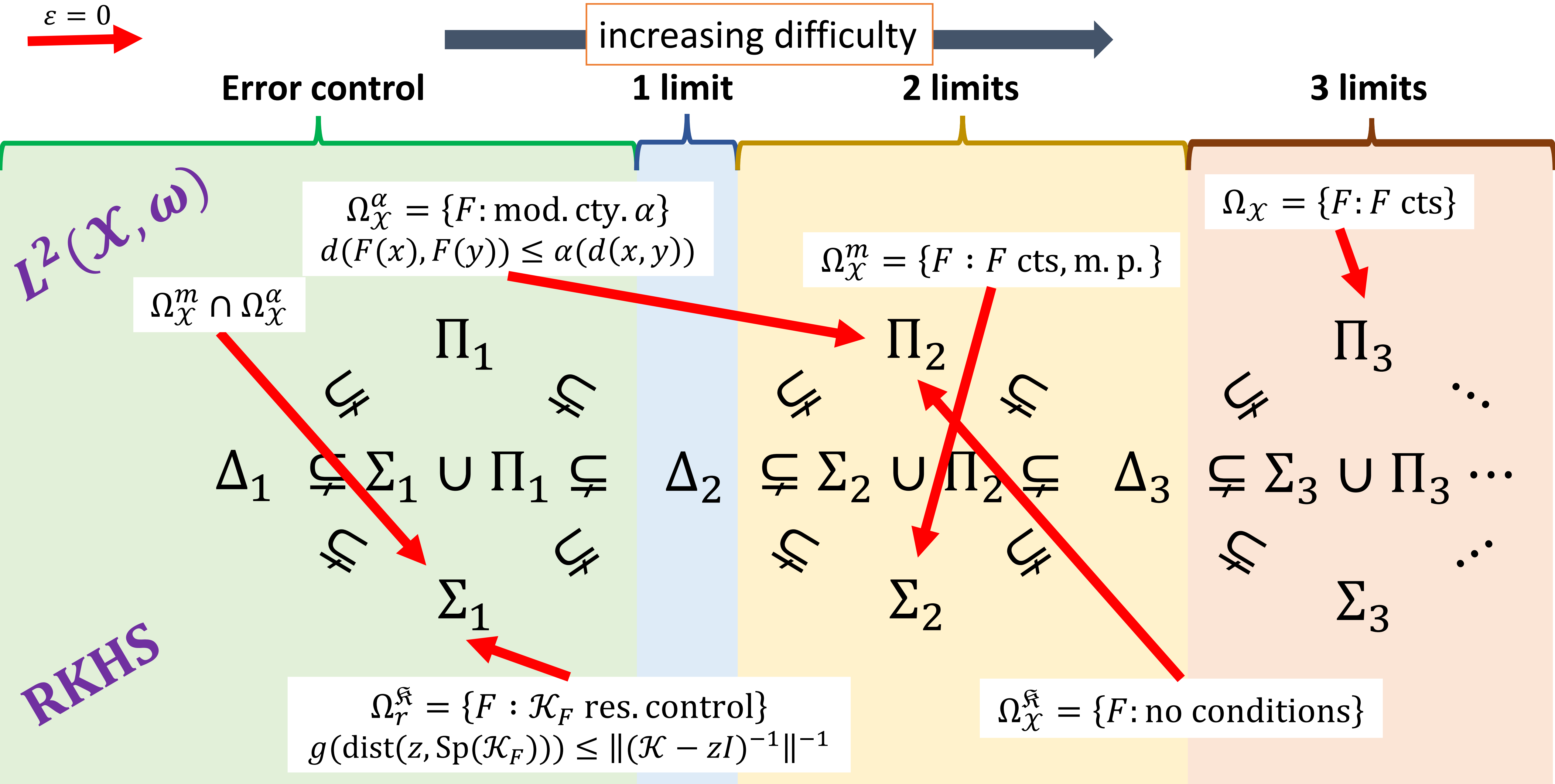
$$\Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

$$\Sigma_1 \qquad \Sigma_2 \qquad \Sigma_3$$

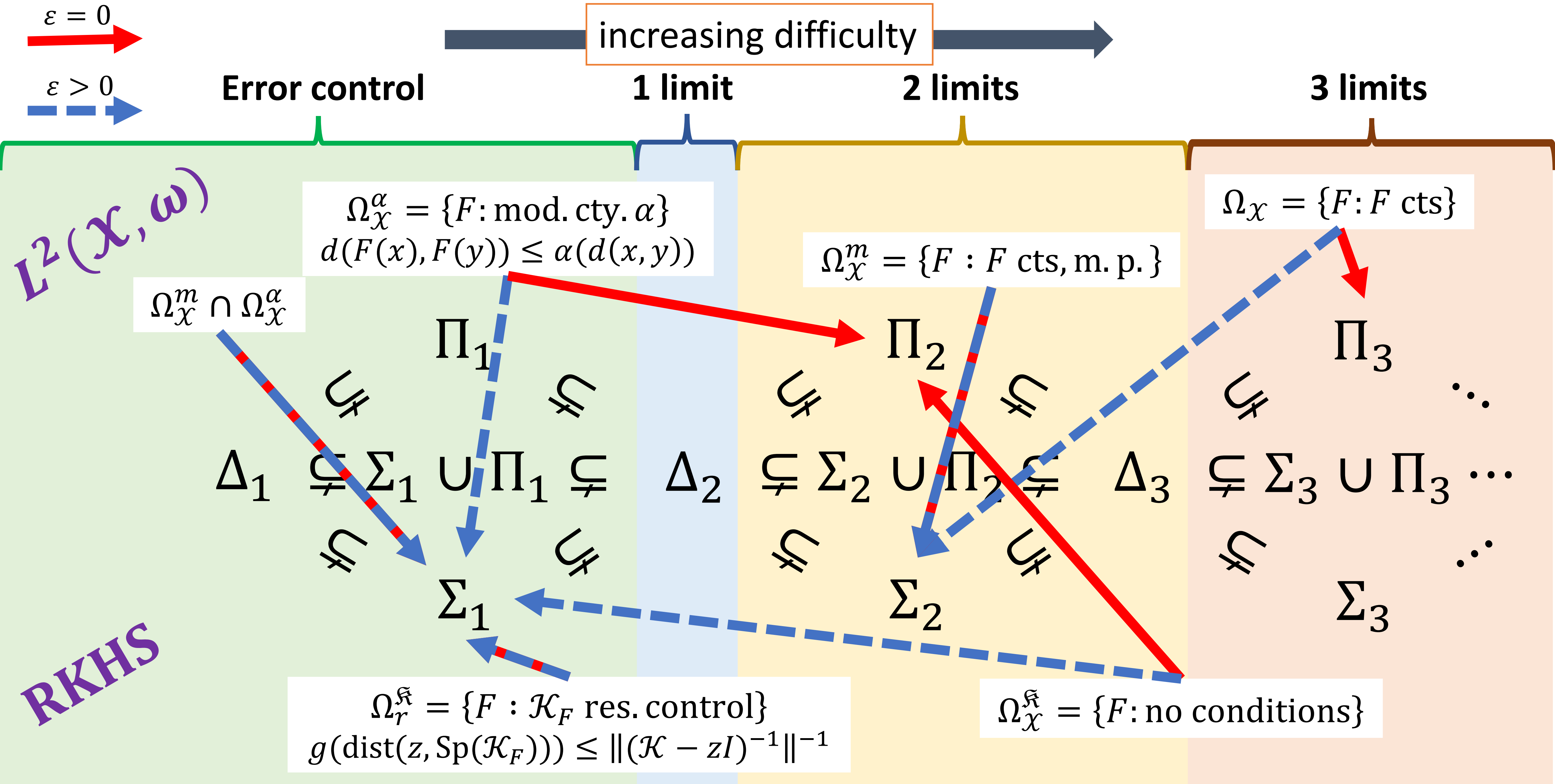
Optimal algorithms and classifications of systems



