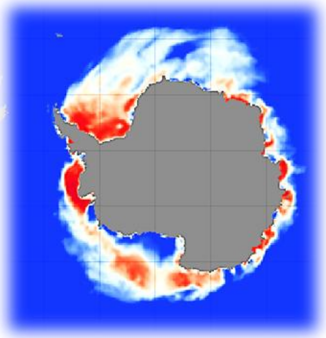
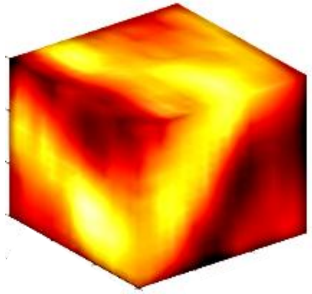
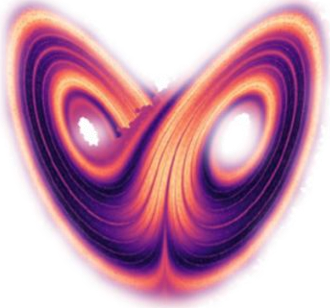






# *Adversaries and classifying the difficulty of data-driven dynamical systems*

Matthew Colbrook

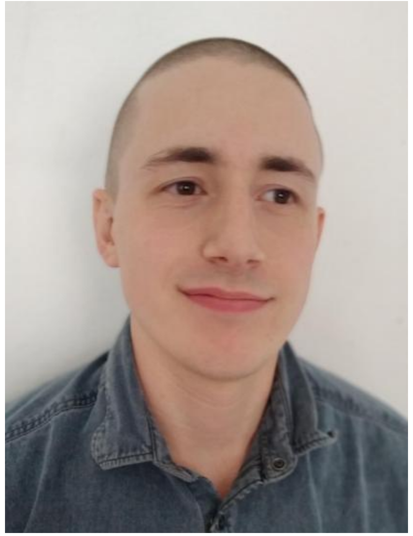
UNIVERSITY OF CAMBRIDGE

6/5/2025

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

**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!**)

# Operator theory for dynamical systems

- Metric space $(\mathcal{X}, d)$ – *the state space*

- $x \in \mathcal{X}$ – *the state*

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

Henri Poincaré
(Sorbonne)

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

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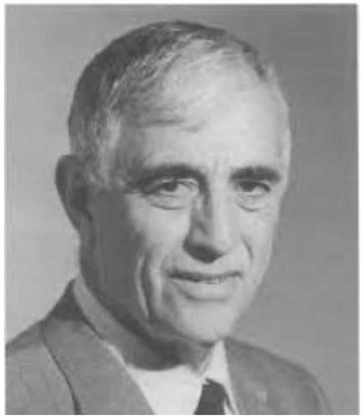
- Function space $L^2 = L^2(\mathcal{X}, \omega)$ (elements $g$ called "observables")
- Koopman operator $\mathcal{K}_F: L^2 \to L^2$; $[\mathcal{K}_F g](x) = g(F(x))$

**NB:** Pointwise definition of $\mathcal{K}_F$ needs $F\#\omega \ll \omega$ – this will hold throughout.
**NB:** $\mathcal{K}_F$ bounded equivalent to $\mathrm{d}F\#\omega/\mathrm{d}\omega \in L^\infty$ – this will hold throughout (can be dropped).

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.

# Operator theory for dynamical systems

- Metric space $(\mathcal{X}, d)$ – *the state space*
- $x \in \mathcal{X}$ – *the state*
- ***Unknown*** cts $F: \mathcal{X} \to \mathcal{X}$ – *the dynamics:* $x_{n+1} = F(x_n)$
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- Koopman operator $\mathcal{K}_F: L^2 \to L^2$; $[\mathcal{K}_F g](x) = g(F(x))$
- ***Available*** snapshot data: $\left\{\left(x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right): m = 1, \ldots, M\right\}$

**Can we compute spectral properties from data?**

# Example

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

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

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

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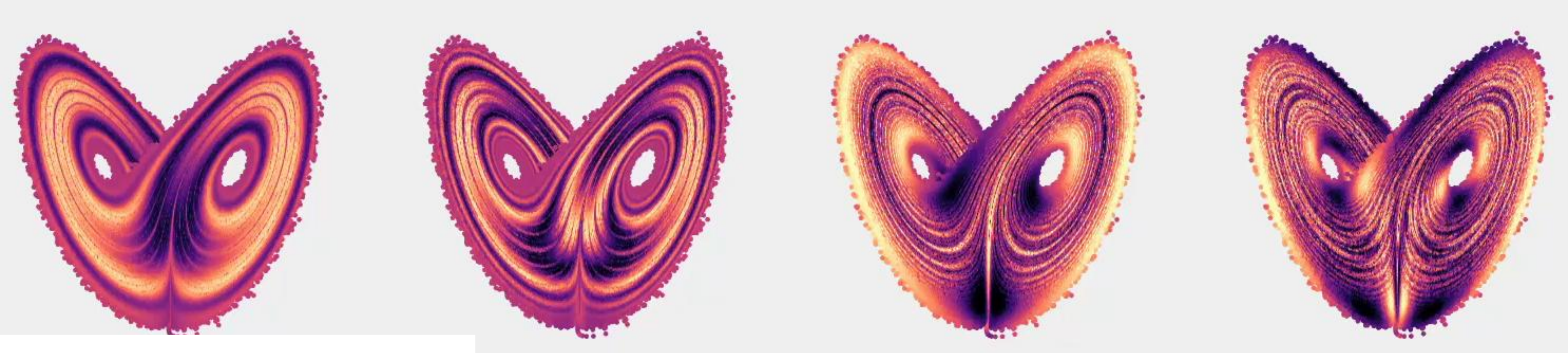

***Coherent features!***

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

# Example

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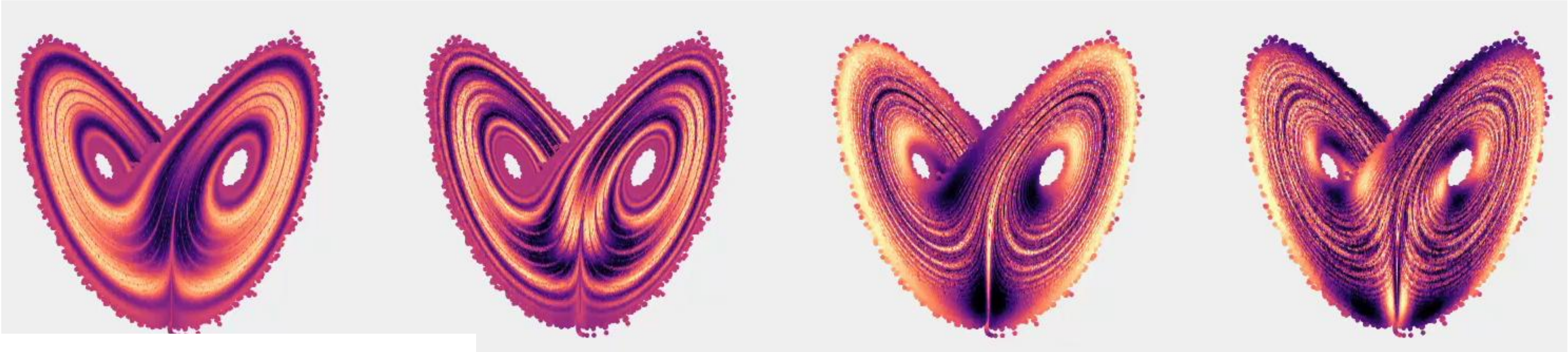


