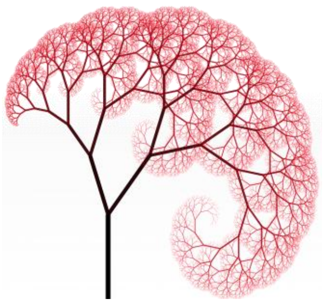
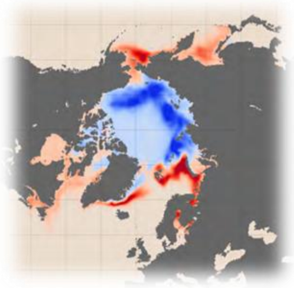
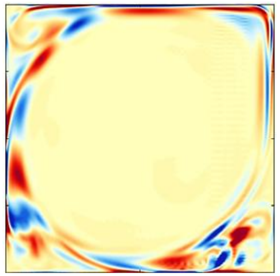





Spectral Computations in Infinite Dimensions: *Classifications and Applications*

Matthew Colbrook
University of Cambridge

19/02/2025

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

For papers and talk slides/videos, visit:
http://www.damtp.cam.ac.uk/user/mjc249/home.html

Outline

- Solvability Complexity Index Hierarchy and spectral problems.
- Example: Spectra with error control.
- Example: Adversaries and data-driven dynamical systems.
- Concluding remarks

Broad goal: classify difficulty of problems, prove optimality of algorithms, figure out what can and cannot be done computationally.

Classical infinite-dimensional spectral problem

$$A \text{"="} \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \qquad A\left(\sum_{k=1}^{\infty} x_k e_k\right) = \sum_{j=1}^{\infty}\left(\sum_{k=1}^{\infty} a_{jk} x_k\right) e_j$$

Canonical basis vectors of $l^2(\mathbb{N})$

Also deal with PDEs, integral operators etc.

Finite-dimensional	$\Longrightarrow$	**Infinite-dimensional**
Eigenvalues of $B \in \mathbb{C}^{n\times n}$	$\Longrightarrow$	Spectrum, $\mathrm{Sp}(A)$
$\{\lambda_j \in \mathbb{C}: \det(B-\lambda_j I)=0\}$	$\Longrightarrow$	$\{\lambda \in \mathbb{C}: A-\lambda I \text{ is not invertible}\}$

Classical infinite-dimensional spectral problem

$$A \text{"="} \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \qquad A\left(\sum_{k=1}^{\infty} x_k e_k\right) = \sum_{j=1}^{\infty}\left(\sum_{k=1}^{\infty} a_{jk} x_k\right) e_j$$

Canonical basis vectors of $l^2(\mathbb{N})$

Also deal with PDEs, integral operators etc.

Finite-dimensional	$\Longrightarrow$	**Infinite-dimensional**
Eigenvalues of $B \in \mathbb{C}^{n\times n}$	$\Longrightarrow$	Spectrum, $\mathrm{Sp}(A)$
$\{\lambda_j \in \mathbb{C}: \det(B - \lambda_j I) = 0\}$	$\Longrightarrow$	$\{\lambda \in \mathbb{C}: A - \lambda I \text{ is not invertible}\}$

*"Most operators that arise in practice are not presented in a representation in which they are diagonalized, and it is often very hard to locate even a single point in the spectrum. Thus, one often has to settle for numerical approximations. Unfortunately, there is a dearth of literature on this basic problem and, so far as we have been able to tell, **there are no proven [general] techniques**."* W. Arveson, Berkeley (1994)

What can go wrong?

Typical approach:

- **Matrix case ($l^2(\mathbb{N})$):** truncate to $\mathcal{P}_n A \mathcal{P}_n^* \in \mathbb{C}^{n\times n}$.
- **PDE on unbounded domain:** truncate domain then discretise.

two sources of error

Some key issues:

- Spectral pollution (evals accumulate at points not in $\mathrm{Sp}(A)$ as $n \to \infty$)
- Spectral invisibility.
- Dealing with essential spectra and continuous spectra.
- Stability, non-normality etc.
- Verification – can we compute spectral properties with error bounds?

Motivation

- **Applications:** Quantum mechanics, structural mechanics, optics, acoustics, statistical physics, number theory, matter physics, PDEs, data analysis, neural networks and AI, nuclear scattering, optics, computational chemistry, …
- **Specific open problems**, e.g., computational quantum mechanics (Schwinger 1960), (Digernes, Varadarajan, Varadhan, 1994):

> Given a self-adjoint Schrödinger operator $-\Delta + V$ on $\mathbb{R}$,
> can we approximate its spectrum from sampling V?

- **Verified computations:** Many **computer-assisted proofs** involve spectra. E.g., $E(Z) =$ ground state energy of $H = \sum_{k=1}^{N}\left(-\Delta_{x_k} - Z|x_k|^{-1}\right) + \sum_{j\leq k}\left|x_j - x_k\right|^{-1}$.

  Dirac-Schwinger conjecture: asymptotics of $E(Z)$ (Fefferman, Seco 1996)
- **Foundations:** What is computationally possible? Beyond spectra etc.

Not all spectral problems are equally hard …

Warm-up: bounded diagonal operators

$$A = \begin{pmatrix} a_1 & & \\ & a_2 & \\ & & \ddots \end{pmatrix}$$

Assumption: Algorithm can query entries of A

Algorithm: $\Gamma_n(A) = \{a_1, a_2, \ldots, a_n\} \to \mathrm{Sp}(A) = \overline{\{a_1, a_2, \ldots\}}$ in Haus. Metric.

One-sided error control: $\Gamma_n(A) \subset \mathrm{Sp}(A)$

$$d_{\mathrm{H}}(X, Y) = \max\left\{\sup_{x\in X} d(x, Y), \sup_{y\in Y} d(y, X)\right\}$$

Optimal: Can't obtain $\hat{\Gamma}_n(A) \to \mathrm{Sp}(A)$ with $\mathrm{Sp}(A) \subset \hat{\Gamma}_n(A)$.

Warm-up: compact self-adjoint operators

classic method
"finite section"

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Algorithm: $\Gamma_n(A) = \mathrm{Sp}(\mathcal{P}_n A \mathcal{P}_n^*)$ converges to $\mathrm{Sp}(A)$ in Haus. Metric.

Question: Can we verify the output?

i.e., Does there exist some alg. $\hat{\Gamma}_n(A) \to \mathrm{Sp}(A)$ with $\hat{\Gamma}_n(A) \subset \mathrm{Sp}(A) + B_{2^{-n}}$?

Warm-up: compact self-adjoint operators

classic method
"finite section"

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Algorithm: $\Gamma_n(A) = \mathrm{Sp}(\mathcal{P}_n A \mathcal{P}_n^*)$ converges to $\mathrm{Sp}(A)$ in Haus. Metric.

Question: Can we verify the output?

i.e., Does there exist some alg. $\hat{\Gamma}_n(A) \to \mathrm{Sp}(A)$ with $\hat{\Gamma}_n(A) \subset \mathrm{Sp}(A) + B_{2^{-n}}$?

Answer: No algorithm can do this on whole class!

What about Jacobi operators?

$$A = \begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & b_2 & a_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix}, \qquad b_k > 0, \qquad a_k \in \mathbb{R}$$

Non-trivial, e.g., spurious eigenvalues.

What about Jacobi operators?

$$A = \begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & b_2 & a_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix}, \qquad b_k > 0, \qquad a_k \in \mathbb{R}$$

Non-trivial, e.g., spurious eigenvalues.

Sparse: finitely many non-zeros in each column

Enlarge class to **sparse normal operators** - surely now much harder?!

What about Jacobi operators?

$$A = \begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & b_2 & a_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix}, \qquad b_k > 0, \qquad a_k \in \mathbb{R}$$

Non-trivial, e.g., spurious eigenvalues.

Sparse: finitely many non-zeros in each column

Enlarge class to **sparse normal operators** - surely now much harder?!

Answer: $\exists\{\Gamma_n\}$ s.t. $\lim_{n\to\infty} \Gamma_n(A) = \mathrm{Sp}(A)$ and $\Gamma_n(A) \subset \mathrm{Sp}(A) + B_{2^{-n}}$,

for any sparse normal operator A

- C., Roman, Hansen, "How to compute spectra with error control," **Phys. Rev. Lett.**,2019.

A curious case of limits

General bounded: $A = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$

Algorithm: $\exists\{\Gamma_{n_3,n_2,n_1}\}$ s.t. $\lim_{n_3\to\infty}\lim_{n_2\to\infty}\lim_{n_1\to\infty}\Gamma_{n_3,n_2,n_1}(A) = \mathrm{Sp}(A)$

Question: Can we do better?

• Hansen, *"On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators,"* **J. Amer. Math. Soc.**, 2011.

A curious case of limits

General bounded: $A = \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$

Algorithm: $\exists\{\Gamma_{n_3,n_2,n_1}\}$ s.t. $\lim_{n_3\to\infty}\lim_{n_2\to\infty}\lim_{n_1\to\infty}\Gamma_{n_3,n_2,n_1}(A) = \mathrm{Sp}(A)$

Question: Can we do better?

Answer: No! Canonically embed problems such as:

Explains Arveson's lament!

Given $B \in \{0,1\}^{\mathbb{N}\times\mathbb{N}}$, does B have a column with infinitely many 1's?

$\Longrightarrow$ lower bound on number of "successive limits" needed (indep. of comp. model).

- Hansen, *"On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators,"* **J. Amer. Math. Soc.**, 2011.
- C., *"On the computation of geometric features of spectra of linear operators on Hilbert spaces,"* **Found. Comput. Math.**, 2022.

General algorithm: beyond recursion theory

Computational problem:

- Class of objects Ω (e.g., operators).
- Metric space $(\mathcal{M}, d)$ (e.g., Hausdorff metric).
- Thing we want to compute $\Xi: \Omega \to \mathcal{M}$.
- Info we can access, Λ a set of functions $\Omega \to \mathbb{C}$ (e.g., matrix entries).

General algorithm: map $\Gamma: \Omega \to \mathcal{M}$ such that for any $A \in \Omega$, $\exists$ a finite non-empty subset $\Lambda_\Gamma(A) \subseteq \Lambda$ such that

$$B \in \Omega, f(B) = f(A) \;\; \forall f \in \Lambda_\Gamma(A) \Rightarrow \Lambda_\Gamma(A) = \Lambda_\Gamma(B), \Gamma(A) = \Gamma(B)$$

A lower bound for general algorithms holds in **ALL** models of computation.

Solvability Complexity Index Hierarchy

- Δ_0: Solved in finite time (v. rare for cts problems).
- Δ_1: Solved in "one limit" with full error control:

$$d(\Gamma_n(A), \Xi(A)) \leq 2^{-n}$$

- Δ_2: Solved in "one limit":

$$\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$$

- Δ_3: Solved in "two successive limits":

$$\lim_{n\to\infty} \lim_{m\to\infty} \Gamma_{n,m}(A) = \Xi(A)$$

⋮

Can work in *any* model. E.g., BSS machine, Turing machine, interval arithmetic, inexact input etc.

- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "*On the solvability complexity index hierarchy and towers of algorithms,*" preprint.
- Hansen, "*On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators,*" **J. Amer. Math. Soc.**, 2011.

Solvability Complexity Index Hierarchy

- Δ_0: Solved in finite time (v. rare for cts problems).
- Δ_1: Solved in "one limit" with full error control:

$$d(\Gamma_n(A), \Xi(A)) \leq 2^{-n}$$

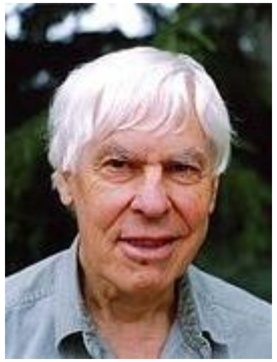
- Δ_2: Solved in "one limit":

$$\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$$

- Δ_3: Solved in "two successive limits":

$$\lim_{n\to\infty} \lim_{m\to\infty} \Gamma_{n,m}(A) = \Xi(A)$$

⋮



Steve Smale: *"Is there any purely [rational] iterative generally convergent algorithm for polynomial zero finding?"*

Curt McMullen: *"Yes, if the degree is three; no, if the degree is higher."*

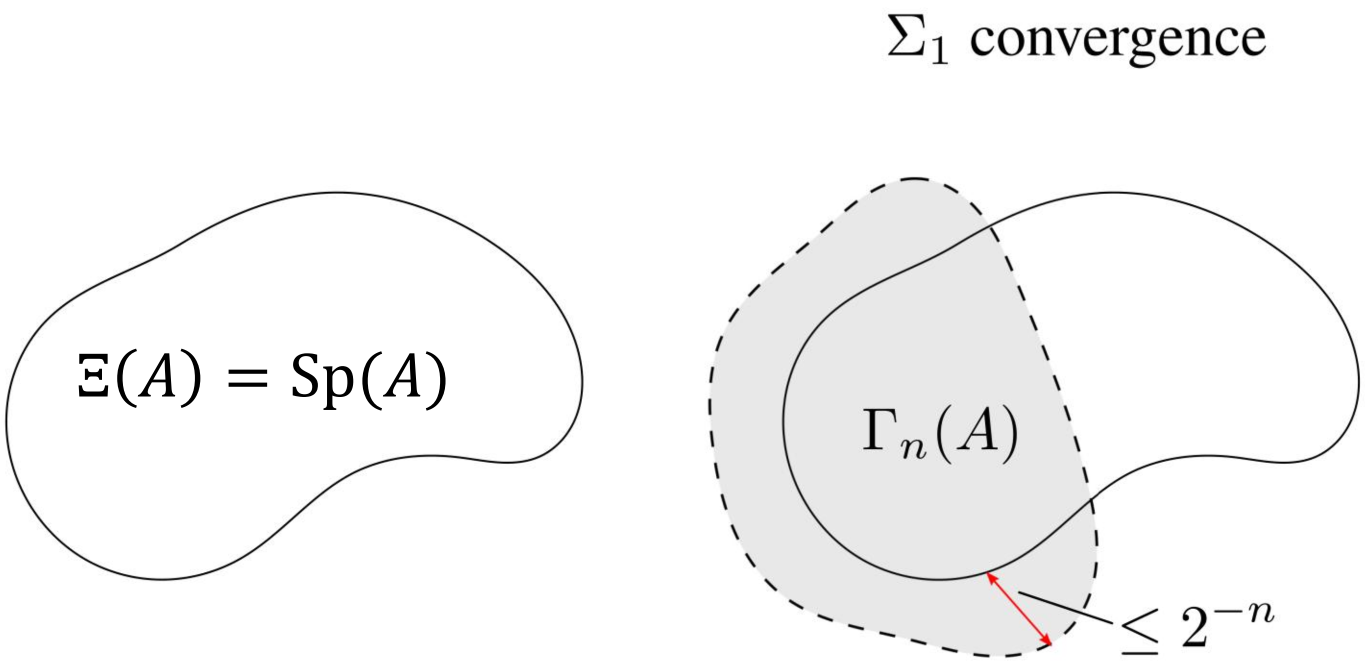
Peter Doyle & Curt McMullen: *"The problem can be solved using successive limits for the quartic and quintic, but not the sextic."*

Can work in *any* model. E.g., BSS machine, Turing machine, interval arithmetic, inexact input etc.

- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, *"On the solvability complexity index hierarchy and towers of algorithms,"* preprint.
- Hansen, *"On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators,"* **J. Amer. Math. Soc.**, 2011.
- McMullen, *"Families of rational maps and iterative root-finding algorithms,"* **Ann. of Math.**, 1987.
- Doyle, McMullen, *"Solving the quintic by iteration,"* **Acta Math.**, 1989.
- Smale, *"The fundamental theorem of algebra and complexity theory,"* **Bull. Amer. Math. Soc.**, 1981.

Error control for spectral problems

$$d_{\mathrm{H}}(X,Y) = \max\left\{\sup_{x\in X} d(x,Y), \sup_{y\in Y} d(y,X)\right\}$$

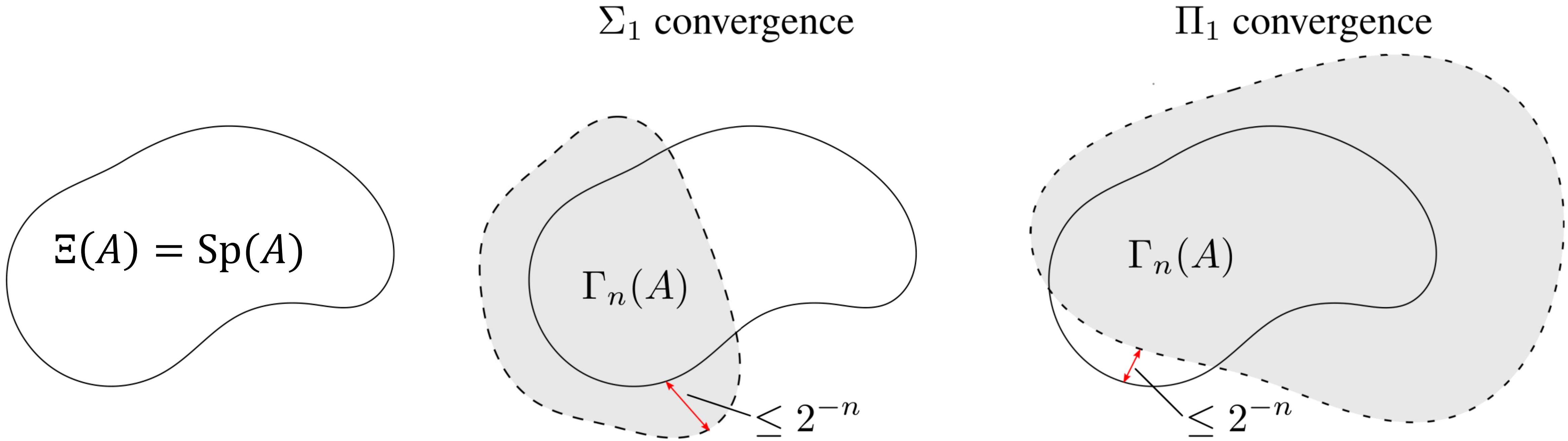


- Σ_1: $\exists$ alg. $\{\Gamma_n\}$ s.t. $\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$, $\max_{z\in\Gamma_n(A)} \mathrm{dist}\big(z, \Xi(A)\big) \leq 2^{-n}$

- C., *"The foundations of infinite-dimensional spectral computations,"* **PhD diss., University of Cambridge**, 2020.

Error control for spectral problems

$$d_{\mathrm{H}}(X,Y) = \max\left\{\sup_{x\in X} d(x,Y), \sup_{y\in Y} d(y,X)\right\}$$



- Σ_1: $\exists$ alg. $\{\Gamma_n\}$ s.t. $\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$, $\max_{z\in\Gamma_n(A)} \mathrm{dist}\big(z, \Xi(A)\big) \leq 2^{-n}$
- Π_1: $\exists$ alg. $\{\Gamma_n\}$ s.t. $\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$, $\max_{z\in\Xi(A)} \mathrm{dist}(z, \Gamma_n(A)) \leq 2^{-n}$

Such problems can be used in a proof!

- C., *"The foundations of infinite-dimensional spectral computations,"* **PhD diss., University of Cambridge**, 2020.

Sampler of results for bounded op. on $l^2(\mathbb{N})$

increasing difficulty →

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

$\Pi_0 = \Delta_0 = \Sigma_0$

$$\Delta_0 \subsetneq \Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

$\Delta_1 \subsetneq \Pi_1 \subsetneq \Delta_2$, $\Delta_1 \subsetneq \Sigma_1 \subsetneq \Delta_2$

$\Delta_2 \subsetneq \Pi_2 \subsetneq \Delta_3$, $\Delta_2 \subsetneq \Sigma_2 \subsetneq \Delta_3$

$\Delta_3 \subsetneq \Pi_3 \cdots$, $\Delta_3 \subsetneq \Sigma_3 \cdots$

Sampler of results for bounded op. on $l^2(\mathbb{N})$

increasing difficulty →

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

Compact operators → Δ_2

$$\Pi_0 = \Delta_0 = \Sigma_0 \subsetneq \Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

$$\Delta_1 \subsetneq \Pi_1 \subsetneq \Delta_2, \quad \Delta_1 \subsetneq \Sigma_1 \subsetneq \Delta_2$$

$$\Delta_2 \subsetneq \Pi_2 \subsetneq \Delta_3, \quad \Delta_2 \subsetneq \Sigma_2 \subsetneq \Delta_3$$

$$\Delta_3 \subsetneq \Pi_3 \cdots, \quad \Delta_3 \subsetneq \Sigma_3 \cdots$$

Sampler of results for bounded op. on $l^2(\mathbb{N})$

increasing difficulty →

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

Compact operators

$$\Pi_0 \qquad \Pi_1 \qquad \Pi_2 \qquad \Pi_3$$

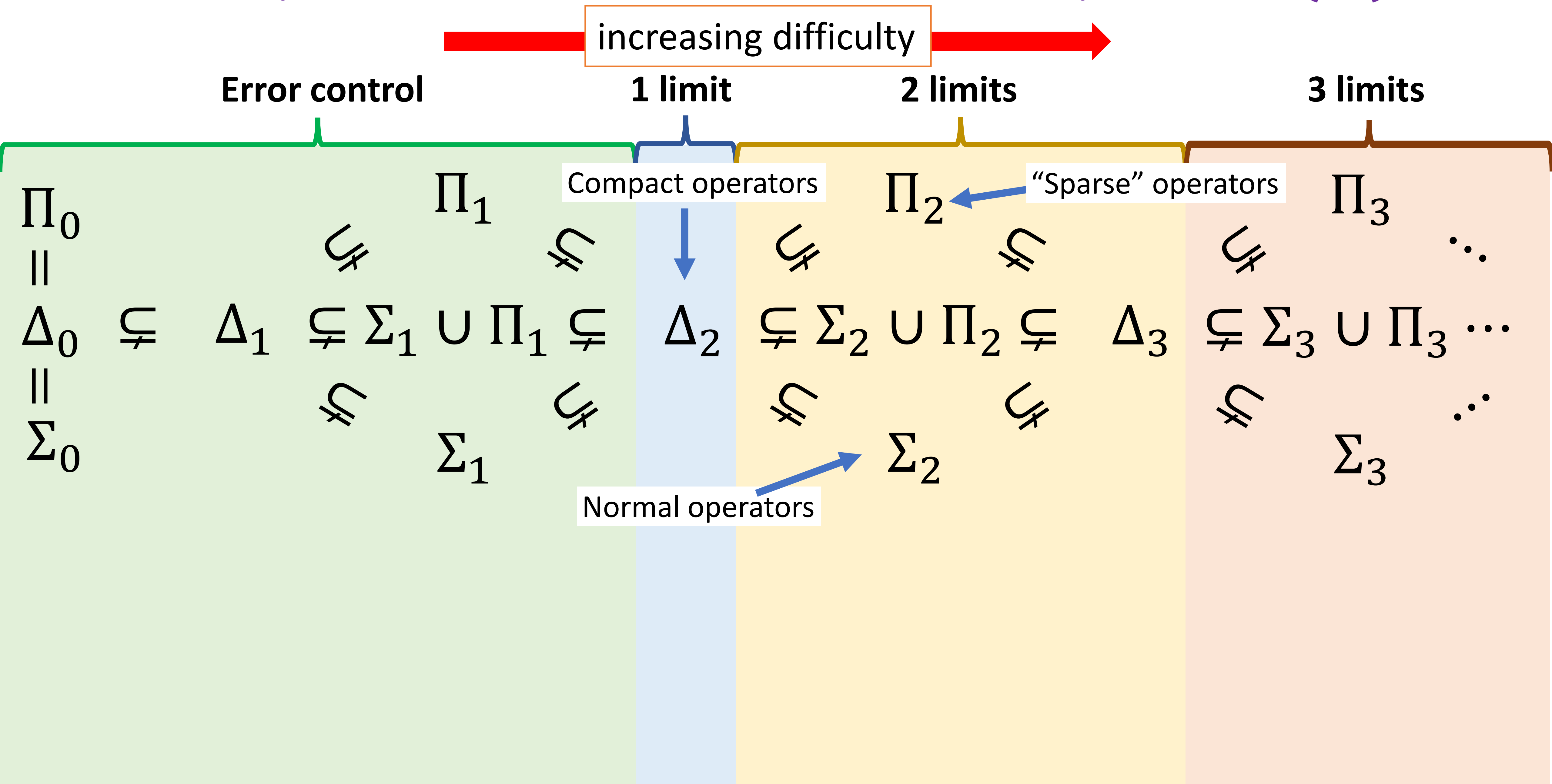
$$\Pi_0 = \Delta_0 = \Sigma_0$$

$$\Delta_0 \subsetneq \Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

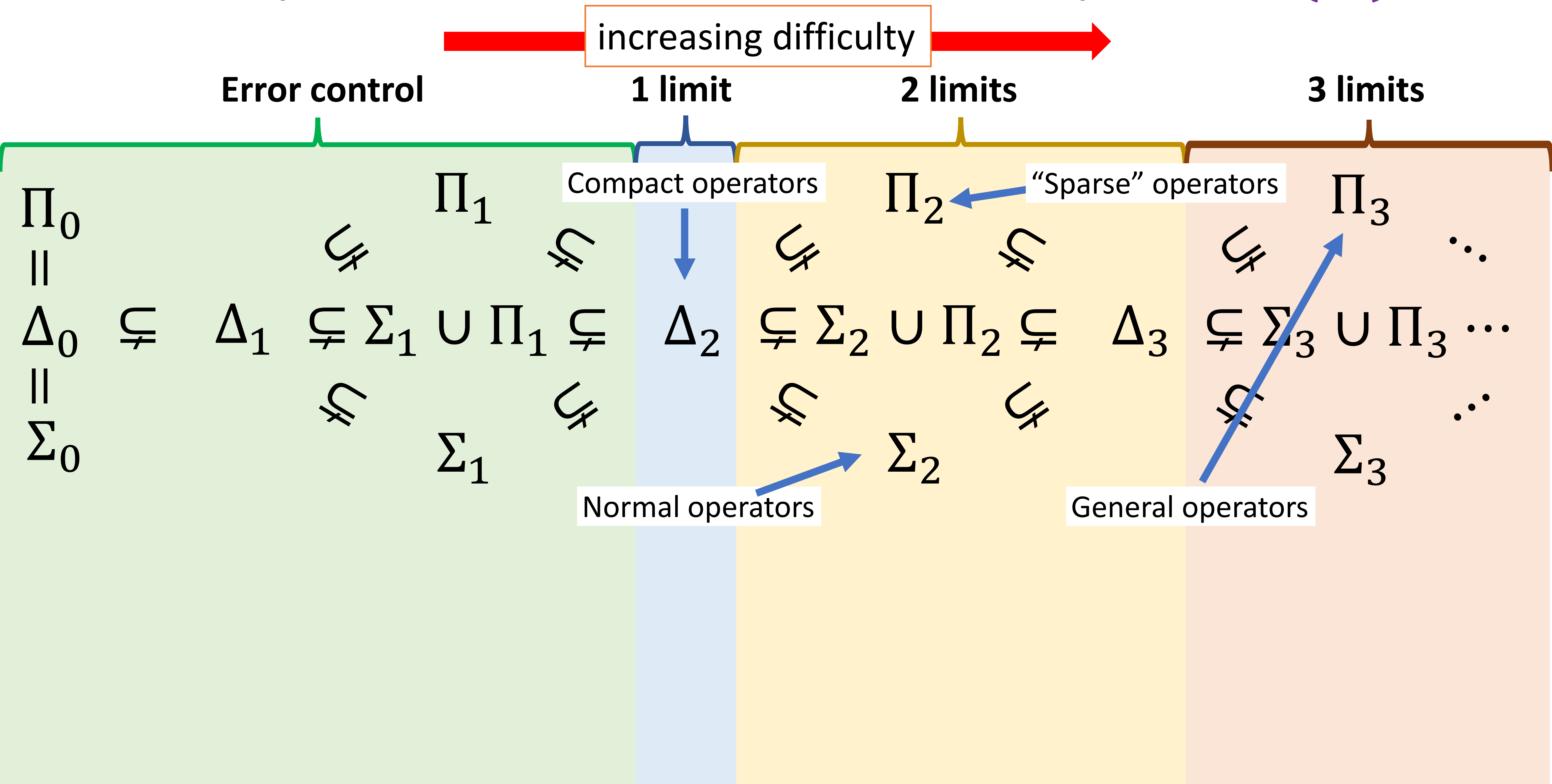
$$\Sigma_0 \qquad \Sigma_1 \qquad \Sigma_2 \qquad \Sigma_3$$