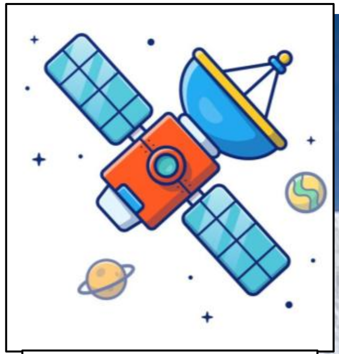
Optimal algorithms and classifications of systems



Optimal algorithms and classifications of systems

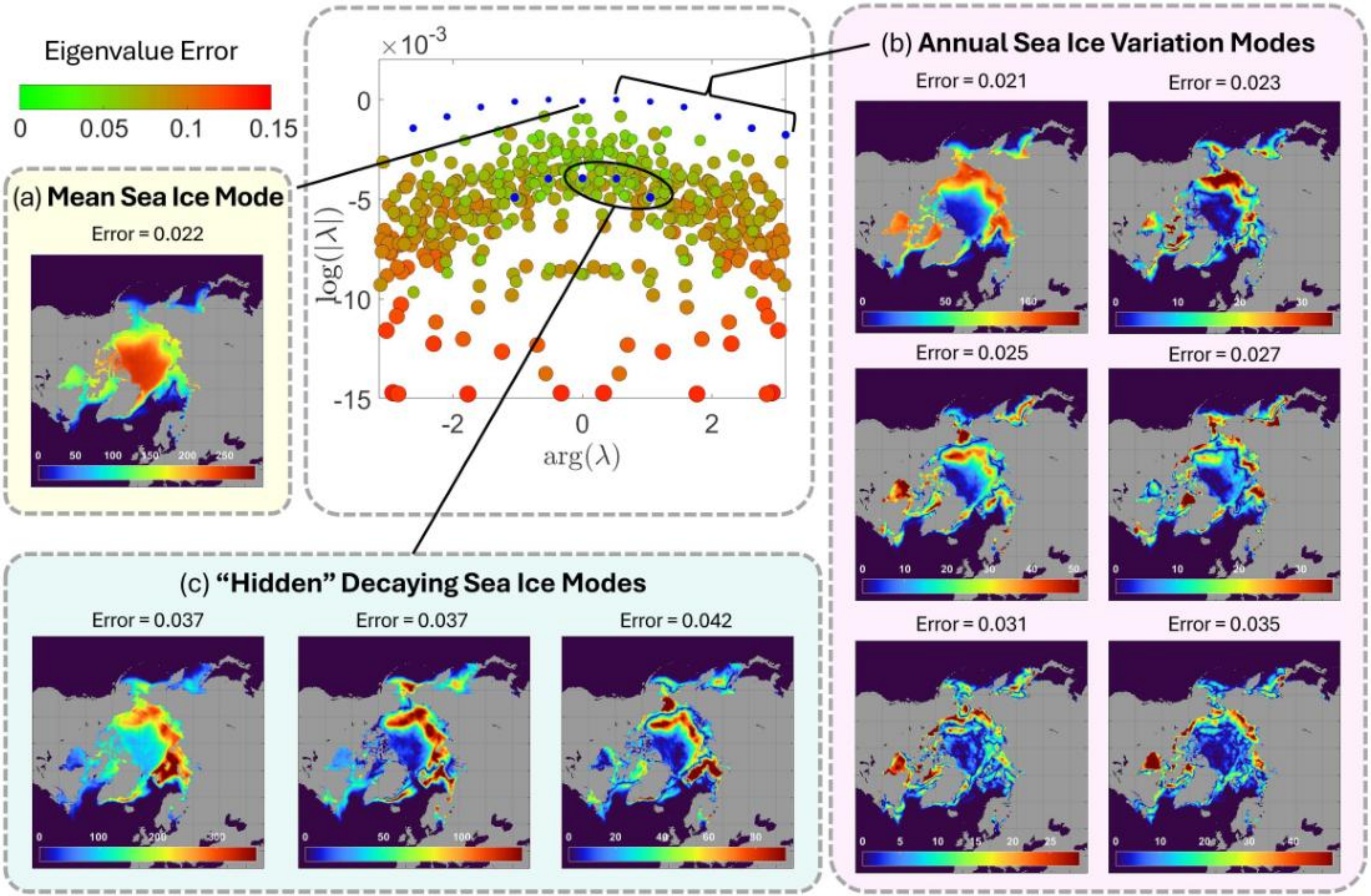


Practical gains: Arctic sea ice forecasting



Satellite data

Problems: 1. Very hard to locate geographical significant regions.
2. Very hard to predict more than two months in advance.