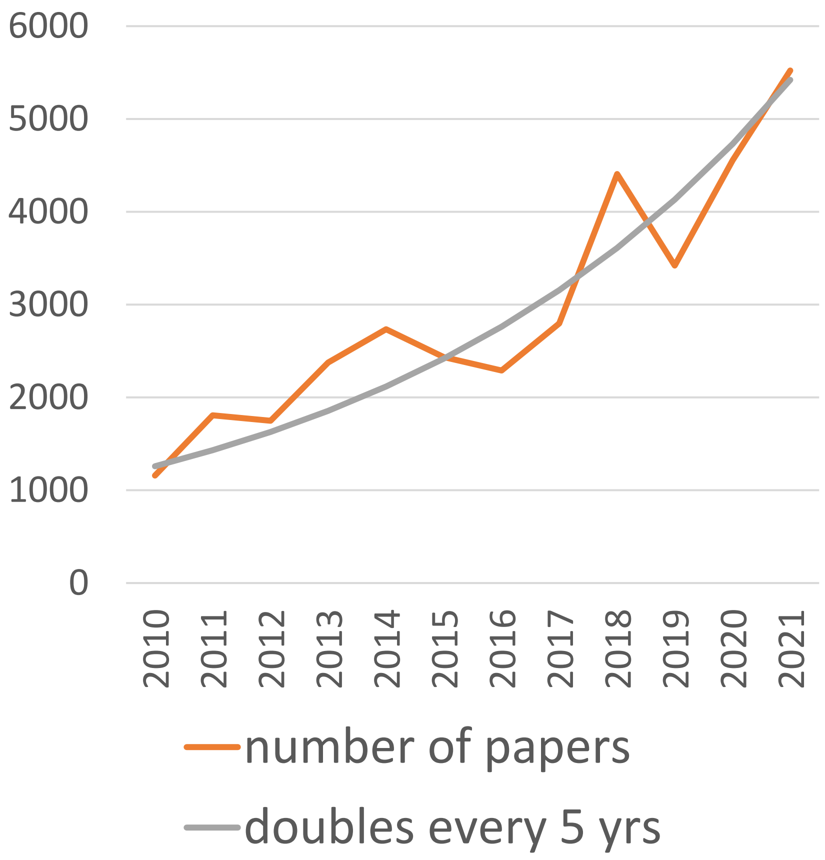
***Coherent features!***

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

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

# Koopmania*: A revolution in the big data era

**New papers on computing Koopman operator spectra**




***Very* little on convergence guarantees. *WHY?***

1. Koopman operators have been largely used in applied domains + distinct from NA.

2. Infinite-dimensional spec. comp. notoriously hard …

Only recently have the tools been developed

# 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!**

# Building the matrix: EDMD

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

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

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

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

**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.

# Residual DMD (ResDMD): Approx. $\mathcal{K}$ and $\mathcal{K}^*\mathcal{K}$

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

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


- C., Townsend, "*Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*," **Commun. Pure Appl. Math.**, 2023.
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- Code: https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition

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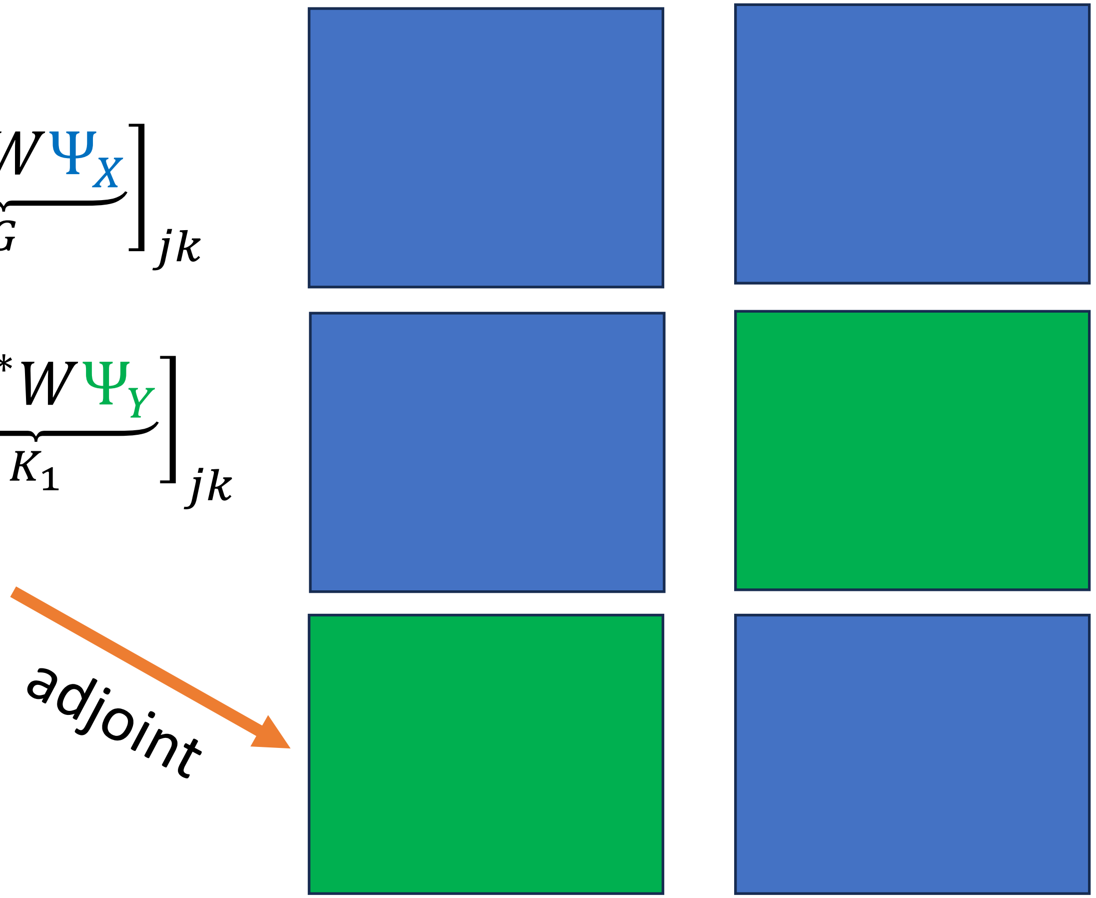



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$$\langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle \approx \sum_{m=1}^{M} w_m \overline{\psi_j(y^{(m)})}\, \psi_k\left(y^{(m)}\right) = \Big[\underbrace{\Psi_Y{}^* W \Psi_Y}_{K_2}\Big]_{jk}$$


- C., Townsend, "*Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*," **Commun. Pure Appl. Math.**, 2023.
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**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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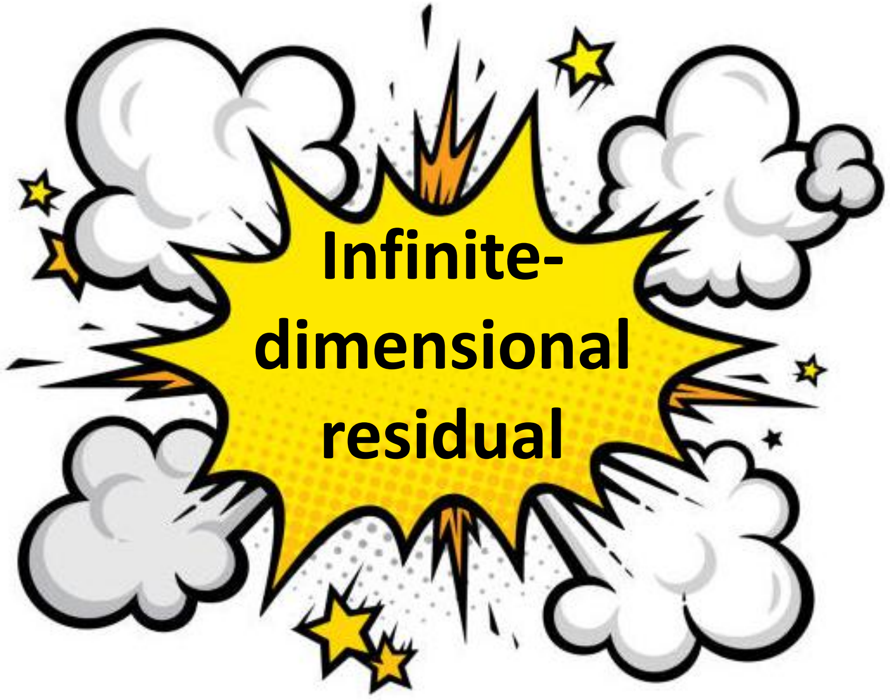


**<u>Residuals:</u>** $g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j$, $\|\mathcal{K}g - \lambda g\|^2 = \lim_{M\to\infty} \mathbf{g}^*[K_2 - \lambda K_1{}^* - \bar{\lambda} K_1 + |\lambda|^2 G]\mathbf{g}$