Normal operators

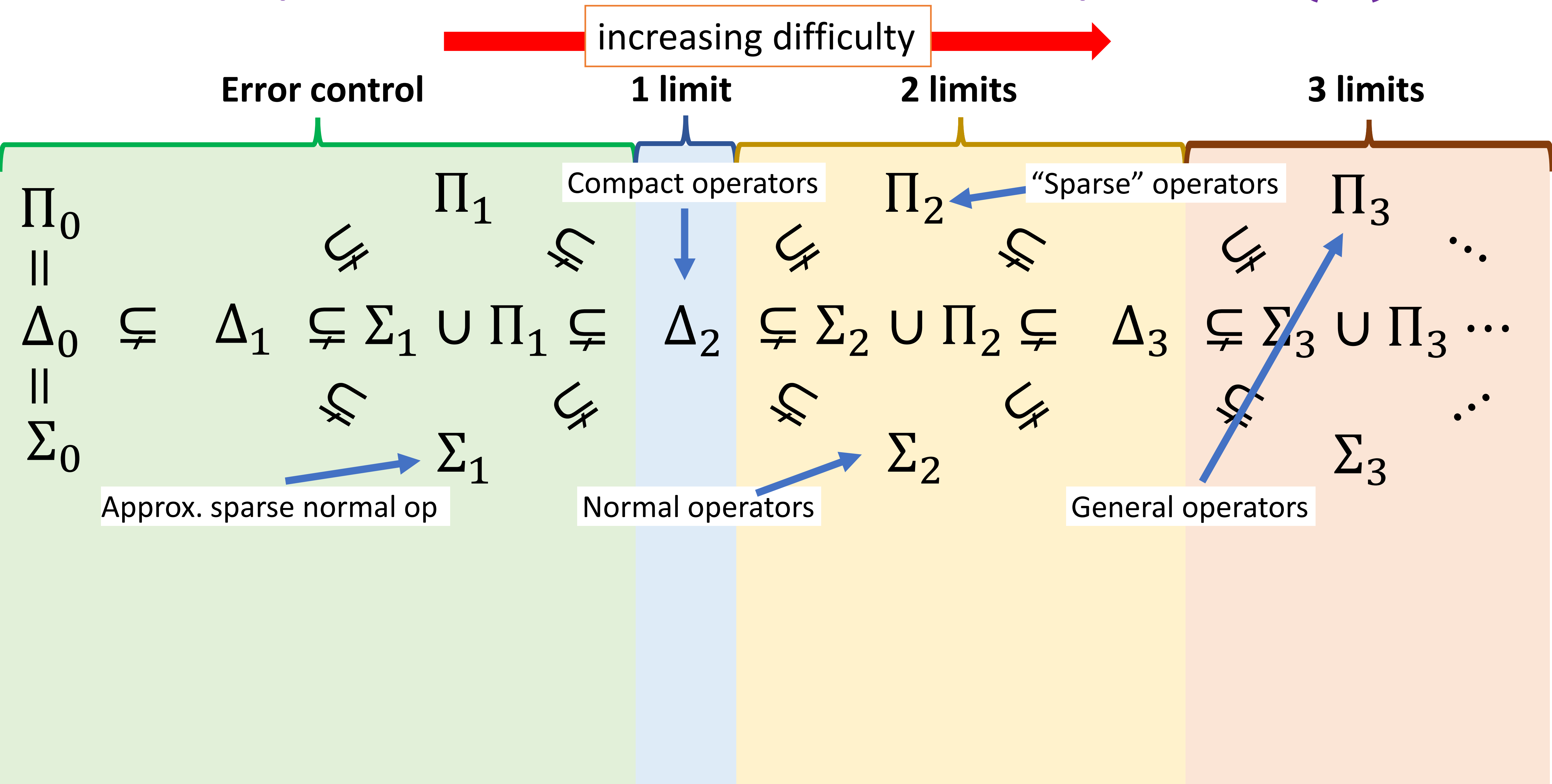
Sampler of results for bounded op. on $l^2(\mathbb{N})$



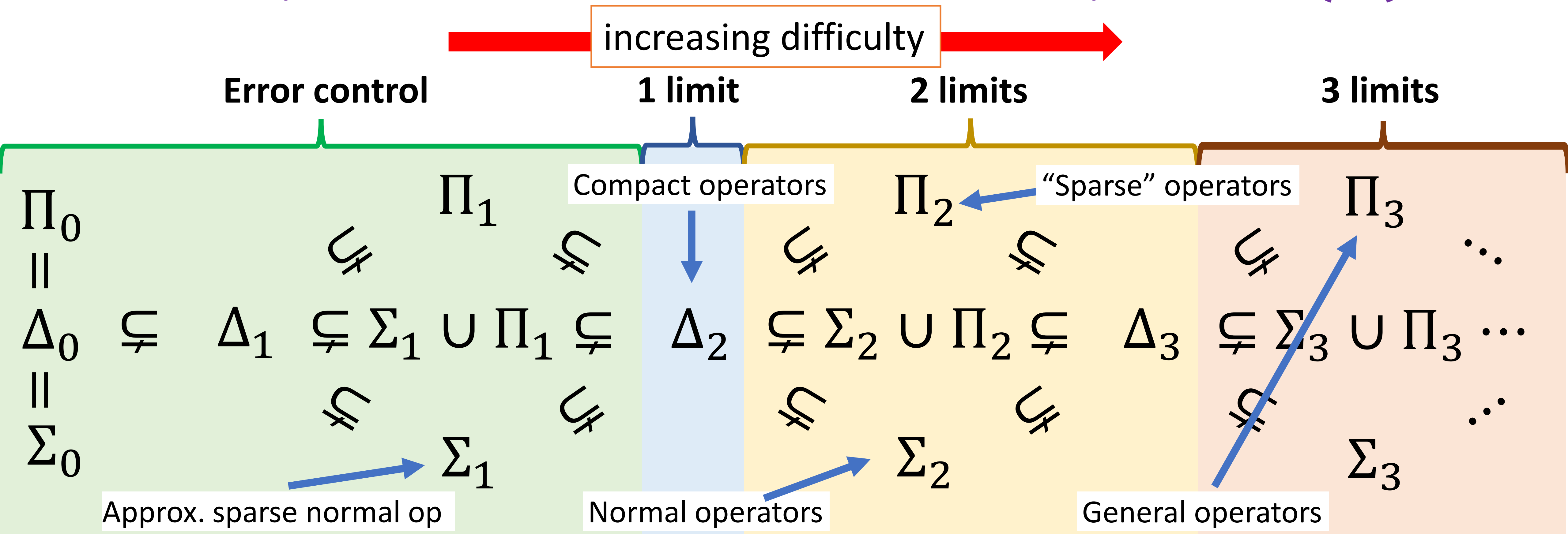
Sampler of results for bounded op. on $l^2(\mathbb{N})$



Sampler of results for bounded op. on $l^2(\mathbb{N})$



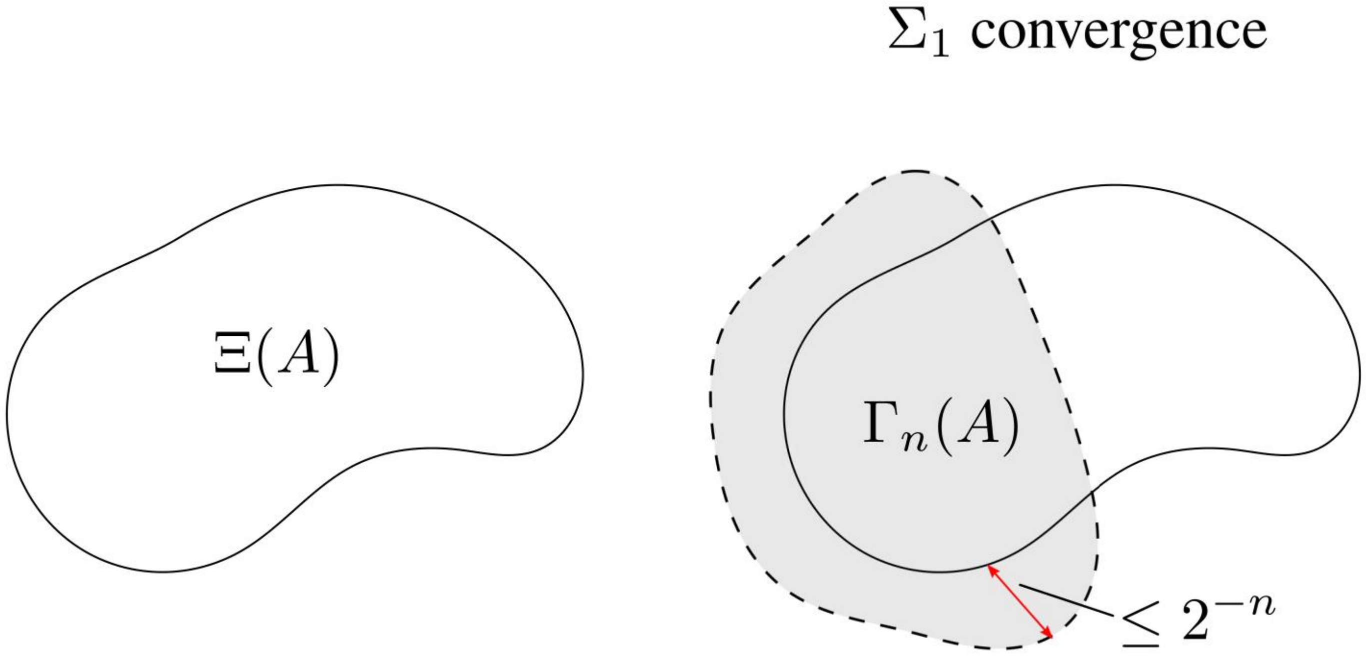
Sampler of results for bounded op. on $l^2(\mathbb{N})$



Zoo of problems: spectral type (pure point, absolutely continuous, singularly continuous), Lebesgue measure and fractal dimensions of spectra, discrete spectra, essential spectra, eigenspaces + multiplicity, spectral radii, essential numerical ranges, geometric features of spectrum (e.g., capacity), spectral gap problem, resonances ...

- C., *"The foundations of infinite-dimensional spectral computations,"* **PhD diss.**, University of Cambridge, 2020.
- C., *"On the computation of geometric features of spectra of linear operators on Hilbert spaces,"* **Found. Comput. Math.**, 2022.
- C., Hansen, *"The foundations of spectral computations via the solvability complexity index hierarchy,"* **J. Eur. Math. Soc.**, 2023.
- C., *"Computing spectral measures and spectral types,"* **Commun. Math. Phys.**, 2021.
- C., Horning, Townsend, *"Computing spectral measures of self-adjoint operators,"* **SIAM Rev.**, 2021.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, *"On the solvability complexity index hierarchy and towers of algorithms,"* preprint.

Example 1: Σ_1 algorithm for spectra



Two reasons its hard!

$$A = \bigoplus_{r=1}^{\infty} J_{l_r}, \qquad J_{l_r} = \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in \mathbb{C}^{l_r \times l_r}$$

Instability

$$\mathrm{Sp}(A) = \begin{cases} \{0\}, & \sup l_r < \infty \\ \{z : |z| \leq 1\}, & \text{otherwise} \end{cases}$$

No algorithm when given $\{l_r\}_{r=1}^{\infty}$ can determine if it is bounded.

$\Longrightarrow$ No algorithm computes spectra of gen. tridiagonal operators.

Two reasons its hard!

$$A = \bigoplus_{r=1}^{\infty} J_{l_r}, \qquad J_{l_r} = \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in \mathbb{C}^{l_r \times l_r}$$

Instability

$$\mathrm{Sp}(A) = \begin{cases} \{0\}, & \sup l_r < \infty \\ \{z : |z| \leq 1\}, & \text{otherwise} \end{cases}$$

No algorithm when given $\{l_r\}_{r=1}^{\infty}$ can determine if it is bounded.

$\Longrightarrow$ No algorithm computes spectra of gen. tridiagonal operators.

Always have:

$$\|(A - z)^{-1}\|^{-1} \leq \mathrm{dist}(z, \mathrm{Sp}(A))$$

Two reasons its hard!

$$A = \bigoplus_{r=1}^{\infty} J_{l_r}, \qquad J_{l_r} = \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in \mathbb{C}^{l_r \times l_r}$$

Instability

$$\mathrm{Sp}(A) = \begin{cases} \{0\}, & \sup l_r < \infty \\ \{z : |z| \leq 1\}, & \text{otherwise} \end{cases}$$

No algorithm when given $\{l_r\}_{r=1}^{\infty}$ can determine if it is bounded.