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Avoid spurious evals ⇒ State-of-the-art forecasts

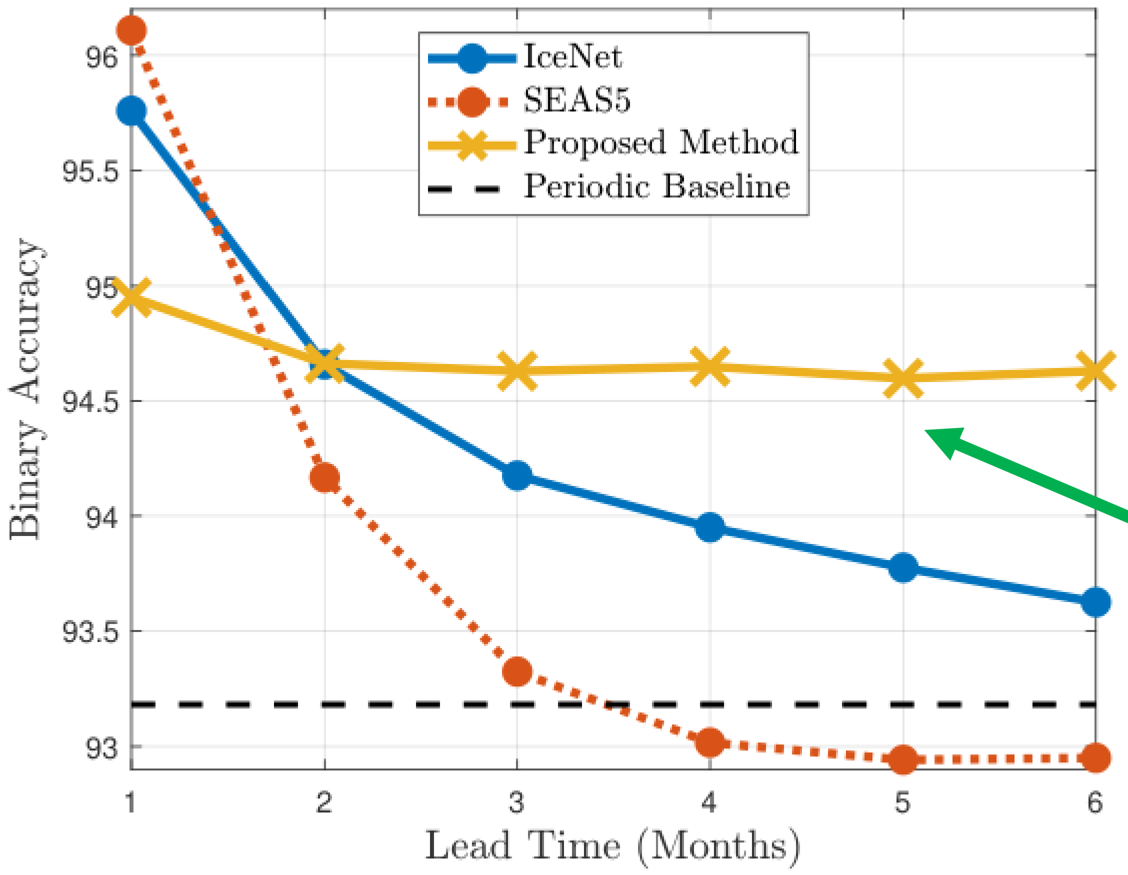


Figure: Mean binary accuracy over test years 2012-2020.
(IceNet: Andersson et al, "Seasonal Arctic sea ice forecasting with probabilistic deep learning." Nature Communications, 2021.)

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

$$\|\mathcal{K}g - \lambda g\| \leq \varepsilon$$
$$\Rightarrow \; g(x_n) = \lambda^n g(x_0) + \mathcal{O}(n\varepsilon)$$

Use ε to filter evals!

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

What about forecast bounds and dictionary learning?

Principle Angle Decomposition (PAD)

Algorithm 3.1 Principal angles and observables between $\mathcal{V}$ and $\mathcal{KV}$.

Input: Matrices $\mathbf{G}$, $\mathbf{A}$ and $\mathbf{L}$ in (2.3) and (2.9) for dictionary $\{\psi_j\}_{j=1}^N$, subspace selection matrix $\mathbf{B} \in \mathbb{C}^{N\times n}$, cut-off tolerance $\epsilon_c \geq 0$. For RKHS, use instead the matrices $\mathbf{G}$, $\mathbf{A}$ and $\mathbf{R}$ (instead of $\mathbf{L}$) from (2.6) and (2.10).

1: Compress the matrices to form $\mathbf{G}_\mathcal{V} = \mathbf{B}^*\mathbf{G}\mathbf{B}$, $\mathbf{A}_\mathcal{V} = \mathbf{B}^*\mathbf{A}\mathbf{B}$, and $\mathbf{L}_\mathcal{V} = \mathbf{B}^*\mathbf{L}\mathbf{B}$.

2: Compute the matrix

$$\mathbf{J}_\mathcal{V} = \begin{pmatrix} \mathbf{G}_\mathcal{V} & \mathbf{A}_\mathcal{V} \\ \mathbf{A}_\mathcal{V}^* & \mathbf{L}_\mathcal{V} \end{pmatrix} \in \mathbb{C}^{2n\times 2n},$$

and its eigendecomposition $\mathbf{J}_\mathcal{V} = \mathbf{U}\mathbf{D}\mathbf{U}^*$.

3: Set $\mathcal{I} = \{j : \mathbf{D}_{jj} > \epsilon_c,\ j = 1,\ldots,2n\}$, and compute

$$\mathbf{C}_1 = \sqrt{\mathbf{D}(\mathcal{I},\mathcal{I})}\,(\mathbf{U}(1:n,\mathcal{I}))^*, \quad \mathbf{C}_2 = \sqrt{\mathbf{D}(\mathcal{I},\mathcal{I})}\,(\mathbf{U}(n+1:2n,\mathcal{I}))^*.$$

4: Compute the principal angles and observables

$$[\{\theta_j\}_{j=1}^q, \mathbf{U}_1, \mathbf{U}_2] = \texttt{subspacea}(\mathbf{C}_1, \mathbf{C}_2), \quad q \leq n,$$

and convert back to the original dictionary via (3.1) and (3.2).