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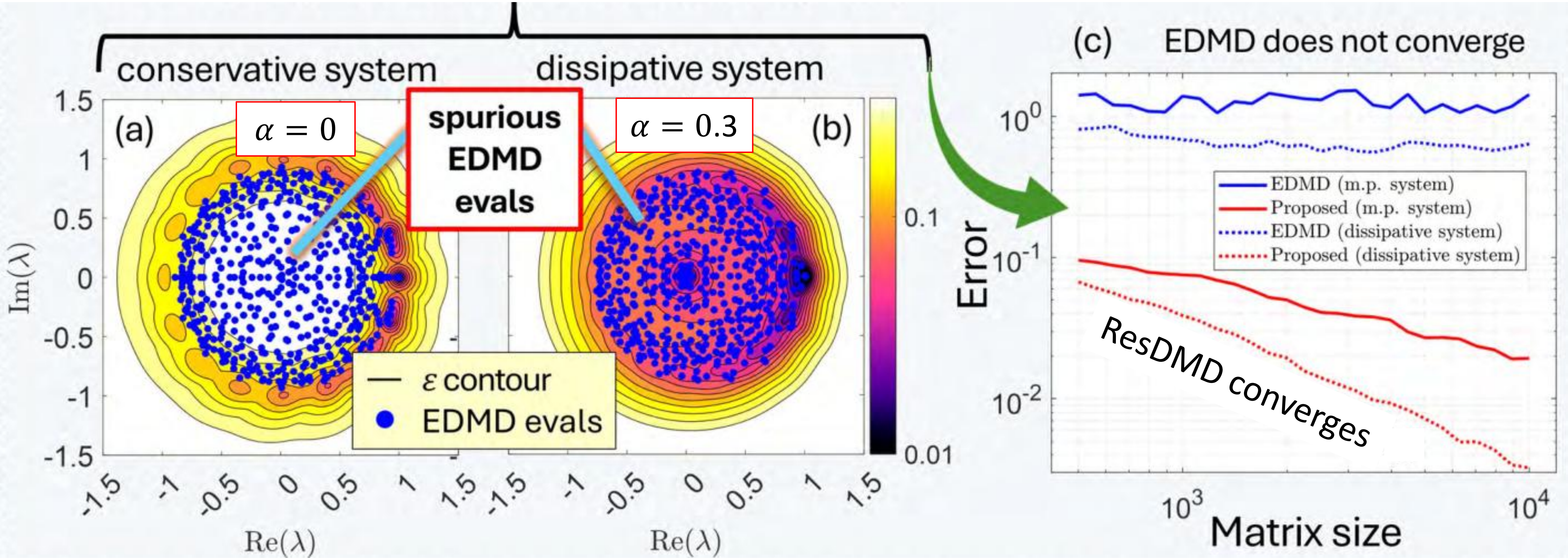
# Example: EDMD doesn't converge

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



# Good news!

**Theorem:** There **exists** *deterministic* 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)**

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

# Question?

**Theorem:** There **exists** *deterministic* 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)**

**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

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

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

**Theorem:** There **does not exist** any sequence of (even random) algorithms $\{\Gamma_n\}$ using $\mathcal{T}_F$ s.t. $\lim_{n\to\infty} \Gamma_n(F) = \mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}_F)$ with probability $> 1/2$ for any $F \in \Omega_{\mathbb{D}}$.

**Universal - any type of algorithm or computational model.**

**$n$ can index anything.**

Adversaries occur with high probability.

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

# What if we change the function space?

$$g: \mathcal{X} \to \mathbb{C}, \qquad [\mathcal{K}_F g](x) = g(F(x))$$

# Reproducing kernel Hilbert space (RKHS)

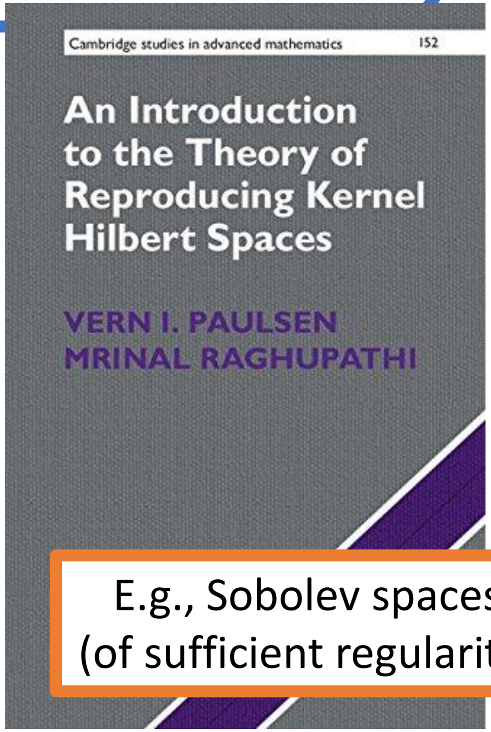
Hilbert space $\mathcal{H}$ of functions on $\mathcal{X}$ s.t. $g \mapsto g(x)$ bounded $\forall x \in \mathcal{X}$.

Generated by a conjugate symmetric positive definite $\mathfrak{K}: \mathcal{X} \times \mathcal{X} \to \mathbb{C}$

$$g(x) = \langle g, \mathfrak{K}_x \rangle_{\mathcal{H}}, \qquad \mathfrak{K}(x, y) = \left\langle \mathfrak{K}_x, \mathfrak{K}_y \right\rangle_{\mathcal{H}} = \mathfrak{K}_x(y)$$

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

- Forecasts: $\|\cdot\|_{\mathcal{H}}$ bounds $\Rightarrow$ pointwise bounds.
- High-dimensional systems practical through kernel trick.
- Fast methods for evaluating $\mathfrak{K}$.
- Different $\mathfrak{K} \Rightarrow$ 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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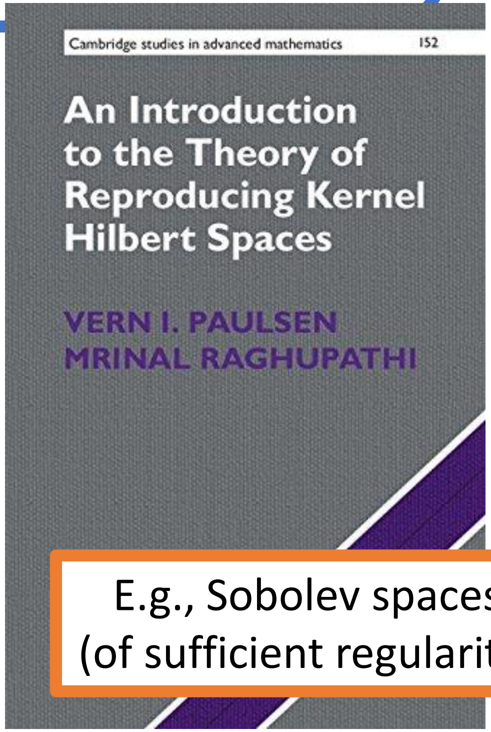



E.g., Sobolev spaces (of sufficient regularity)

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

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

Evolution of functionals.

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

*No quadrature needed:*

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

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

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

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


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

# SpecRKHS: Example algorithm

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

1. Compute $G, A, R \in \mathbb{C}^{N\times N}$ $(N=M)$
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:** $\{z_k:\tau_k<\varepsilon\}$, $\{g_k:\tau_k<\varepsilon\}$ ($\varepsilon$-pseudoeigenfunctions).