$\Longrightarrow$ No algorithm computes spectra of gen. tridiagonal operators.

Always have:

$$\|(A-z)^{-1}\|^{-1} \leq \mathrm{dist}(z, \mathrm{Sp}(A))$$

Assume:

$$g(\mathrm{dist}(z, \mathrm{Sp}(A))) \leq \|(A-z)^{-1}\|^{-1}$$

known function

Two reasons its hard!

$$A = \bigoplus_{r=1}^{\infty} A_{l_r}, \qquad A_{l_r} = \begin{pmatrix} 1 & & & & 1 \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ 1 & & & & 1 \end{pmatrix} \in \mathbb{C}^{l_r \times l_r}$$

Info at ∞

$$\mathrm{Sp}(A) = \{0,2\}, \qquad \mathrm{Sp}\big(\mathrm{diag}(1,0,\ldots)\big) = \{0,1\}$$

More involved: choose $\{l_r\}_{r=1}^{\infty}$ to trick any supposed algorithm (try it!)

Two reasons its hard!

$$A = \bigoplus_{r=1}^{\infty} A_{l_r}, \qquad A_{l_r} = \begin{pmatrix} 1 & & & & 1 \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ 1 & & & & 1 \end{pmatrix} \in \mathbb{C}^{l_r \times l_r}$$

Info at ∞

$$\mathrm{Sp}(A) = \{0,2\}, \qquad \mathrm{Sp}\big(\mathrm{diag}(1,0,\dots)\big) = \{0,1\}$$

More involved: choose $\{l_r\}_{r=1}^{\infty}$ to trick any supposed algorithm (try it!)

Assume:

We have access (Λ) to inner products

$\langle Ae_j, e_i \rangle, \qquad \langle Ae_j, Ae_i \rangle, \qquad \langle A^*e_j, A^*e_i \rangle$

Sketch of method

$\mathcal{P}_n$ = orthog-projection onto span$\{e_1, \dots, e_n\}$
$\mathcal{P}_n : l^2(\mathbb{N}) \longrightarrow \mathbb{C}^n, \qquad \mathcal{P}_n^* : \mathbb{C}^n \longrightarrow l^2(\mathbb{N})$

Spectra through injection moduli (smallest singular value)

$$\sigma_{\inf}(T) = \inf\{\|Tv\| : v \in \mathfrak{D}(T), \|v\| = 1\}$$

$$\|(A - z)^{-1}\|^{-1} = \min\{\sigma_{\inf}(A - z), \sigma_{\inf}(A^* - \bar{z})\}$$

$$\sqrt{\sigma_{\inf}(\mathcal{P}_n(A - z)^*(A - z)\mathcal{P}_n^*)} = \sigma_{\inf}([A - z]\mathcal{P}_n^*) \downarrow \sigma_{\inf}(A - z)$$

$$g^{-1}\left(\sqrt{\sigma_{\inf}(\mathcal{P}_n[A - z]^*[A - z]\mathcal{P}_n^*)}\right) \downarrow g^{-1}(\|(A - z)^{-1}\|^{-1}) \geq \mathrm{dist}\big(z, \mathrm{Sp}(A)\big)$$

$$\|(A - z)^{-1}\|^{-1} \geq g(\mathrm{dist}(z, \mathrm{Sp}(A)))$$

Error control!

Final ingredient: adaptive search for local minimisers.

What did we do?

See conditions to make possible!

- **Lower bound:** embed a problem of known difficulty.

  Now have canonical ways to do this.

  Holds regardless of computational model.

- **Upper bound:** build an algorithm.

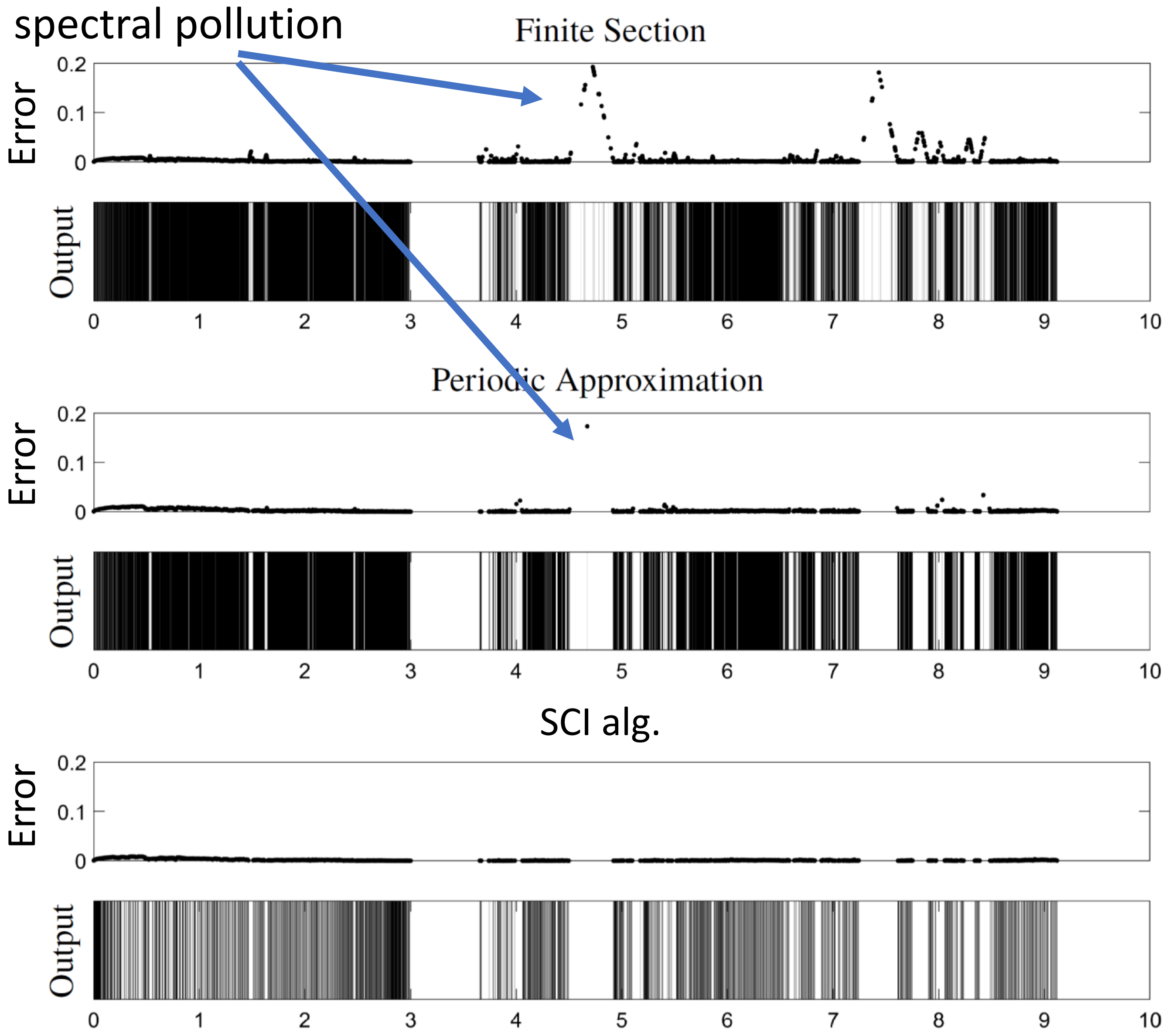
  Problem dependent.

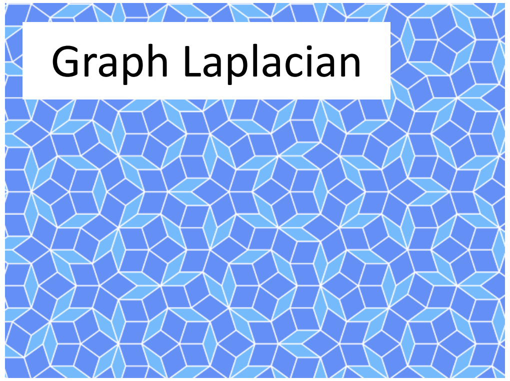
  Typically involves resolvent $(A-z)^{-1}$ for spectral problems.

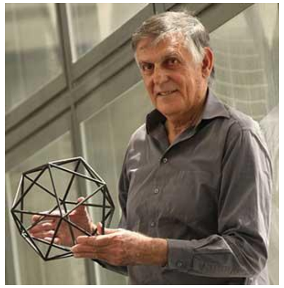
Often, infinite-dimensional solve-then-discretise needed

NB: One can show without g or $\langle Ae_j, Ae_i\rangle$, $\langle A^*e_j, A^*e_i\rangle$, $\mathrm{SCI} \geq 2$.

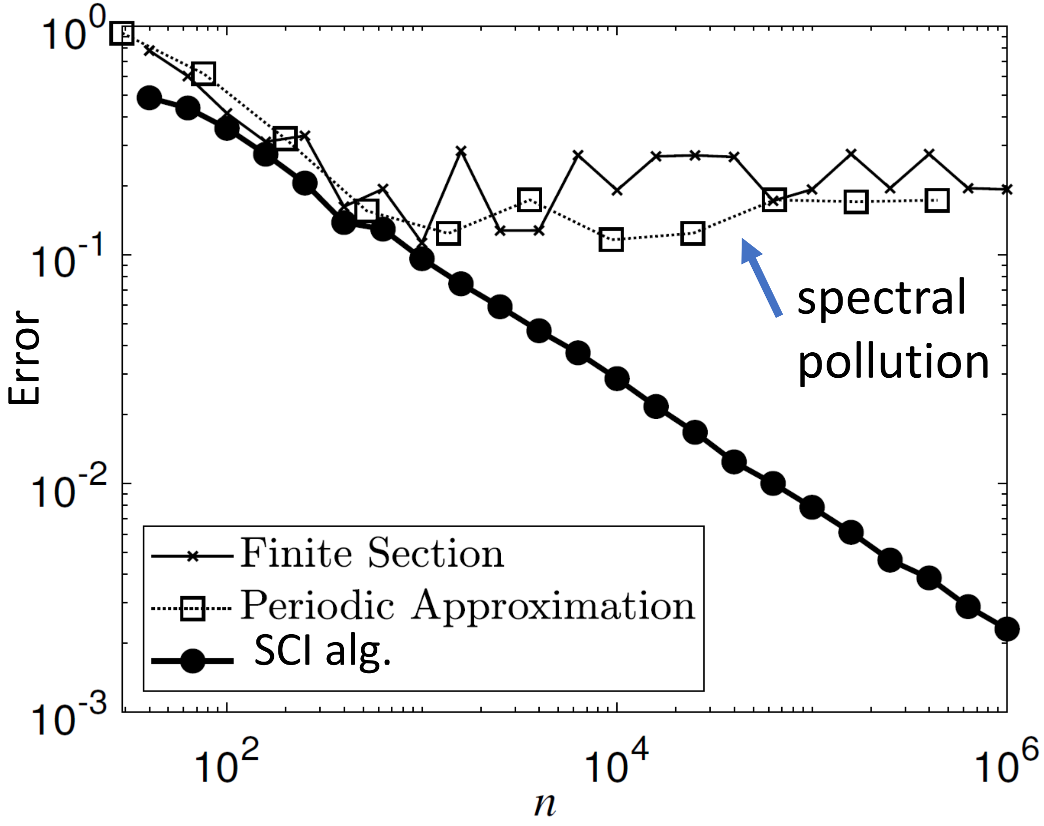
Example: Quasicrystal



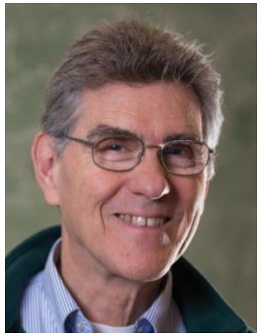




Dan Shechtman (Nobel Prize in Chemistry 2011.)



Example with non-trivial g

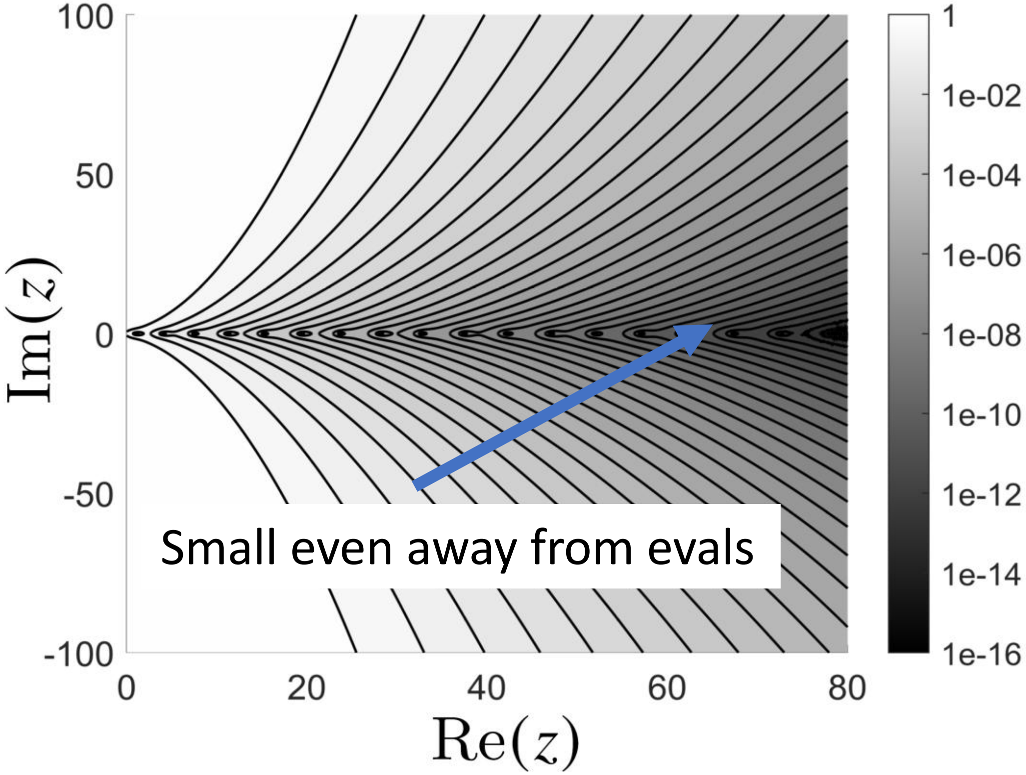


Carl Bender

Michael Berry

$$T = -\frac{d^2}{dx^2} + ix^3 \text{ on } \mathbb{R}$$

$\|(T-z)^{-1}\|^{-1}$



j	E_j to 30 digits with int. arith.
1	1.156 267 071 988 113 293 799 219 177 999 9
2	4.109 228 752 809 651 535 843 668 478 561 3
3	7.562 273 854 978 828 041 351 809 110 631 4
4	11.314 421 820 195 804 402 233 783 948 426 9
5	15.291 553 750 392 532 388 181 630 791 751 9
6	19.451 529 130 691 728 314 686 111 714 104 4
7	23.766 740 435 485 819 131 558 025 968 789 9
8	28.217 524 972 981 193 297 595 053 878 268 9
9	32.789 082 781 862 957 492 447 371 485 046 3
10	37.469 825 360 516 046 866 428 873 594 530 5
100	627.694 712 248 436 511 352 673 702 901 153 6

- C., *“INFINITE-DIMENSIONAL SPECTRAL COMPUTATIONS, Foundations, Algorithms, and Modern Applications.,”* **CUP**, to appear.