Output: Principal angles $\{\theta_j\}_{j=1}^q$ and principal observables $\{(u_j, v_j)\}_{j=1}^q$.

Algorithm 3.2 Principal Angle Decomposition (PAD).

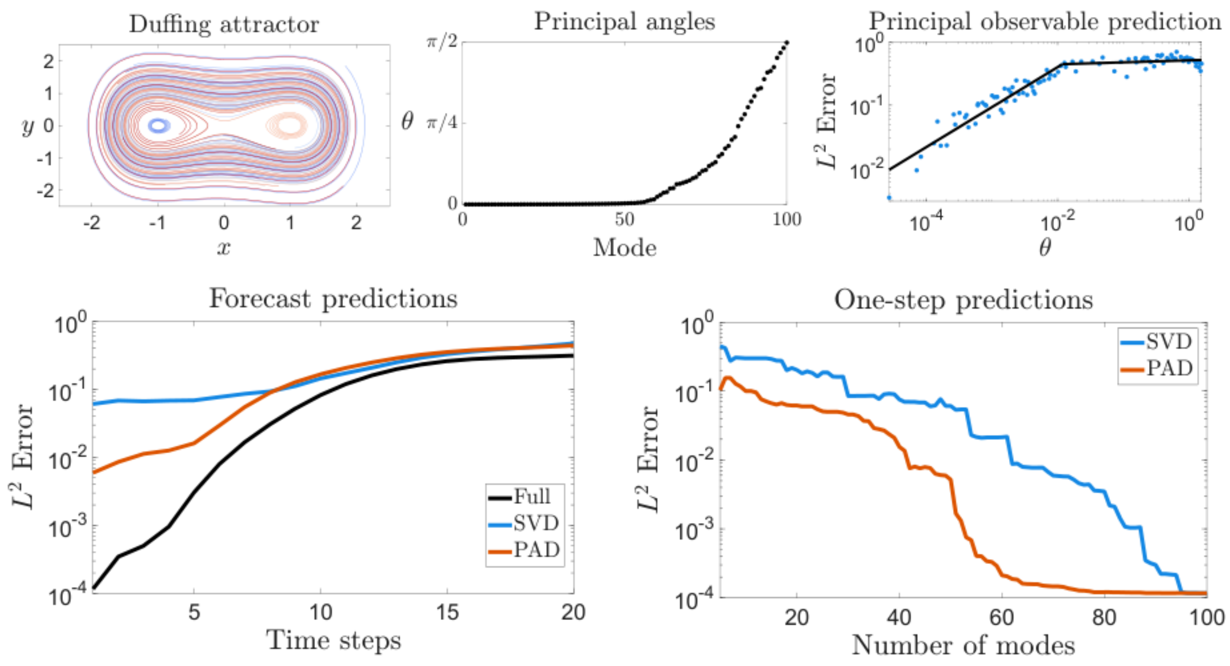
Input: Matrices $\mathbf{G}$, $\mathbf{A}$, $\mathbf{K}$ and $\mathbf{L}$ in (2.3), (2.4), and (2.9) for dictionary $\{\psi_j\}_{j=1}^N$, cut-off tolerance $\epsilon_c \geq 0$, number of post-compression modes $r > 0$.

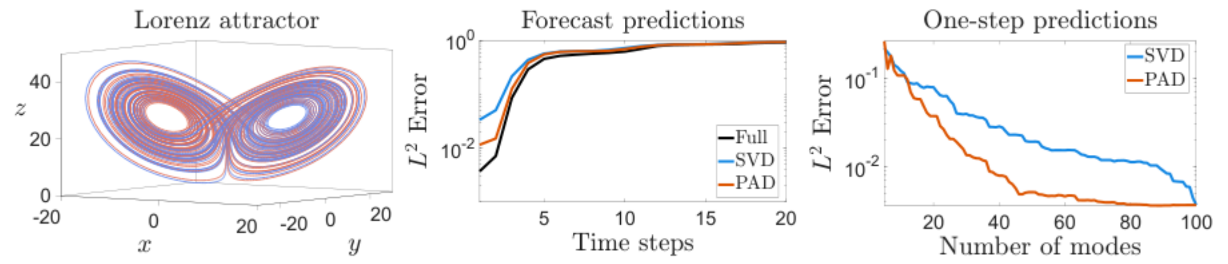
1: Compute principal angles $\{\theta_j\}_{j=1}^q$ and observables $\mathbf{U}_1$ via Algorithm 3.1 ($\mathbf{B} = \mathbf{I}_N$).

2: Define $\mathbf{U}_1' = \mathbf{U}_1(1:q,:) + \mathbf{K}\mathbf{U}_1(q+1:2q,:)$, and truncate to $\mathbf{U} = \mathbf{U}_1'(:,1:r)$.

3: Construct the matrices $\mathbf{A}_{\text{pad}} = \mathbf{U}^*\mathbf{A}\mathbf{U} = \mathbf{K}_{\text{pad}}$ and $\mathbf{L}_{\text{pad}} = \mathbf{U}^*\mathbf{L}\mathbf{U}$.

Output: The compressed matrices $\mathbf{A}_{\text{pad}}$, $\mathbf{K}_{\text{pad}}$ and $\mathbf{L}_{\text{pad}}$.