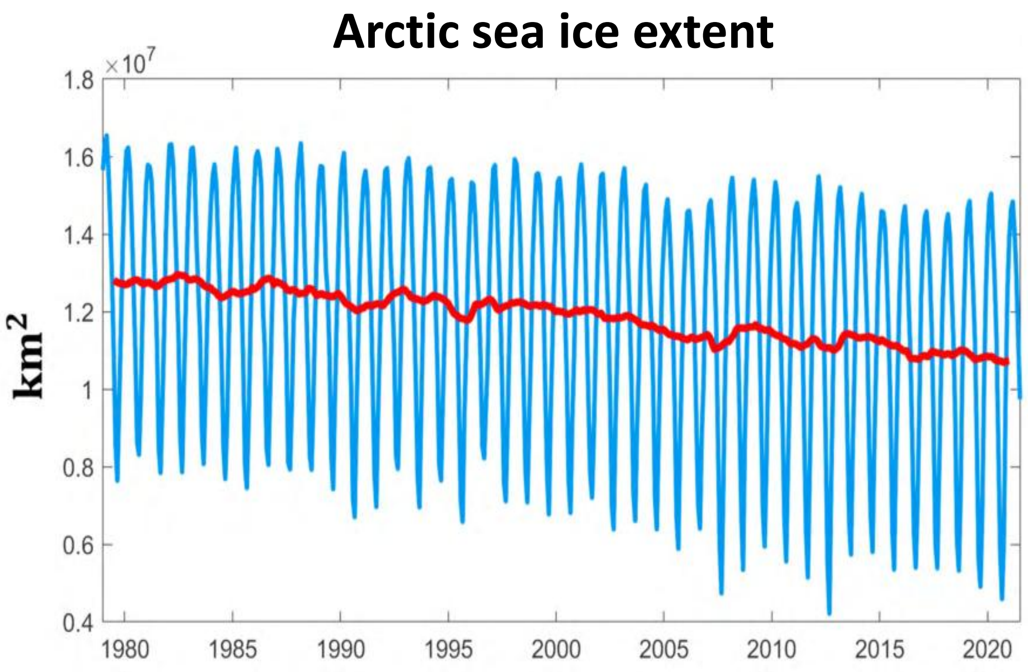
**First convergent method for general $\mathcal{K}$**

**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.

# Practical gains: Sea ice forecasting



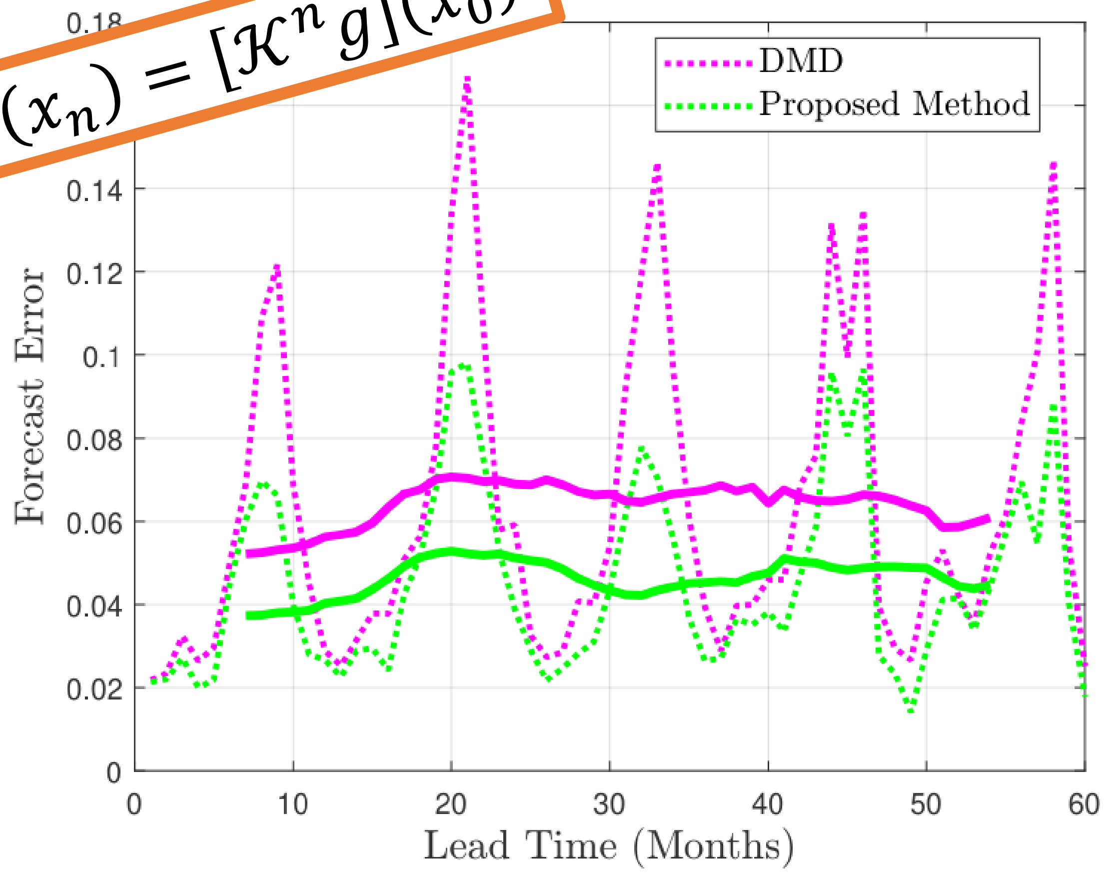

Monthly average from satellite passive microwave sensors.

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

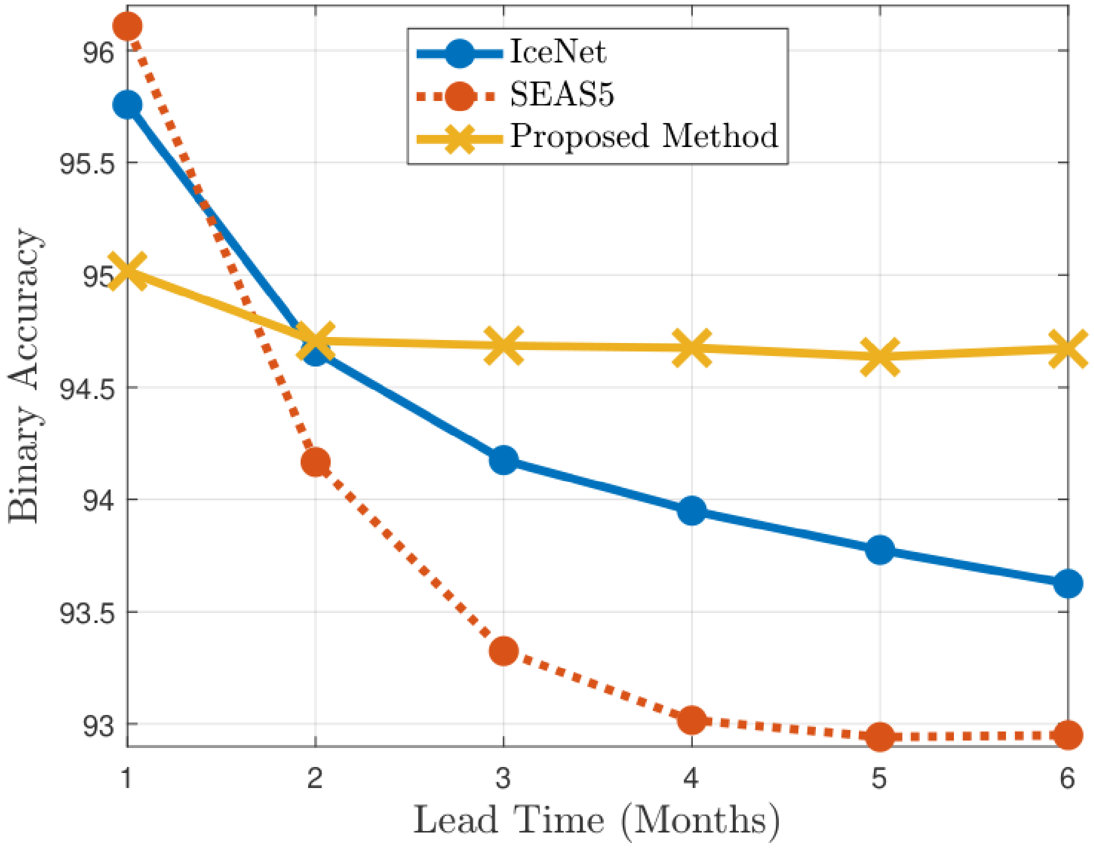
**Problem:** Very hard to predict more than two months in advance.

# Arctic case: Avoiding spurious eigenvalues helps!

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



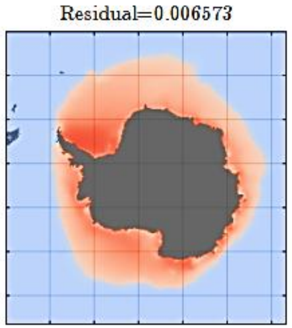

Relative mean squared error over 2016-2020. Model built from 2005-2015 data. (Solid lines moving 12-month mean.)