Example 2: Data-driven learning for dynamical systems

"Very often, the creation of a technological artifact precedes the science that goes with it. The steam engine was invented before thermodynamics. Thermodynamics was invented to explain the steam engine, essentially the ***limitations*** *of it.* ***What we are after is the equivalent of thermodynamics for intelligence.****"* Yann LeCun

Lower bounds: The method of adversarial dynamical systems.

randomized general algorithms → **capture adaptive and probabilistic choice of training data, stochastic gradient descent etc.**

Data-driven dynamical systems

- Compact metric space $(\mathcal{X}, d)$ – the state space
- $x \in \mathcal{X}$ – the state

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

Dynamics (geometry)
19th century

- Borel measure ω on $\mathcal{X}$
- Function space $L^2 = L^2(\mathcal{X}, \omega)$ (elements g called "observables")
- Koopman operator $\mathcal{K}_F: L^2 \to L^2$; $[\mathcal{K}_F g](x) = g(F(x))$
- ***Available*** snapshot data: $\left\{\left(x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right): m = 1, \ldots, M\right\}$

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).

Data-driven dynamical systems

- Compact metric space $(\mathcal{X}, d)$ – the state space
- $x \in \mathcal{X}$ – the state

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

Dynamics (geometry)
19th century

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

Analysis
20th century

- ***Available*** snapshot data: $\left\{\left(x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right) : m = 1, \dots, M\right\}$

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

Data-driven dynamical systems

- Compact metric space $(\mathcal{X}, d)$ – the state space
- $x \in \mathcal{X}$ – the state
- ***Unknown*** cts $F: \mathcal{X} \to \mathcal{X}$ – the dynamics: $x_{n+1} = F(x_n)$

Dynamics (geometry)
19th century

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

Analysis
20th century

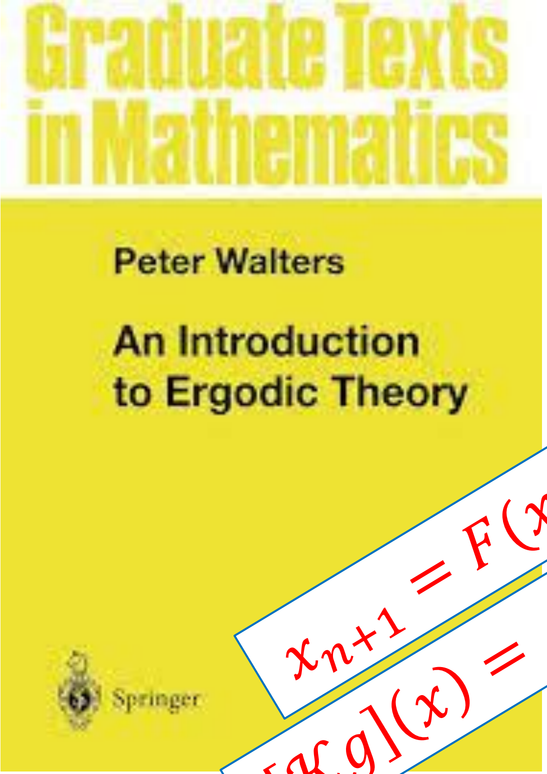
- ***Available*** snapshot data: $\left\{\left(x^{(m)}, y^{(m)} = F\left(x^{(m)}\right)\right): m = 1, \ldots, M\right\}$

Data
21st century

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).

Why you should care about Koopman

Fundamental in ergodic theory



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

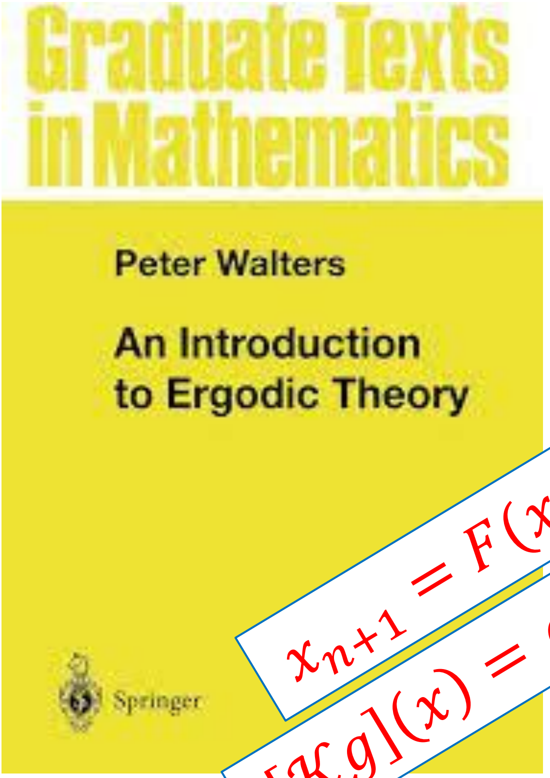
$$[\mathcal{K}g](x) = g(F(x))$$

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

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

Why you should care about Koopman

Fundamental in ergodic theory



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

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

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

Can provide a *diagonalization* of a nonlinear system.

eigenfunction of $\mathcal{K}$

continuous spectrum

$$g(x) = \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \varphi_{\lambda_j}(x) + \int_{-\pi}^{\pi} \phi_{\theta,g}(x)\, d\theta$$

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

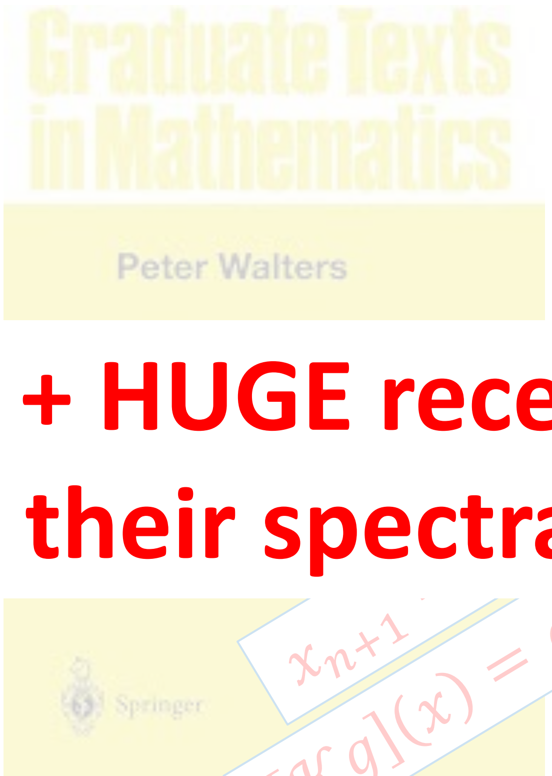
$$= \sum_{\text{eigenvalues } \lambda_j} c_{\lambda_j} \lambda_j{}^n \varphi_{\lambda_j}(x_0) + \int_{-\pi}^{\pi} e^{in\theta} \phi_{\theta,g}(x_0)\, d\theta$$

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

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

Why you should care about Koopman

Fundamental in ergodic theory



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

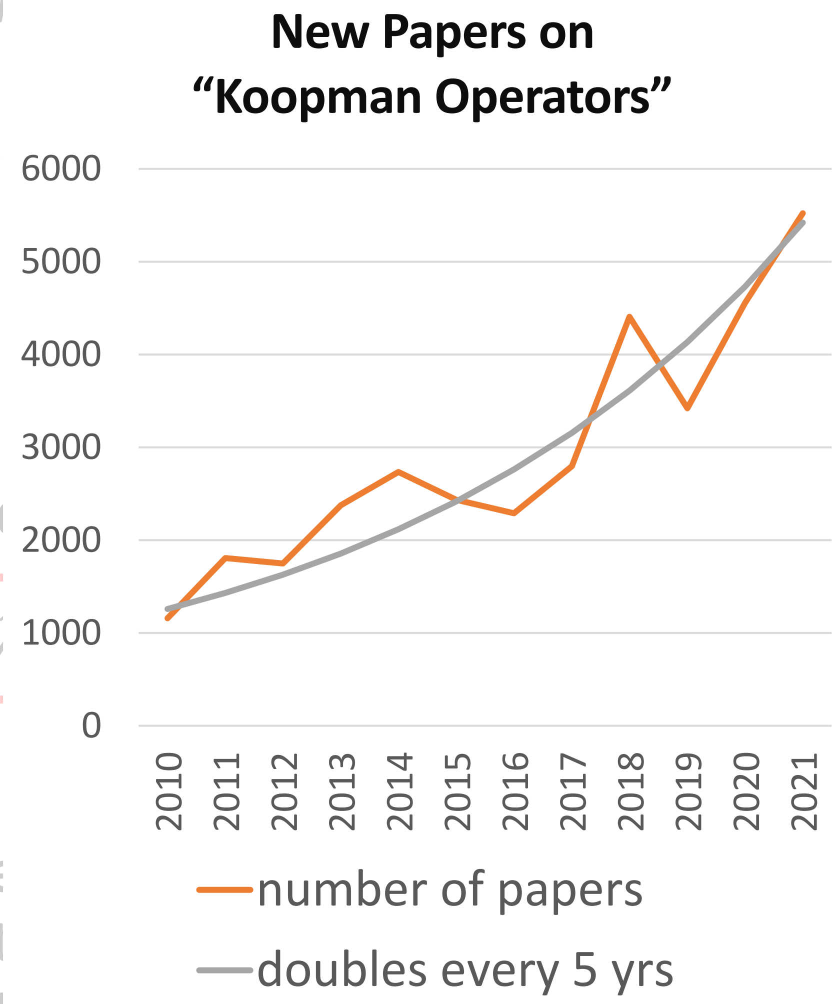
Can provide a *diagon*

$g(x) = \sum$ eigenvalues

$\sum$ eigenvalues λ_j

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

+ HUGE recent interest in their spectral properties!



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

Extended Dynamic Mode Decomposition (EDMD)

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

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

quadrature points

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

quadrature weights

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

- 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.

Extended Dynamic Mode Decomposition (EDMD)

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

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

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

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

Galerkin Approximation

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

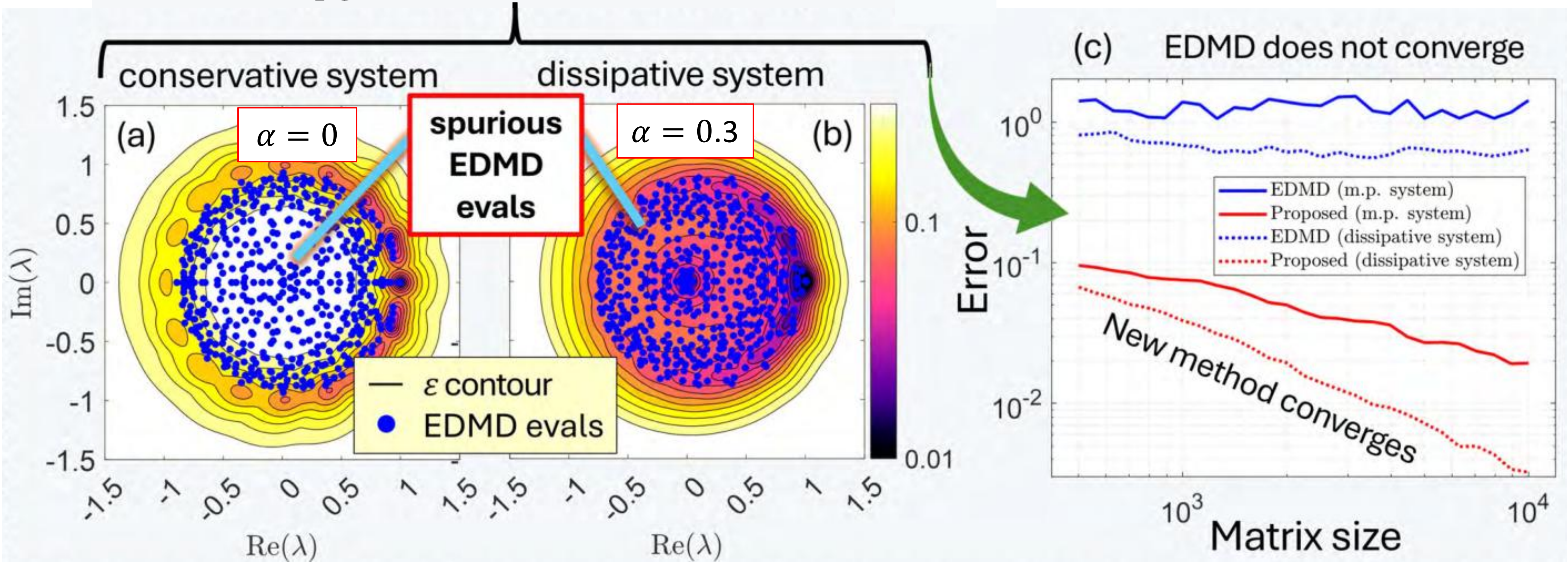
- Schmid, *"Dynamic mode decomposition of numerical and experimental data,"* **J. Fluid Mech.**, 2010.
- Rowley, Mezić, Bagheri, Schlatter, Henningson, *"Spectral analysis of nonlinear flows,"* **J. Fluid Mech.**, 2009.
- Williams, Kevrekidis, Rowley *"A data-driven approximation of the Koopman operator: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