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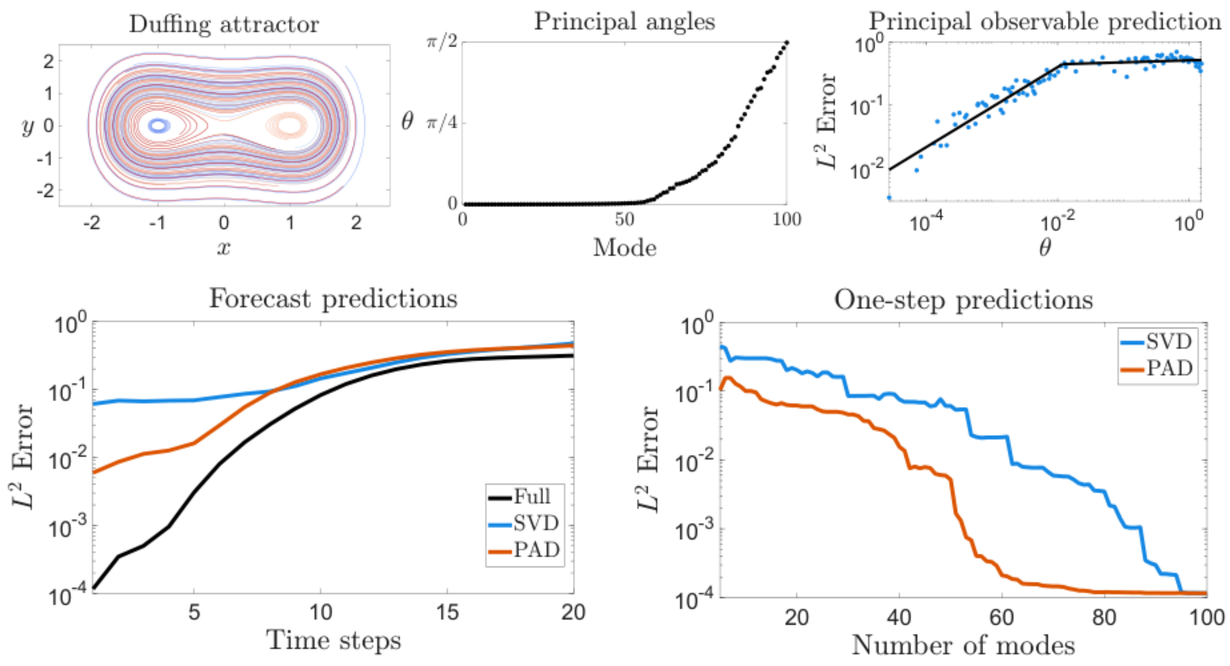

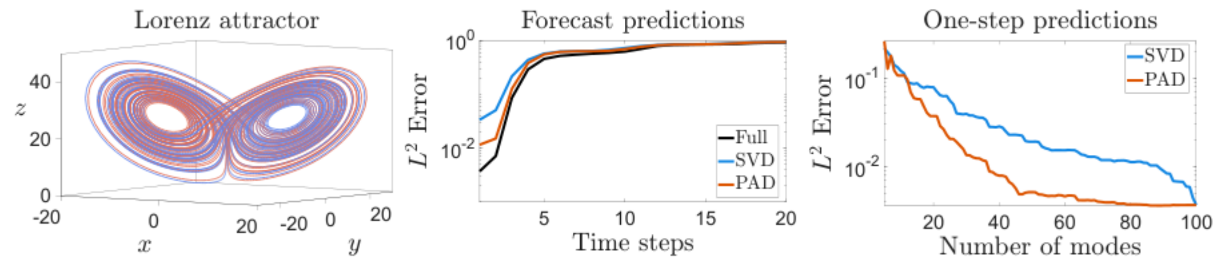

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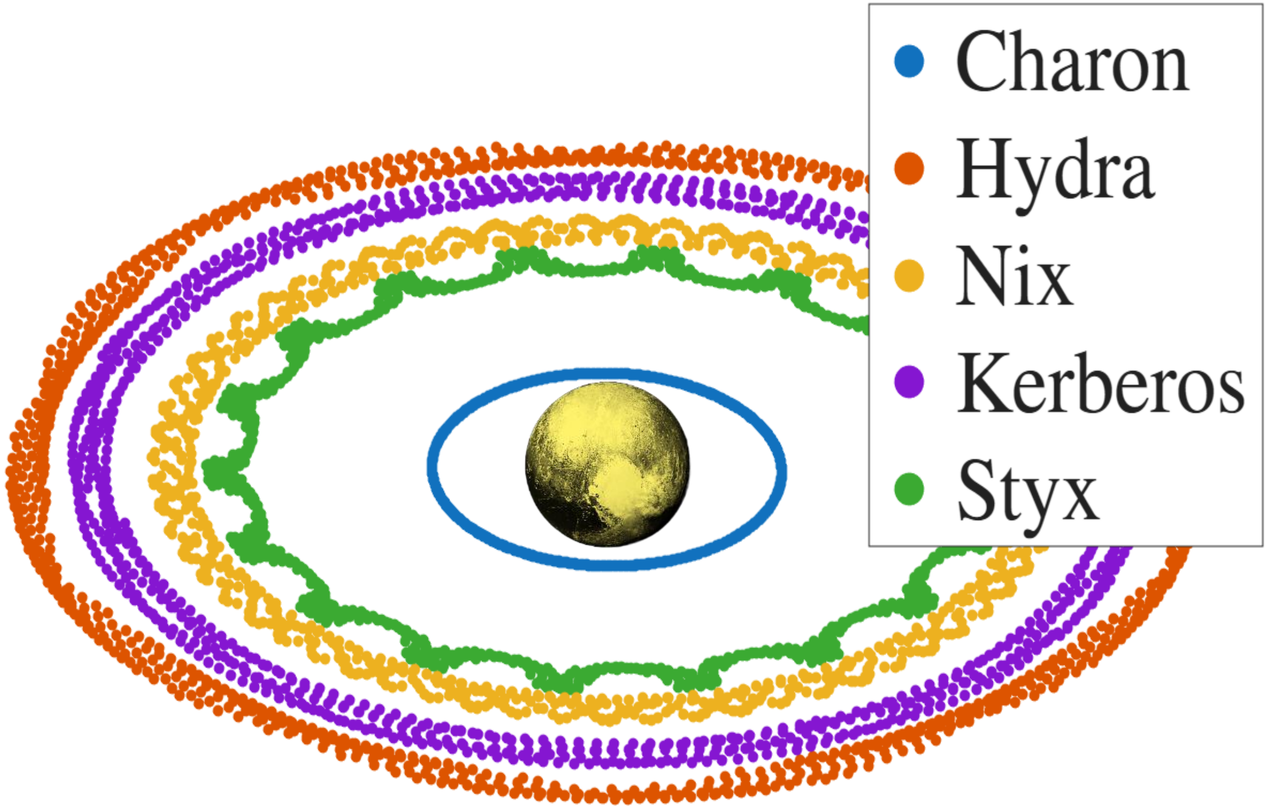
Dictionary learning and forecast multistep bounds