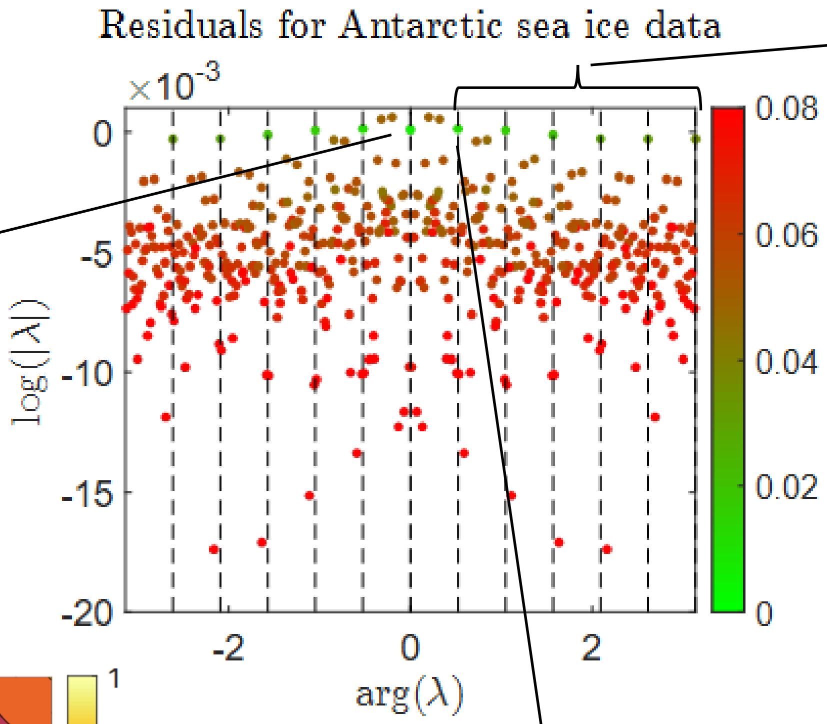



Mean binary accuracy over test years 2012-2020. *(IceNet: Andersson et al, "Seasonal Arctic sea ice forecasting with probabilistic deep learning." Nature Communications, 2021.)*

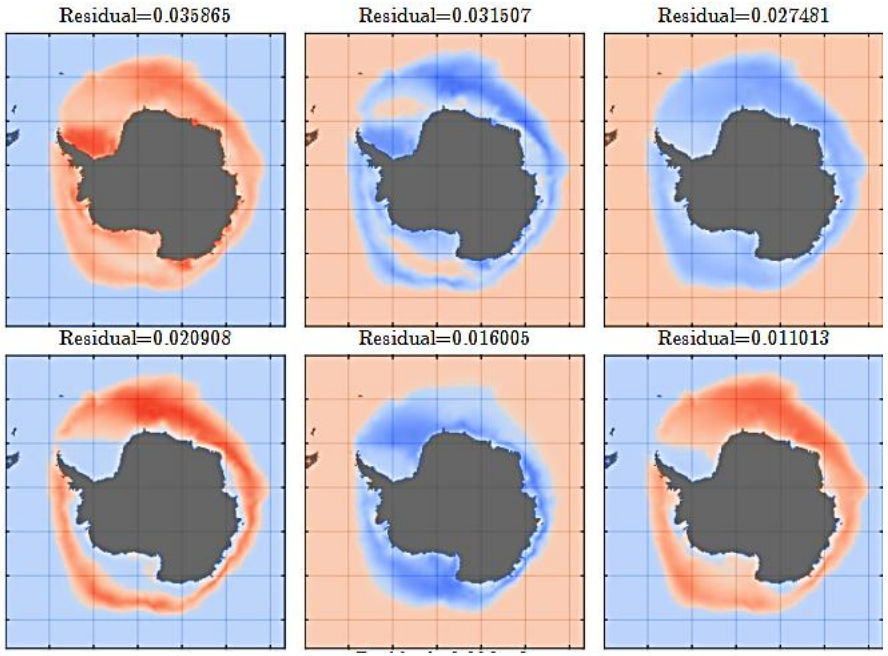
# Antarctic case

Mean Sea Ice Mode

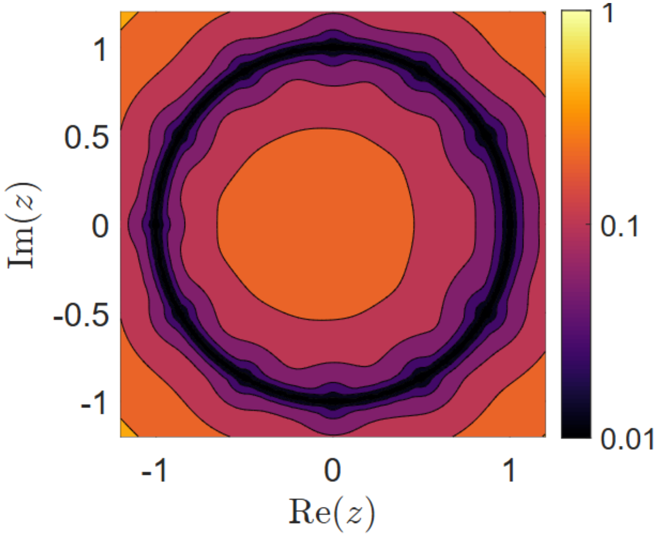


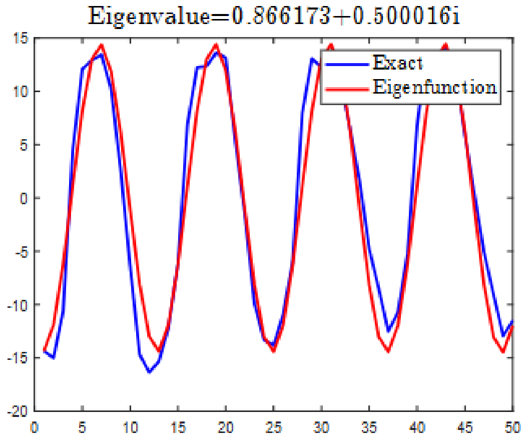




Annual Sea Ice Variation Modes




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




State space dimension: 82907

$N = M = 550$

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

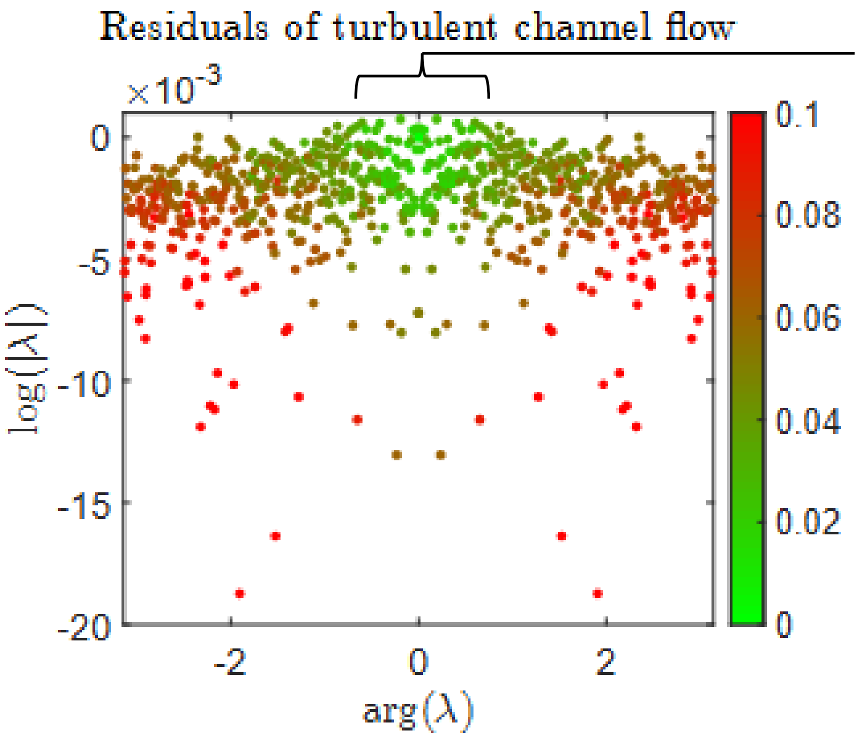
Matérn kernel

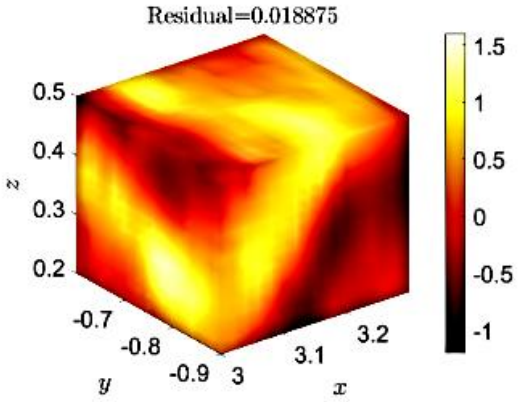
$$\propto (\sigma\|x-y\|_2)^{1/2} K_{-1/2}(\sigma\|x-y\|_2)$$