Example: EDMD does NOT converge

- Duffing oscillator: $\dot{x} = y, \dot{y} = -\alpha y + x(1 - x^2)$, sampled $\Delta t = 0.3$.
- Gaussian radial basis functions, Monte Carlo integration ($M = 50000$)

Compute Sp_ε, local adaptive control on $\varepsilon \downarrow 0$

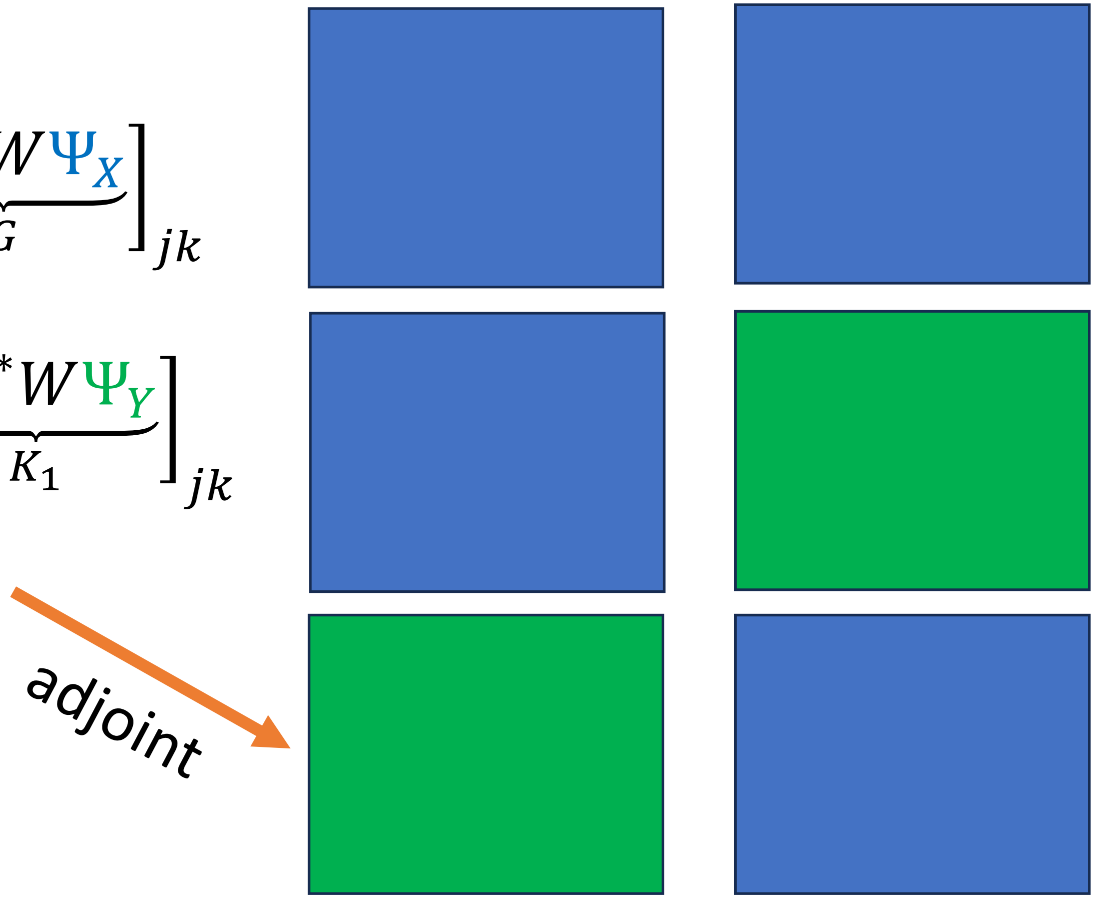
$\mathrm{Sp}_\varepsilon(\mathcal{K}_F) = \{z \in \mathbb{C}: \|(\mathcal{K}_F - zI)^{-1}\|^{-1} \leq \varepsilon\}$



Residual DMD (ResDMD)

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

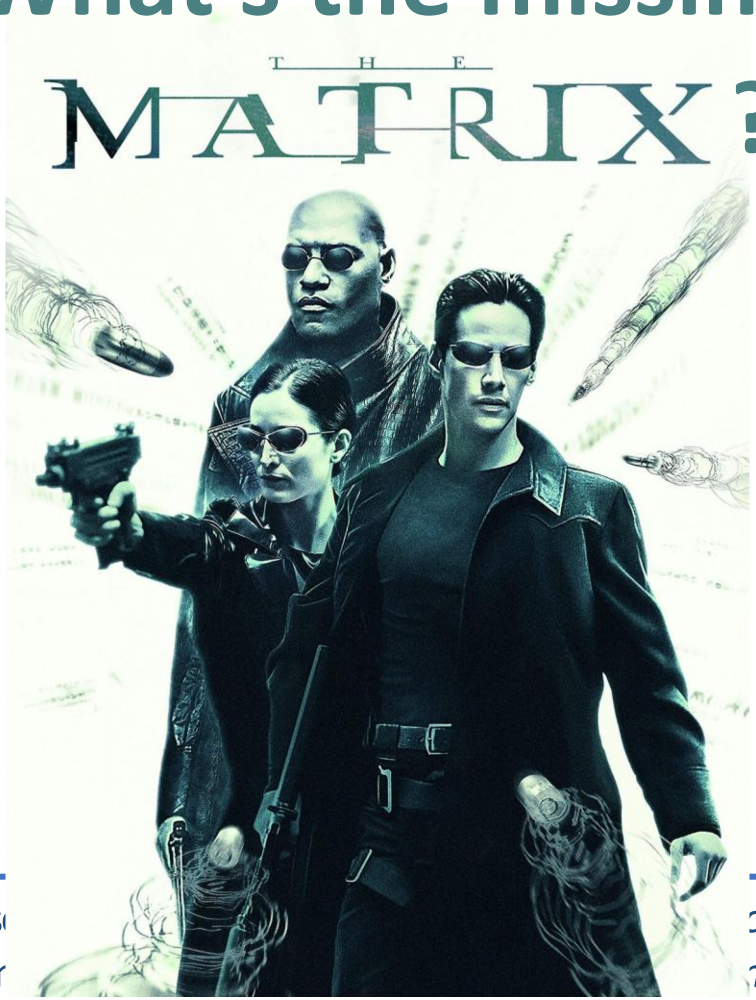
$$\langle \mathcal{K}\psi_k, \psi_j \rangle \approx \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})}\, \underbrace{\psi_k\left(y^{(m)}\right)}_{[\mathcal{K}\psi_k](x^{(m)})} = \Big[\underbrace{{\Psi_X}^* W \Psi_Y}_{K_1}\Big]_{jk}$$



- 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.
- Code: https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition

Residual DMD (ResDMD)

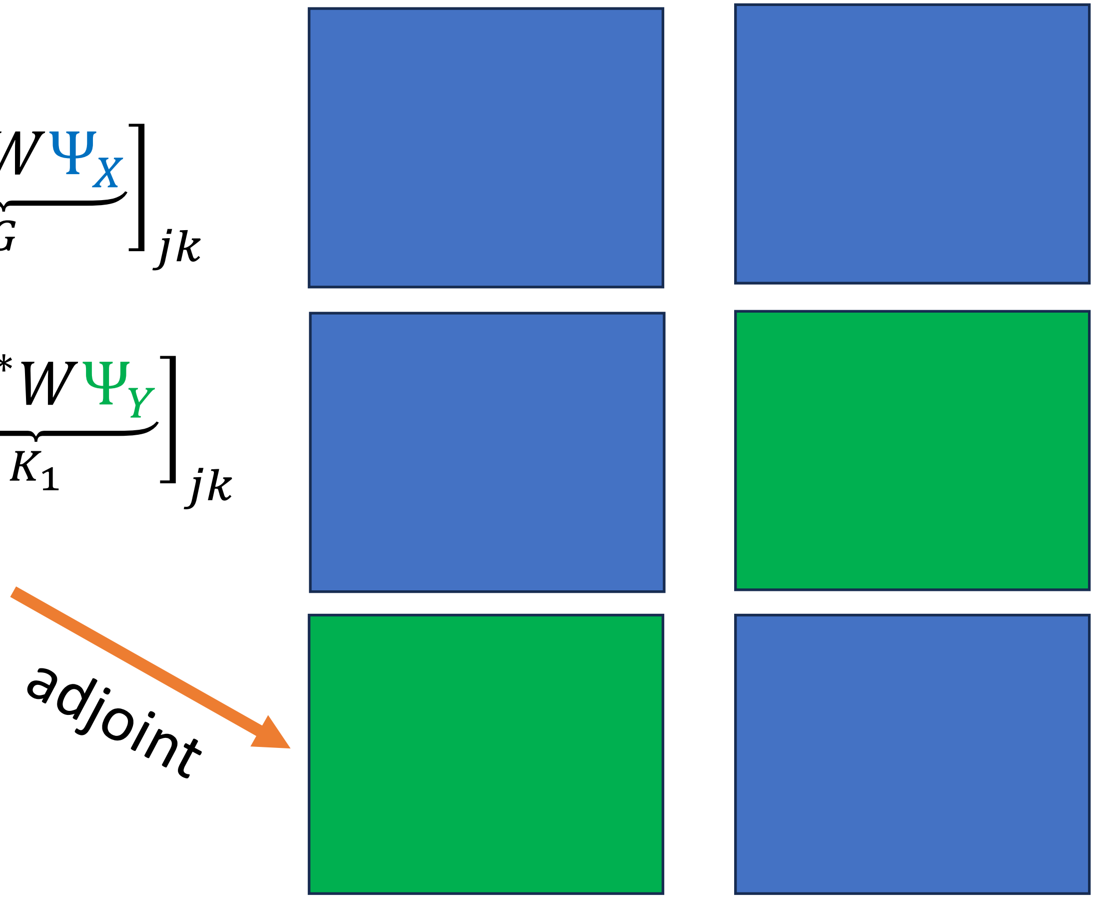
What's the missing



?

$$= \Big[\underbrace{{\Psi_X}^{*} W \Psi_X}_{G}\Big]_{jk}$$

$$) \quad = \Big[\underbrace{{\Psi_X}^{*} W \Psi_Y}_{K_1}\Big]_{jk}$$



- C., Towns ... ctral properties of Koopman operators for dynamical systems," **Commun. Pure Appl. Math.**, 2023.
- C., Aytor ... nposition," **J. Fluid Mech.**, 2023.
- Code: https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition

Residual DMD (ResDMD)

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

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

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

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

Residual DMD (ResDMD)

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

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

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

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

- 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.
- Code: https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition

Residual DMD (ResDMD)

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

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

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

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

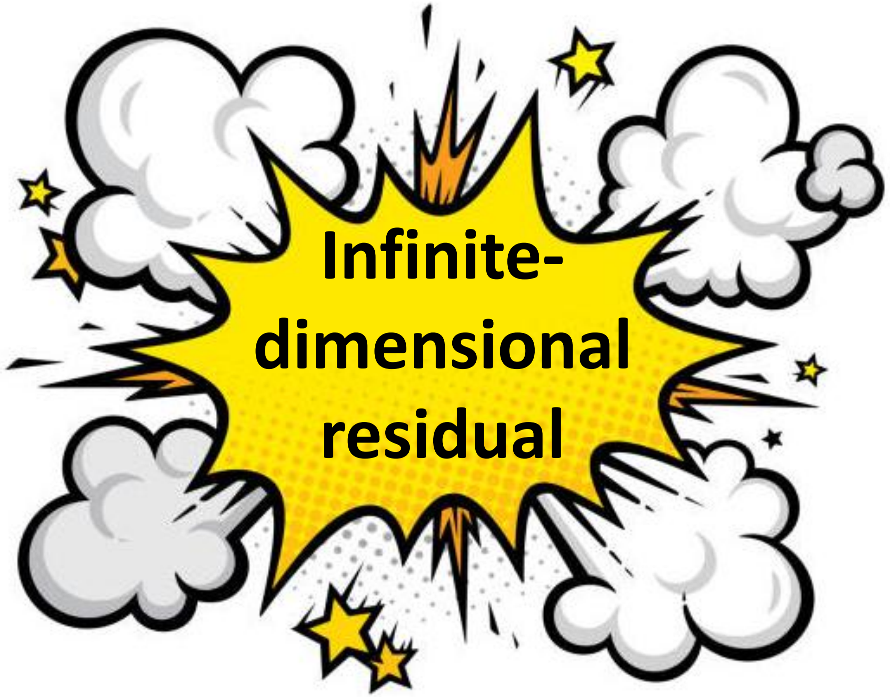
- C., Townsend, "*Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*," **Commun. Pure Appl. Math.**, 2023.
- C., Ayton, Szőke, "*Residual Dynamic Mode Decomposition*," **J. Fluid Mech.**, 2023.
- Code: https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition

Bound projection errors!