- Pluto and its 5 satellites
- Comparable mass of Pluto and Charon → **complex dynamics**
- Obtain error bounds for both L^2 and RKHS cases



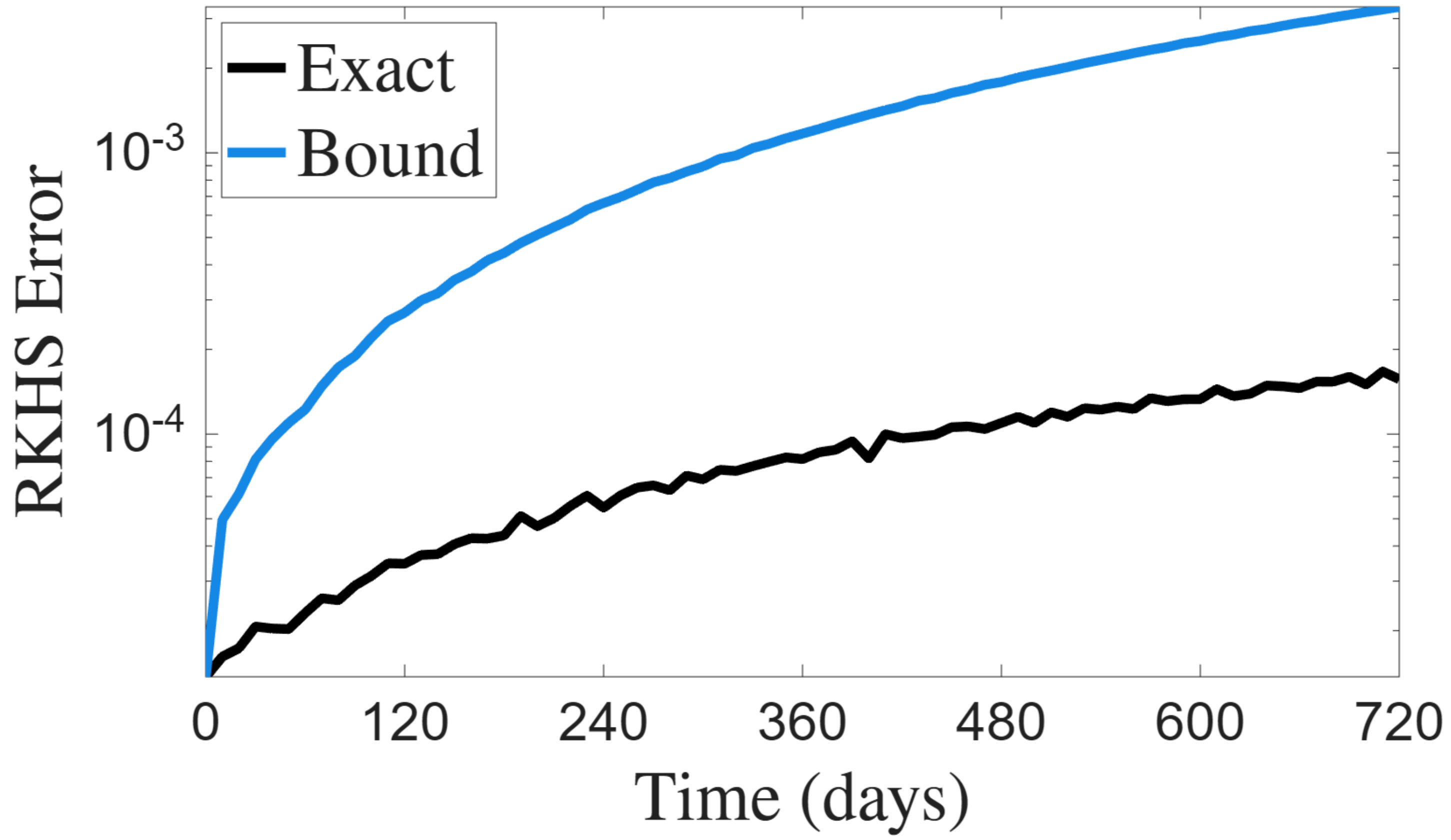
apply to dictionary refinement

obtain pointwise error bounds, expected error surrogates

- Conradie, Boullé, Loiseau, Brunton, C., *"Trustworthy Koopman Operator Learning: Invariance Diagnostics and Error Bounds,"* **preprint**, 2026.