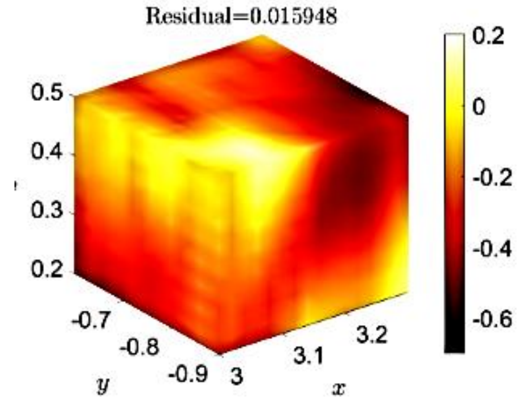
Modified Bessel function of second kind of order -1/2

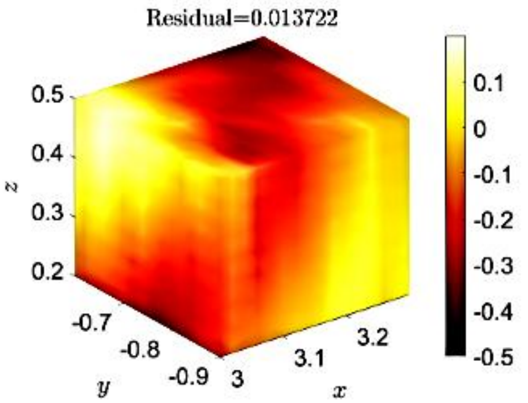
scaling parameter

# 3D turbulence ($Re \approx 1000$)



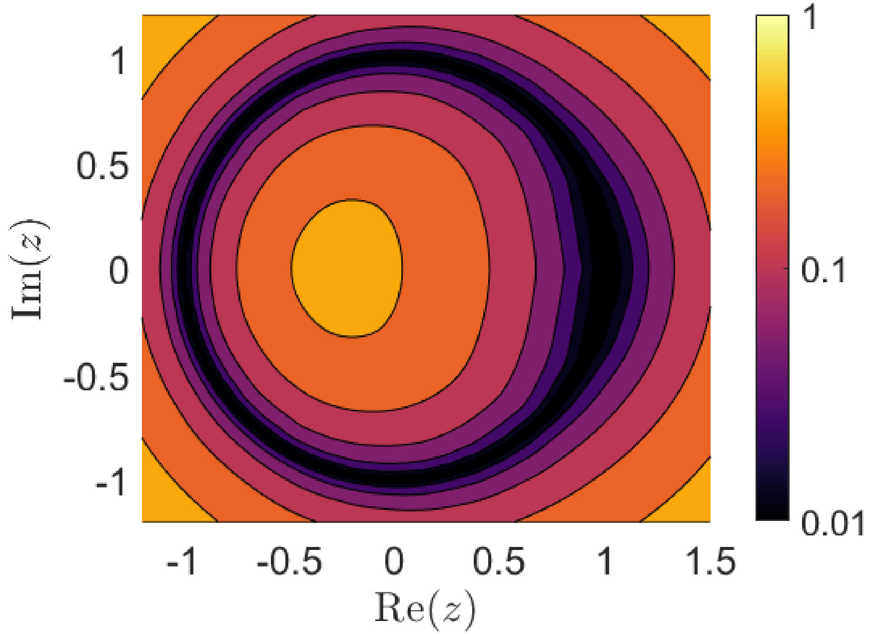




Can handle very non-normal systems!

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




State space dimension: 4096

$N = M = 800$

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

Matérn kernel

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

# Example of the method of adversarial dynamical systems

# What about $\varepsilon = 0$? (i.e., the spectrum)

If $\mathcal{K}_F$ is normal, $\mathrm{dist}\big(z, \mathrm{Sp}(\mathcal{K}_F^*)\big) = \min\{\varepsilon : z \in \mathrm{Sp}_{\mathrm{ap},\varepsilon}(\mathcal{K}_F^*)\}$, adaptive search for local minimisers. Otherwise…


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

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*Input class:* $\Omega_{\mathbb{I}} = \{F: (0,1) \to (0,1) |\, F \text{ smooth bijection}\}$.

*Data algorithm can use:* $\mathcal{T}_F = \{(x, y) | x \in (0,1), y = F(x)\}$

**Theorem:** Consider Koopman operators on $H^r((0,1))$ ($r \geq 1/2$). There **does not exist** any sequence of deterministic algorithms $\{\Gamma_n\}$ using $\mathcal{T}_F$ such that $\lim_{n\to\infty} \Gamma_n(F) = \mathrm{Sp}_{\mathrm{ap}}(\mathcal{K}_F^*)$ $\forall F \in \Omega_{\mathbb{I}}$.

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$n$ can index anything. Universal - any type of algorithm or comp. model.

Adversaries occur with high probability. → No random algorithms converging with probability $> 1/2$.

Extends to higher dimensions + other domains by embedding this proof.

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

# Lemma

If $F'(x) = \alpha \in (0,1)$ in a neighborhood of 1,

$F'(x) = 1/\alpha$ in a neighborhood of – 1

Then:

$$\alpha^{-1/2} \leq \sup\{|z|: z \in \mathrm{Sp}_{\mathrm{ap}}(\mathcal{K}_F^*)\} \leq \alpha^{1/2-r}$$

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

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

# Proof idea

$$\boxed{\alpha^{-1/2} \leq \sup\{|z| : z \in \mathrm{Sp}_{\mathrm{ap}}(\mathcal{K}_F^*)\} \leq \alpha^{1/2-r}}$$

Suppose $\{\Gamma_n\}$ converges.

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Suppose $\{\Gamma_n\}$ converges.

Pick $\alpha_1, \alpha_2 \in (0,1)$ and $\tau > 0$ with $(1+2\tau)\alpha_1^{1/2-r} < (1-2\tau)\alpha_2^{-1/2}$

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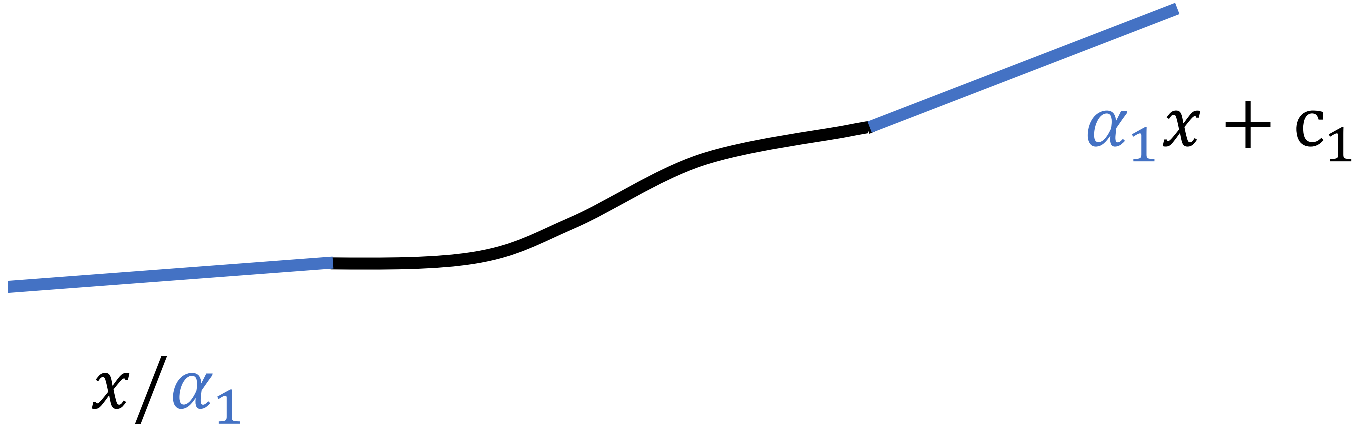
$F_1$:

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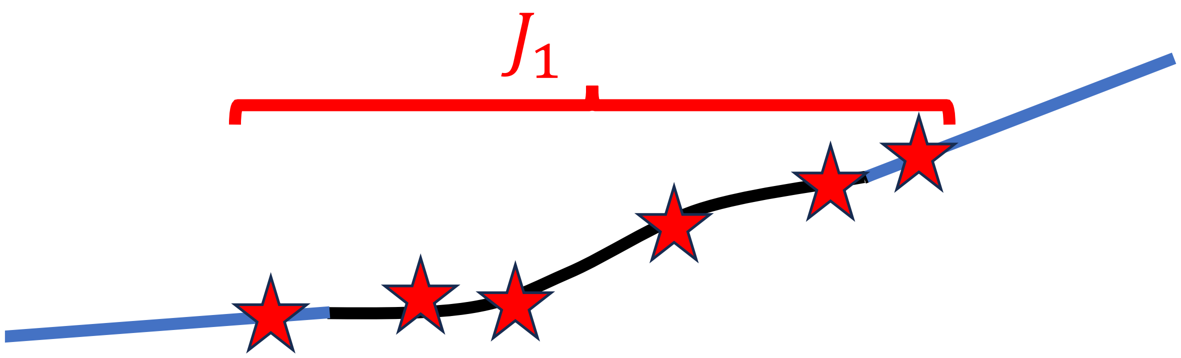


Lemma $\Rightarrow \exists$ subinterval $J_1 \subset (0,1), n_1 \in \mathbb{N}$ such that, when given input $F_1$, $\Gamma_{n_1}$ only samples from $J_1$ and $\sup\{|z| : z \in \Gamma_{n_1}(F_1)\} \le (1+\tau)\alpha_1^{1/2-r}$

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

# Proof idea

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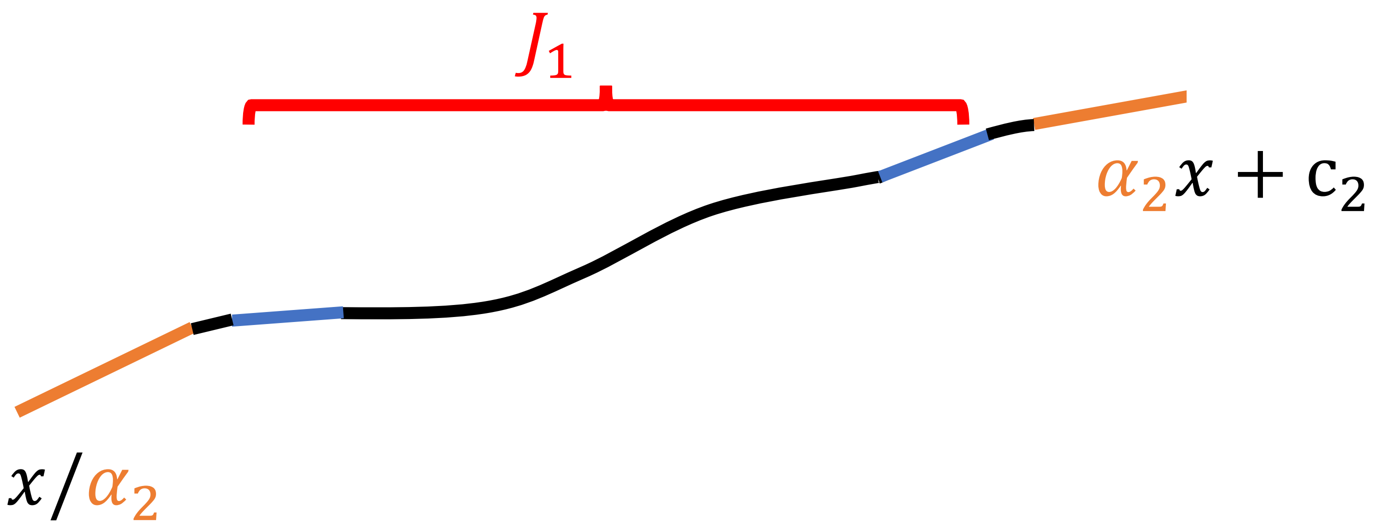
Pick $\alpha_1, \alpha_2 \in (0,1)$ and $\tau > 0$ with $(1+2\tau)\alpha_1^{1/2-r} < (1-2\tau)\alpha_2^{-1/2}$

$F_2$:

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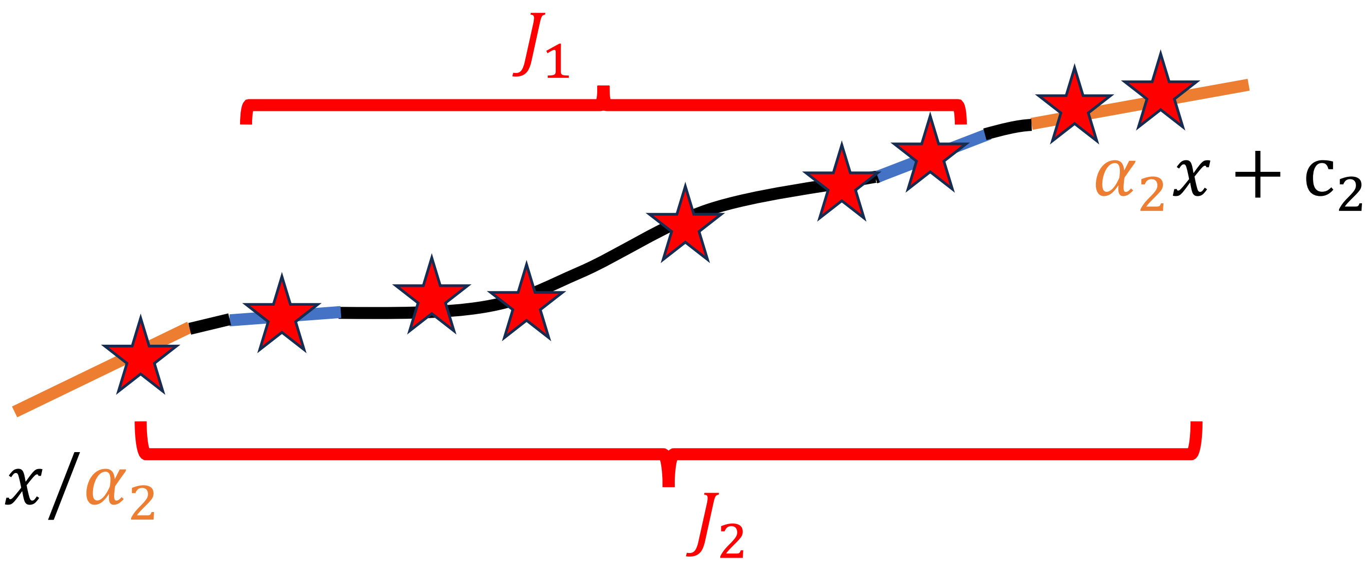


Lemma ⇒ ∃ subinterval $J_2 \subset (0,1)$, $n_2 \in \mathbb{N}$ such that, when given input $F_2$, $\Gamma_{n_2}$ only samples from $J_2$ and $\sup\{|z| : z \in \Gamma_{n_2}(F_2)\} \ge (1-\tau)\alpha_2^{-1/2}$

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# Proof idea

$$\boxed{\alpha^{-1/2} \leq \sup\{|z| : z \in \mathrm{Sp}_{\mathrm{ap}}(\mathcal{K}_F^*)\} \leq \alpha^{1/2-r}}$$

Suppose $\{\Gamma_n\}$ converges.

Pick $\alpha_1, \alpha_2 \in (0,1)$ and $\tau > 0$ with $(1+2\tau)\alpha_1^{1/2-r} < (1-2\tau)\alpha_2^{-1/2}$

Inductively:

$$\sup\{|z| : z \in \Gamma_{n_k}(F_k)\} \begin{cases} \leq (1+\tau)\alpha_1^{1/2-r}, & k \text{ odd} \\ \geq (1-\tau)\alpha_2^{-1/2}, & k \text{ even} \end{cases}$$

$F = \lim_{k\to\infty} F_k$ , data consistency implies $\Gamma_{n_k}(F) = \Gamma_{n_k}(F_k)$.

$\therefore \Gamma_n(F)$ cannot converge, contradiction!