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

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

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

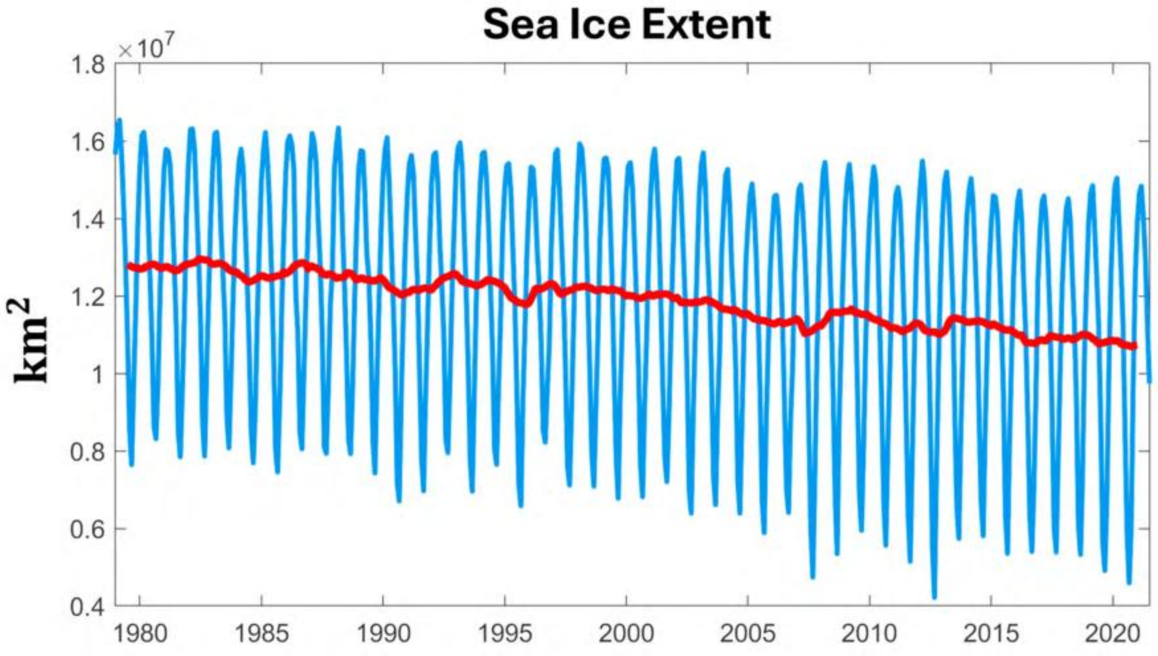


Residuals: $g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j$, $\|\mathcal{K}g - \lambda g\|^2 = \lim_{M\to\infty} \mathbf{g}^*[K_2 - \lambda K_1{}^* - \bar{\lambda} K_1 + |\lambda|^2 G]\mathbf{g}$

- 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.
- Code: https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition

Practical Gains: Arctic Sea Ice Forecasting

Monthly average from satellite passive microwave sensors.



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

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

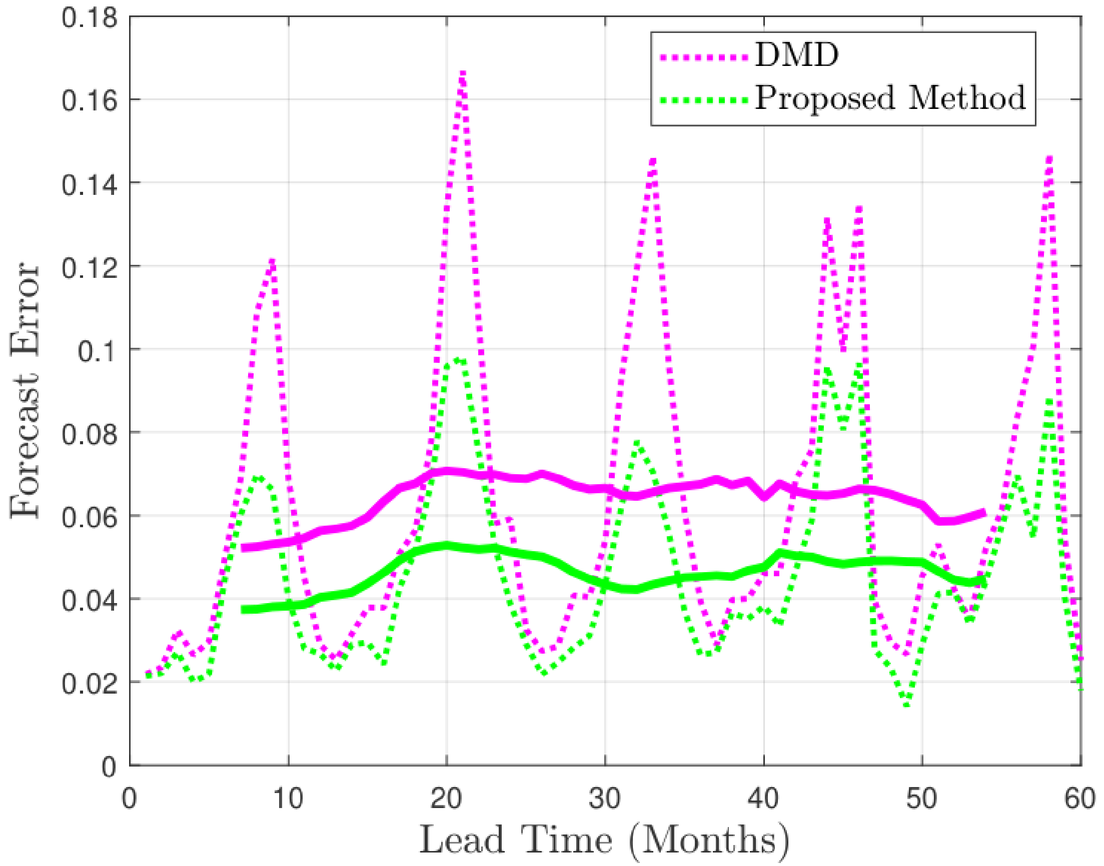


Figure 4: Forecast error for entire sea ice concentration. The relative mean squared error of forecasts over five years. The solid lines show the moving 12-month mean. In each case, the model is built using the data from the years 2005–2015, and then tested on 2016-2020. The proposed method consistently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

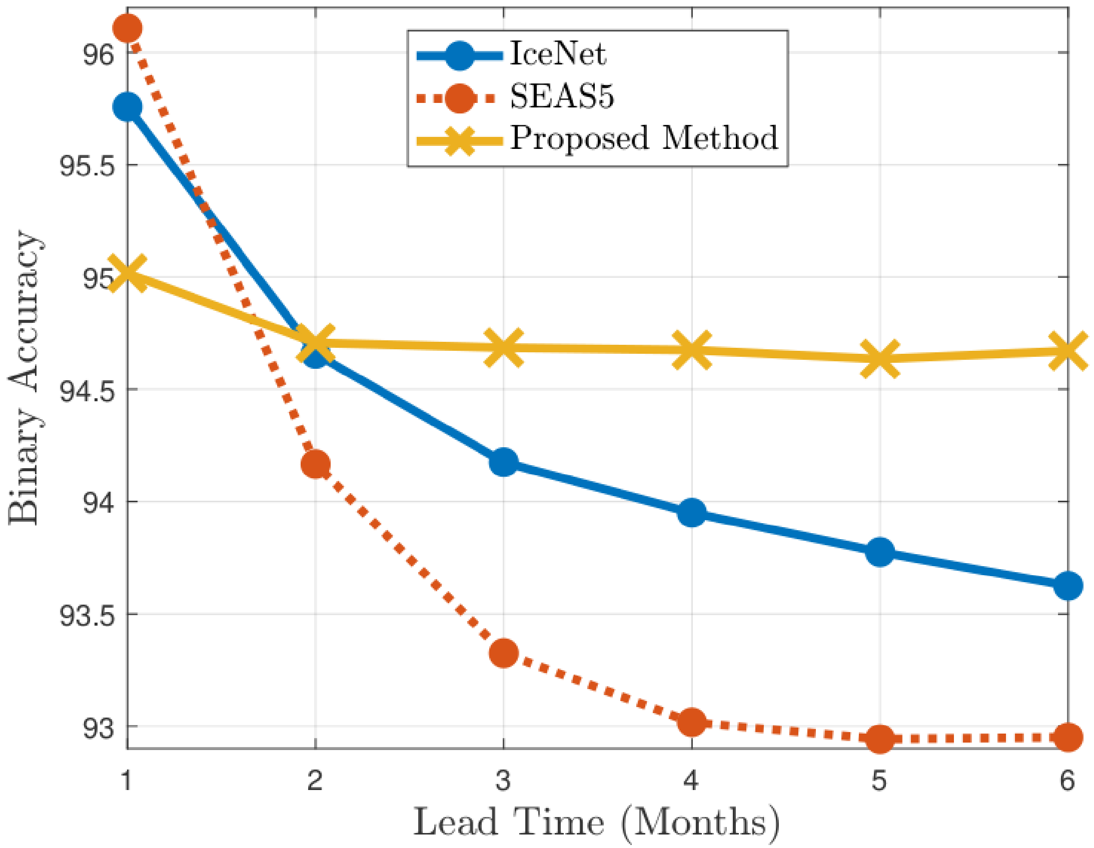


Figure 5: Comparison with machine learning and statistical prediction benchmarks. Mean binary accuracy over the test years 2012–2020, shown for IceNet, SEAS5, and our proposed method that avoids spurious Koopman eigenvalues. Our proposed method achieves better accuracy for lead times greater than one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

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

Theorem (impossibility)

Implies $\mathcal{K}$ is unitary

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

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

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

NB: Similarly, no random algorithms converging with probability $> 1/2$.

Double limit is necessary!

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> ($x_j \rightarrow y_j$) with F_0

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

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

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…

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

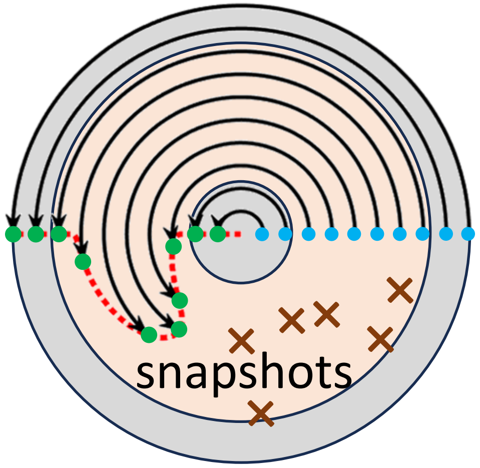
Proof idea: Constructing an adversary

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...

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

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

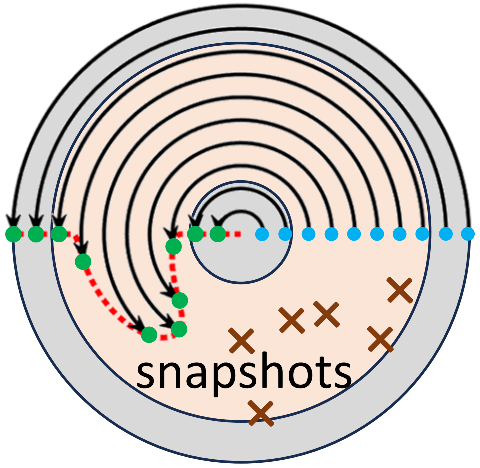


$\mathcal{T}_F = \{(x, y_m) \mid \|F(x) - y_m\| \leq 2^{-m}\}$

Proof idea: Constructing an adversary

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

Build an adversarial F…



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

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

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

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

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

Build an adversarial F…

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

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

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

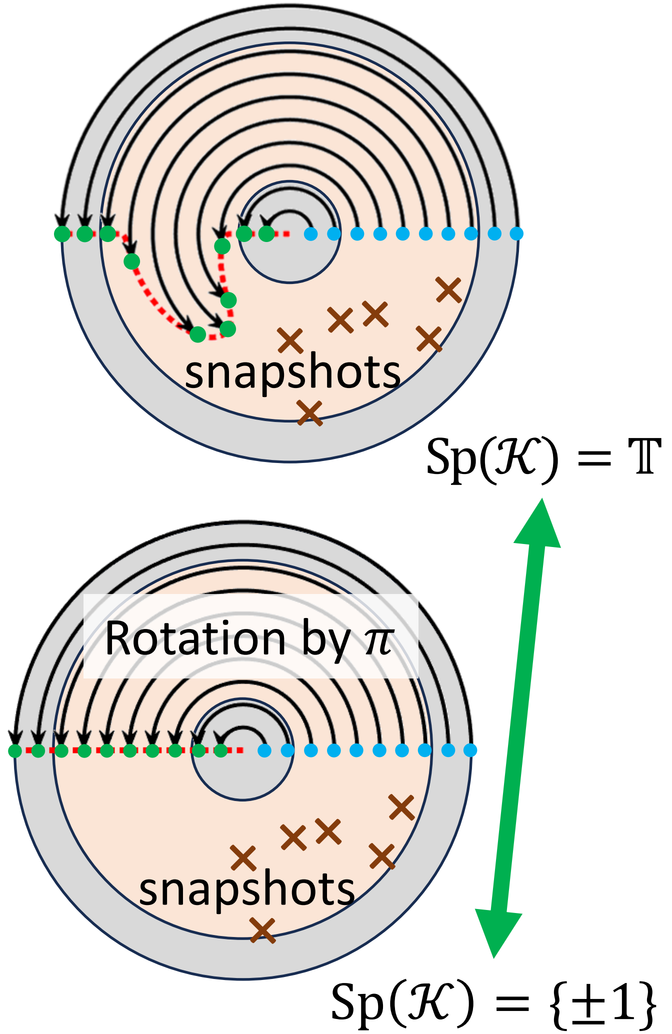
BUT Γ_{n_1} uses finite amount of info to output $\Gamma_{n_1}\big(\widetilde{F_1}\big)$.