Dictionary learning and forecast bounds

- Apply algorithms to RKHS setting using Matérn kernel



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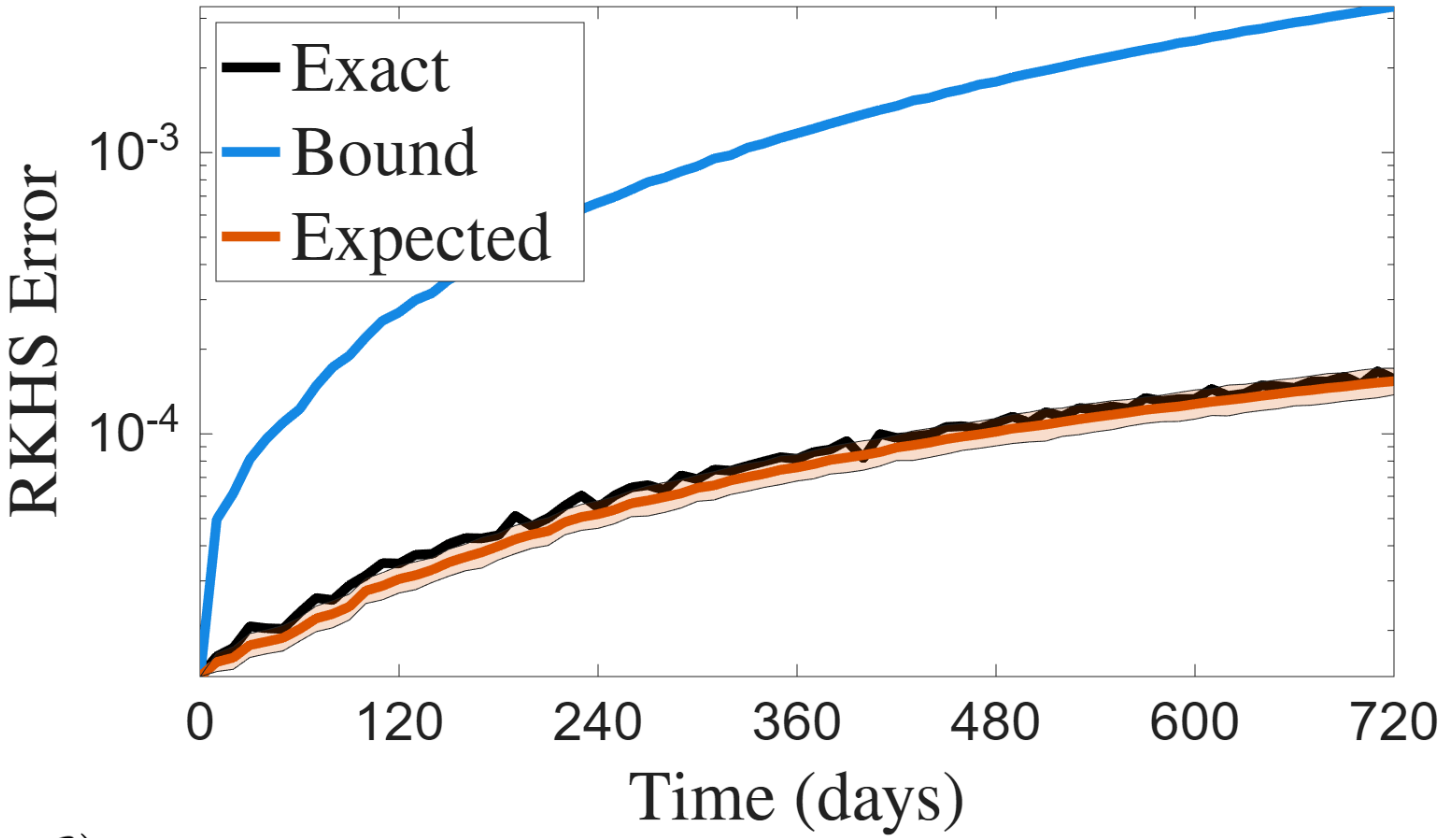
Dictionary learning and forecast bounds

- Apply algorithms to RKHS setting using Matérn kernel
- Expected errors using **Gaussian processes** avoid overestimation
- E.g., replace $\|Ax\| \leq \|A\|\|x\|$ with $\|Ax\| \approx \mathbb{E}_{\mathcal{C}}[A]\|x\|$ where

$$\mathbb{E}_{\mathcal{C}}[A] = \mathbb{E}\left[\frac{\|Ax\|}{\|x\|}\right], \quad x \sim \mathcal{GP}(0, \mathcal{C})$$



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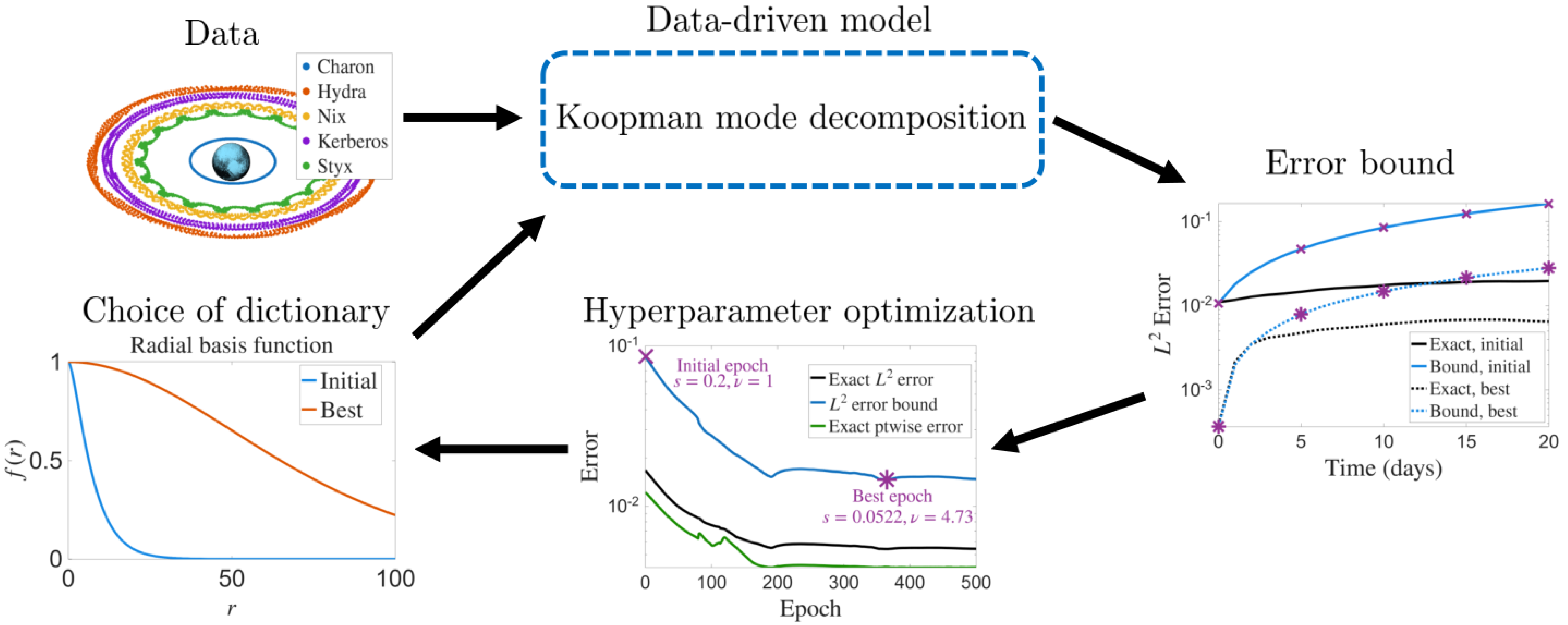
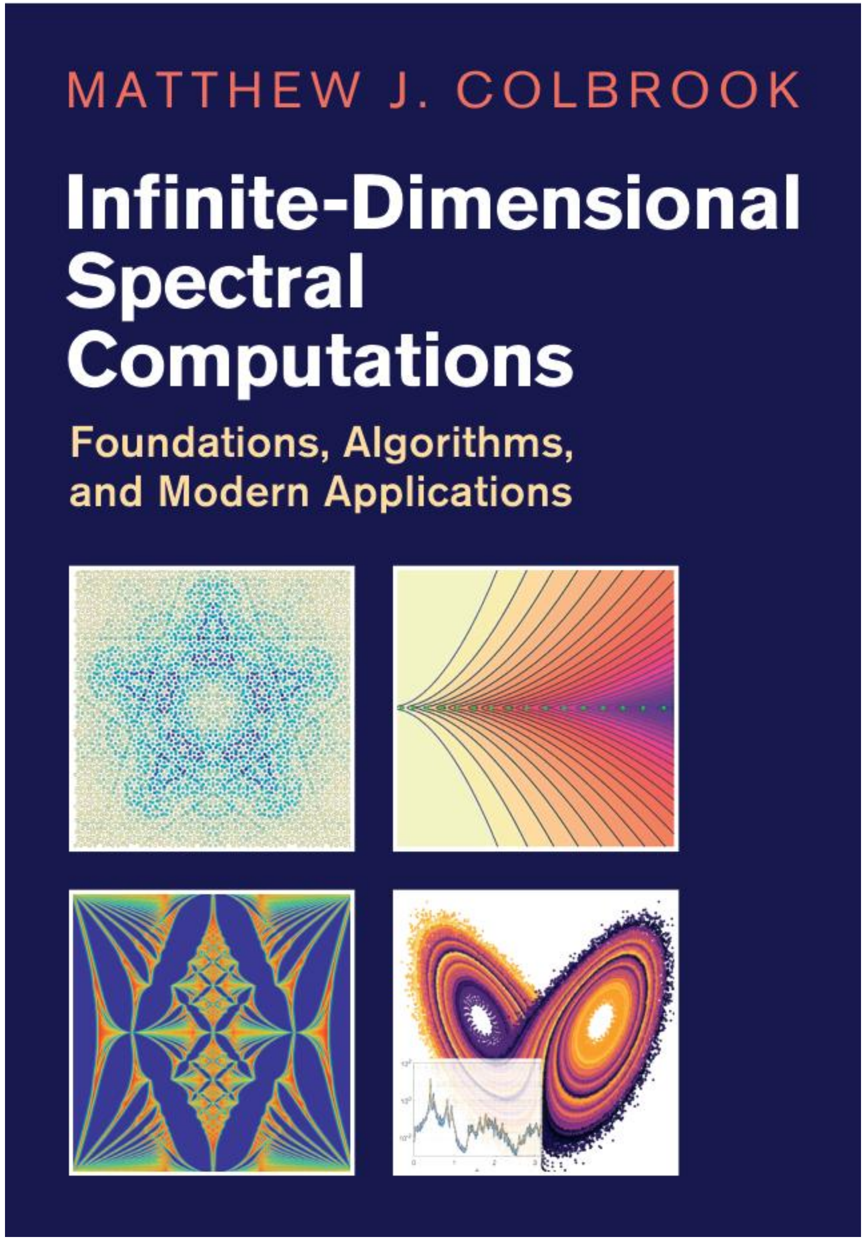
Dictionary learning and forecast bounds