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

# Classifications: *Solvability Complexity Index (SCI)*

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

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

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

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- C., Hansen, "*The foundations of spectral computations via the solvability complexity index hierarchy,*" **J. Eur. Math. Soc.**, 2022.
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verification

trust output

covers spectrum


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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** | | | |
|---|---|---|---|---|---|
| | | *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]<br>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)<br>$\mathrm{SCI} \leq 1$ (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. $+\ \omega$ 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 $\nabla F$<br>(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,…

# Optimal algorithms and classifications of systems

increasing difficulty

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

$$\begin{tikzcd}
 & \Pi_1 \arrow[dr, phantom, sloped, "\subsetneq"] & & \Pi_2 \arrow[dr, phantom, sloped, "\subsetneq"] & & \Pi_3 \arrow[r, phantom, "\cdots"] & \\
\Delta_1 \arrow[ur, phantom, sloped, "\subsetneq"] \arrow[dr, phantom, sloped, "\subsetneq"] \arrow[r, phantom, "\subsetneq"] & \Sigma_1 \cup \Pi_1 \arrow[r, phantom, "\subsetneq"] & \Delta_2 \arrow[ur, phantom, sloped, "\subsetneq"] \arrow[dr, phantom, sloped, "\subsetneq"] \arrow[r, phantom, "\subsetneq"] & \Sigma_2 \cup \Pi_2 \arrow[r, phantom, "\subsetneq"] & \Delta_3 \arrow[ur, phantom, sloped, "\subsetneq"] \arrow[dr, phantom, sloped, "\subsetneq"] \arrow[r, phantom, "\subsetneq"] & \Sigma_3 \cup \Pi_3 \arrow[r, phantom, "\cdots"] & {} \\
 & \Sigma_1 \arrow[ur, phantom, sloped, "\subsetneq"] & & \Sigma_2 \arrow[ur, phantom, sloped, "\subsetneq"] & & \Sigma_3 \arrow[r, phantom, "\cdots"] & 
\end{tikzcd}$$

# Optimal algorithms and classifications of systems

$\varepsilon = 0$

increasing difficulty

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

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

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

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

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

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

$$
\begin{array}{ccccccccccccccc}
 & & \Pi_1 & & & & & & \Pi_2 & & & & & \Pi_3 & \\
 & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & & \rotatebox{45}{$\subsetneq$} & & \iddots \\
\Delta_1 & \subsetneq & \Sigma_1 \cup \Pi_1 & \subsetneq & \Delta_2 & \subsetneq & & \Sigma_2 \cup \Pi_2 & & \subsetneq & \Delta_3 & \subsetneq & \Sigma_3 \cup \Pi_3 & \cdots & \\
 & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & & \rotatebox{-45}{$\subsetneq$} & & \ddots \\
 & & \Sigma_1 & & & & & & \Sigma_2 & & & & & \Sigma_3 &
\end{array}
$$

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 & & \Pi_1 & & & & & & \Pi_2 & & & & & \Pi_3 & \\
 & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & & \rotatebox{45}{$\subsetneq$} & & \cdots \\
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\end{array}$$

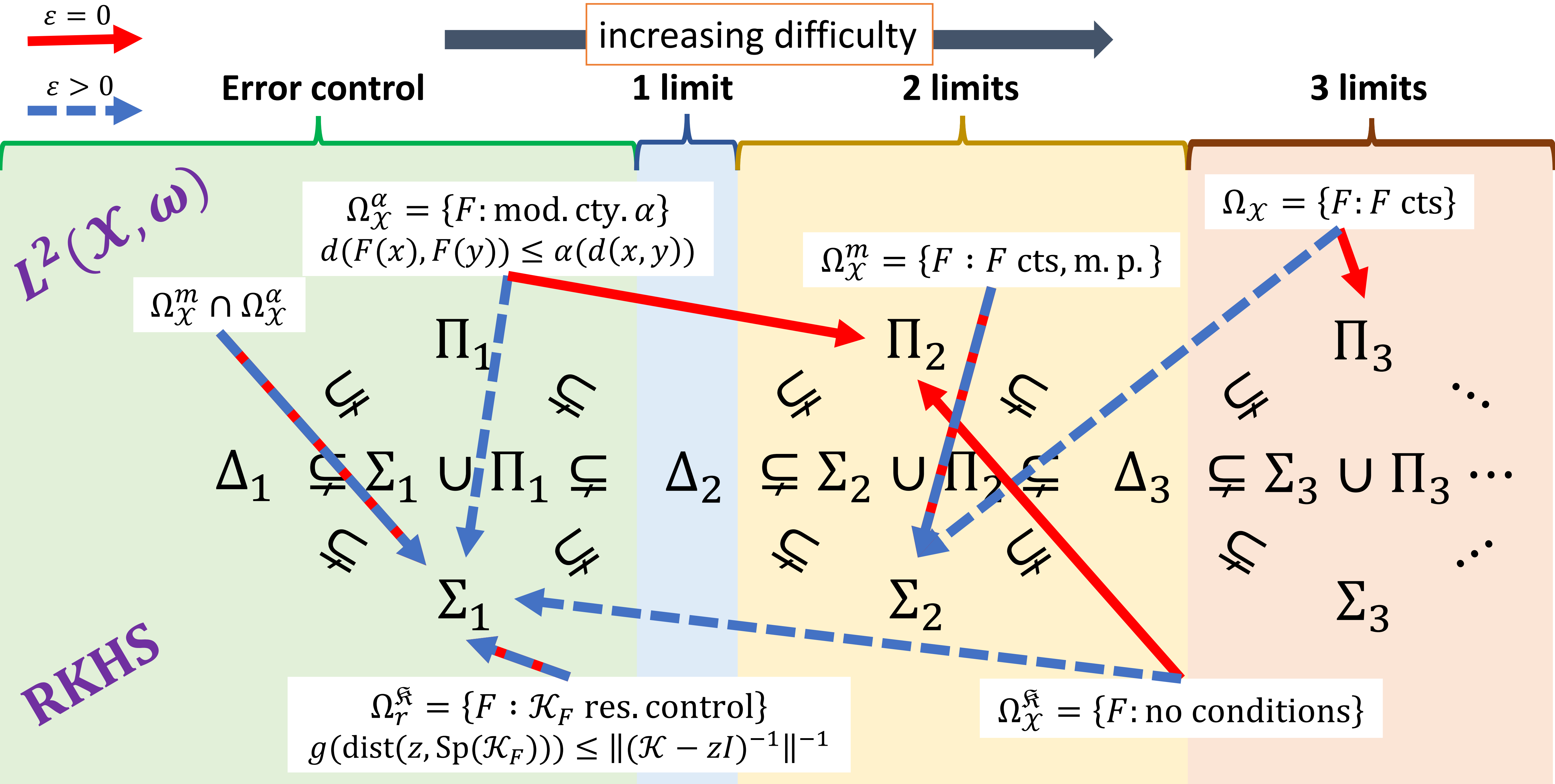
**RKHS**

$\Omega_{r}^{\mathfrak{K}} = \{F : \mathcal{K}_F \text{ res. control}\}$

$g(\mathrm{dist}(z, \mathrm{Sp}(\mathcal{K}_F))) \leq \|(\mathcal{K} - zI)^{-1}\|^{-1}$

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

# Optimal algorithms and classifications of systems



# Conclusion: FOUNDATIONS $\longleftrightarrow$ METHODS

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

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

$\boxed{\mathcal{K}^*\mathfrak{K}_x = \mathfrak{K}_{F(x)}}$ *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).*

# Shameless final plug...

Upcoming book with CUP:

**INFINITE-DIMENSIONAL SPECTRAL COMPUTATIONS**

**Foundations, Algorithms, and Modern Applications**

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

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

Contents

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

# SpecRKHS: Verifying eigenpairs

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

Algorithm 1 (can be combined with kernel singular value decomp.):

1. Compute $G, A, R \in \mathbb{C}^{N\times N}$ and eigendecomposition $AV = GV\Lambda$.
2. For each eigenpair $(\lambda, \mathbf{v})$, compute $\text{res}^*(\lambda, \mathbf{v})$.
3. **Output:** subset of e-vectors $V_{(\varepsilon)}$ & e-vals $\Lambda_{(\varepsilon)}$ with $\text{res}^*(\lambda,\mathbf{v}) \leq \varepsilon$ ($\varepsilon$ = input tol).

**Theorem (coherency within tol):** $\limsup_{N\to\infty} \max_{\lambda\in\Lambda_{(\varepsilon)}} \|(\mathcal{K}^* - \lambda I)^{-1}\|^{-1} \leq \varepsilon$

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

# SpecRKHS: Verifying eigenpairs

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**BUT:** Evals may not approximate all of spectrum (e.g., shift example).

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