Let X, Y correspond to these snapshots.

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

<u>Consistent data</u> $\Rightarrow \Gamma_{n_1}(F_1) = \Gamma_{n_1}\big(\widetilde{F_1}\big)$, $\mathrm{dist}(i, \Gamma_{n_1}(F_1)) \leq 1$

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



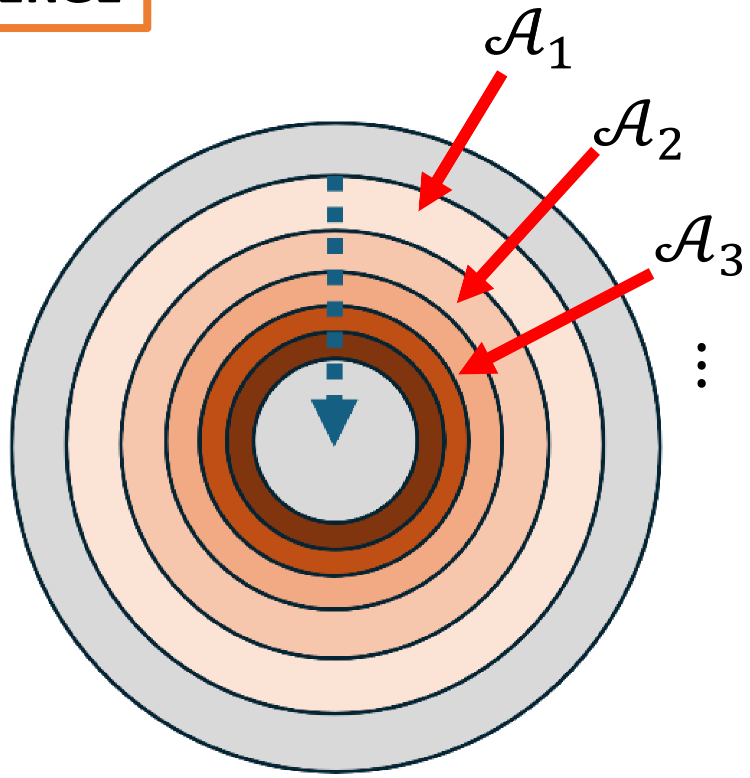
Proof idea: Constructing an adversary

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

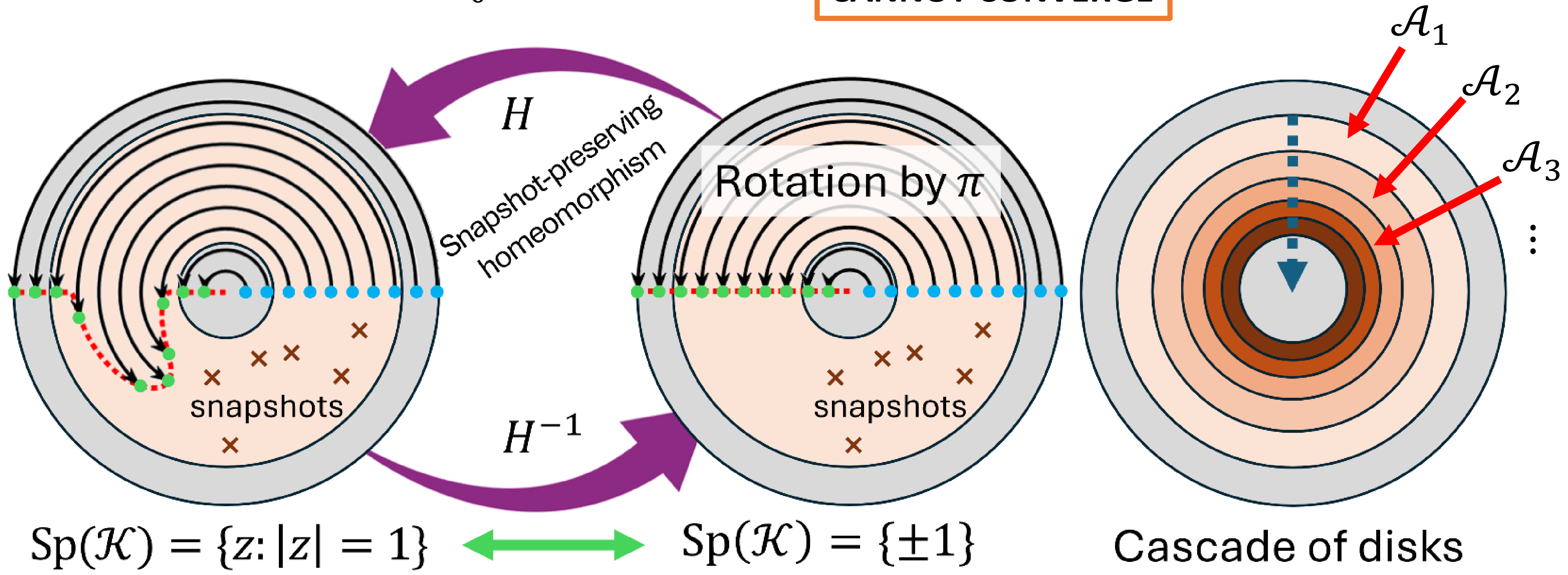
Proof idea: Constructing an adversary

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

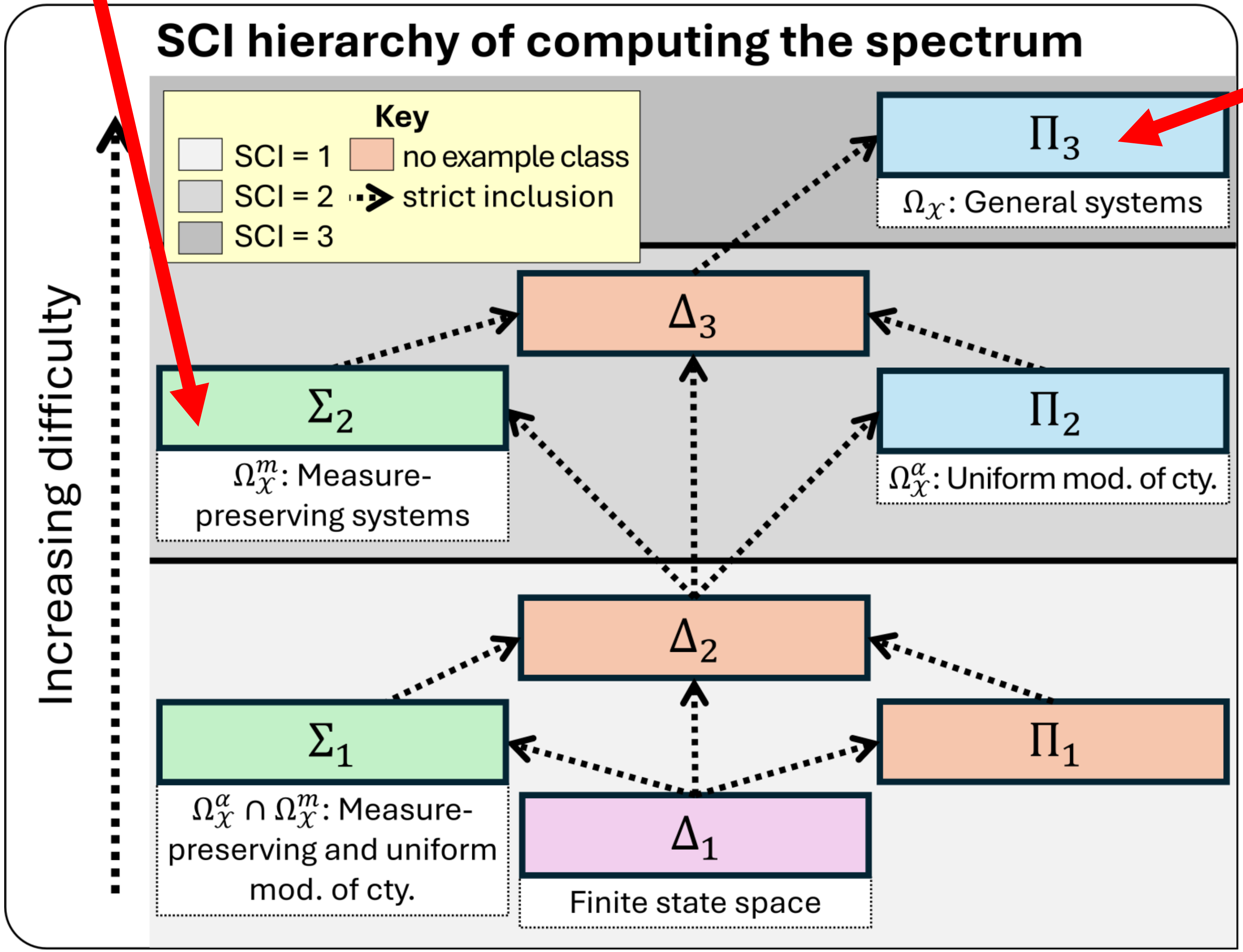
BUT $\mathrm{Sp}(\mathcal{K}_F) = \mathrm{Sp}(\mathcal{K}_{F_0}) = \{\pm 1\}$

CANNOT CONVERGE



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.

Why study this hierarchy?

- Optimality: understand boundaries of what's possible.
- Lower bounds $\Longrightarrow$ spot assumptions needed to lower SCI.
- Upper bounds $\Longrightarrow$ new algorithms and methods.

FOUNDATIONS $\longleftrightarrow$ METHODS

- $\Sigma_1 \cup \Pi_1 \Longrightarrow$ computer-assisted proofs.
- Much of computational literature not sharp!

Remarks:

- Can use any model of computation.
- Existing hierarchies (e.g., arithmetic, Baire etc.) included as particular cases.

Summary

SCI hierarchy is a tool for discovering the foundations of computation.

Example 1: The zoo of spectral problems.

- Many spectral problems in infinite dimensions are impossible.
  Some are more impossible than others!
- New suite of "infinite-dimensional" algorithms for spectral problems.
  Rigorous, optimal, practical.

Example 2: Need for foundations in data-driven learning.

- **Adversarial dynamical systems:** Widespread and prevent learning of properties.
- New provably convergent and optimal algorithms for Koopman operators.

Examples not covered: foundations of AI, optimization, PDEs, resonances, computer-assisted proofs, spectral measures,…

Could this framework be useful in your area?

- C., *"The foundations of infinite-dimensional spectral computations,"* **PhD diss.**, University of Cambridge, 2020.
- Ben-Artzi, Marletta, Rösler, *"Computing scattering resonances,"* **J. Eur. Math. Soc.**, 2022.
- Bastounis, Hansen, Vlačić, *"The extended Smale's 9th problem,"* preprint.
- Webb, Olver, *"Spectra of Jacobi operators via connection coefficient matrices,"* **CIMP**, 2021.
- C., Antun, Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem,*" **PNAS**, 2022.
- C., Horning, Townsend, *"Computing spectral measures of self-adjoint operators,"* **SIAM Rev.**, 2021.

References

[1] 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.

[2] Antun, V., M. J. Colbrook, and A. C. Hansen. "Proving existence is not enough: Mathematical paradoxes unravel the limits of neural networks in artificial intelligence." SIAM News 55.4 (2022): 1-4.

[3] Colbrook, Matthew, Vegard Antun, and Anders Hansen. "Mathematical paradoxes unearth the boundaries of AI." TheScienceBreaker 8.3 (2022).

[4] Adcock, Ben, Matthew J. Colbrook, and Maksym Neyra-Nesterenko. "Restarts subject to approximate sharpness: A parameter-free and optimal scheme for first-order methods." arXiv preprint arXiv:2301.02268 (2023).

[5] Colbrook, Matthew J. "WARPd: A linearly convergent first-order primal-dual algorithm for inverse problems with approximate sharpness conditions." SIAM Journal on Imaging Sciences 15.3 (2022): 1539-1575.

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

[7] 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.

[8] 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).

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

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

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

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

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

[14] Colbrook, Matthew. "Pseudoergodic operators and periodic boundary conditions." Mathematics of Computation 89.322 (2020): 737-766.

[15] Colbrook, Matthew J., and Alex Townsend. "Avoiding discretization issues for nonlinear eigenvalue problems." arXiv preprint arXiv:2305.01691 (2023).

[16] Colbrook, Matthew, Andrew Horning, and Alex Townsend. "Resolvent-based techniques for computing the discrete and continuous spectrum of differential operators." XXI Householder Symposium on Numerical Linear Algebra. 2020.

[17] Johnstone, Dean, et al. "Bulk localized transport states in infinite and finite quasicrystals via magnetic aperiodicity." Physical Review B 106.4 (2022): 045149.

[18] Colbrook, Matthew J., et al. "Computing spectral properties of topological insulators without artificial truncation or supercell approximation." IMA Journal of Applied Mathematics 88.1 (2023): 1-42.

[19] Colbrook, Matthew J., and Andrew Horning. "Specsolve: spectral methods for spectral measures." arXiv preprint arXiv:2201.01314 (2022).

[20] Colbrook, Matthew J., and Alex Townsend. "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems." arXiv preprint arXiv:2111.14889 (2021).

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

[22] 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.

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

[24] Colbrook, Matthew J. "Computing semigroups with error control." SIAM Journal on Numerical Analysis 60.1 (2022): 396-422.

[25] Colbrook, Matthew J., and Lorna J. Ayton. "A contour method for time-fractional PDEs and an application to fractional viscoelastic beam equations." Journal of Computational Physics 454 (2022): 110995.