Shameless plug 1: CUP book out August 2026…



Contents

100s of:

- Classifications
- Algorithms
- Examples (full code)
- Exercises (full solutions)

If something of interest – speak to me!

This talk

Shameless plug 2: Issac Newton Institute Programme

Operator Methods for Dynamical Systems

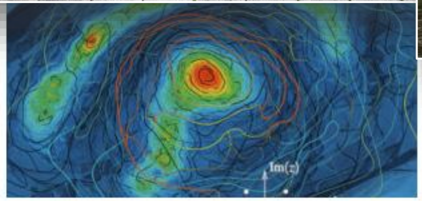
OMD

3 August 2026 to 28 August 2026

Programme theme

Dynamical systems lie at the heart of our understanding of complex phenomena, whether in modelling weather and ocean currents, molecular dynamics, population growth or stock market fluctuations. However, the nonlinear nature of systems poses a challenge to describing their behaviour. Operator methods offer a powerful way to tackle this challenge. By representing a finite-dimensional nonlinear system's evolution as a linear operator acting on an infinite-dimensional space of functions, tools from linear algebra and spectral analysis can be used to gain insights into the system's long-term behaviour. This operator-based perspective has roots in 20th-century mathematics. It has proven fruitful in classical settings like statistical mechanics, where it helped connect chaotic systems with well-understood linear techniques.

In recent years, interest in operator methods for dynamical systems has surged, driven by data-driven techniques to approximate and analyse these operators from real-world or simulated data. A wide range of frameworks and algorithms have emerged, creating an exciting opportunity and need to develop a unifying foundation for these approaches. This programme aims to bring together experts and young researchers from various communities who use operator-theoretic perspectives (for example, the Koopman and transfer operator frameworks) to study dynamics. By uniting participants from pure theory to practical applications, the programme will spark new collaborations and jointly tackle key open questions, building a more cohesive research community. In particular, a significant focus will be on exploring the spectral properties of these operators—essentially, understanding their eigenvalues, modes, and related features—as these provide crucial insights into a system's long-term behaviour and how such behaviour can be effectively analysed and computed.



Organisers

- Matthew Colbrook *University of Cambridge*
- Gary Froyland *University of New South Wales*
- Nathan Kutz *University of Washington*
- Julia Slipantschuk *University of Warwick; Universität Bayreuth*
- Caroline Wormell *University of Sydney*

Participants

- Wael Bahsoun *Loughborough University*
- Steve Brunton *University of Washington*
- Christopher Budd *University of Bath; Institute of Mathematics and its Applications*

Visit to find out more about operator theory and machine learning in dynamical systems!

(and to enjoy Cambridge in the summer!)

Pointers

1. Data-driven spectral problems for Koopman operators are hugely popular.
   BUT: Standard truncation methods can fail – NEED TO GO INF-DIM!

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

   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 spectral picture for K. on $L^2(\mathcal{X}, \omega)$ and RKHS!**

4. **Matrix L** leads to forecast bounds, ways to train dictionary, and PAD.

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	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,…

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