Robust and Verified Koopmania!

Infinite-dimensional spectral computations for nonlinear systems

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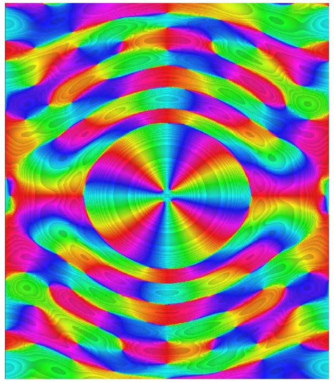
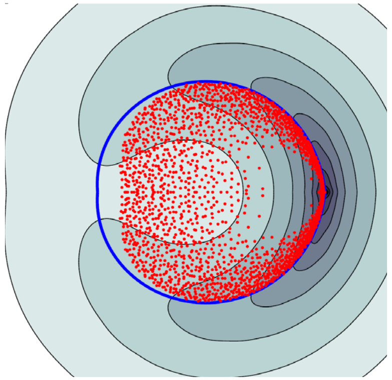




Analysis: C., Townsend, *"Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems"*

Applications: C., Ayton, Szőke, *"Residual Dynamic Mode Decomposition: Robust and verified Koopmanism"*

http://www.damtp.cam.ac.uk/user/mjc249/home.html: slides, papers, and code

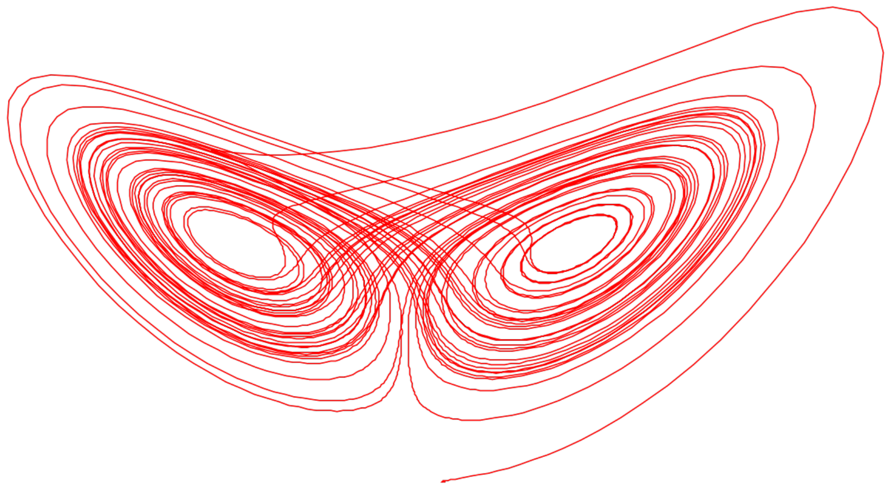
Data-driven dynamical systems

- State $x \in \Omega \subseteq \mathbb{R}^d$, ***unknown*** function $F: \Omega \rightarrow \Omega$ governs dynamics

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

- **Goal:** Learn about system from data $\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^{M}$
  - E.g., **data from** trajectories, experimental measurements, simulations, …
  - E.g., **used for** forecasting, control, design, understanding, …

- **Applications:** chemistry, climatology, electronics, epidemiology, finance, fluids, molecular dynamics, neuroscience, plasmas, robotics, video processing, …



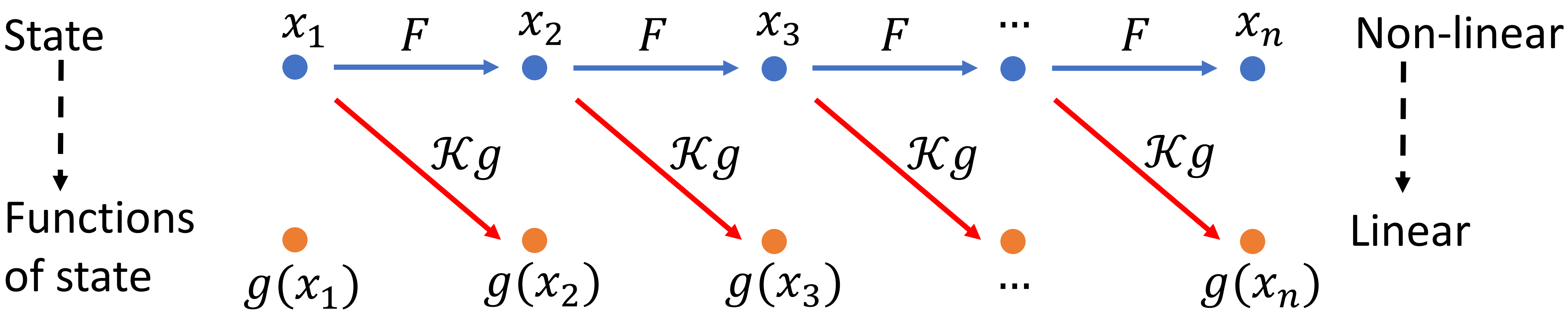
Can we develop verified methods?

Operator viewpoint

- **Koopman operator** $\mathcal{K}$ acts on functions $g: \Omega \to \mathbb{C}$

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

- $\mathcal{K}$ is ***linear*** but acts on an ***infinite-dimensional*** space.



- Work in $L^2(\Omega, \omega)$ for positive measure ω, with inner product $\langle\cdot,\cdot\rangle$.

- Koopman, "*Hamiltonian systems and transformation in Hilbert space,*" **Proceedings of the National Academy of Sciences**, 1931.
- Koopman, v. Neumann, "*Dynamical systems of continuous spectra,*" **Proceedings of the National Academy of Sciences**, 1932.

Koopman mode decomposition

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

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

eigenfunction of $\mathcal{K}$

generalised eigenfunction of $\mathcal{K}$

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

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

Encodes: geometric features, invariant measures, transient behaviour, long-time behaviour, coherent structures, quasiperiodicity, etc.

GOAL: Data-driven approximation of $\mathcal{K}$ and its spectral properties.

- Mezić, "*Spectral properties of dynamical systems, model reduction and decompositions,*" **Nonlinear Dynamics**, 2005.

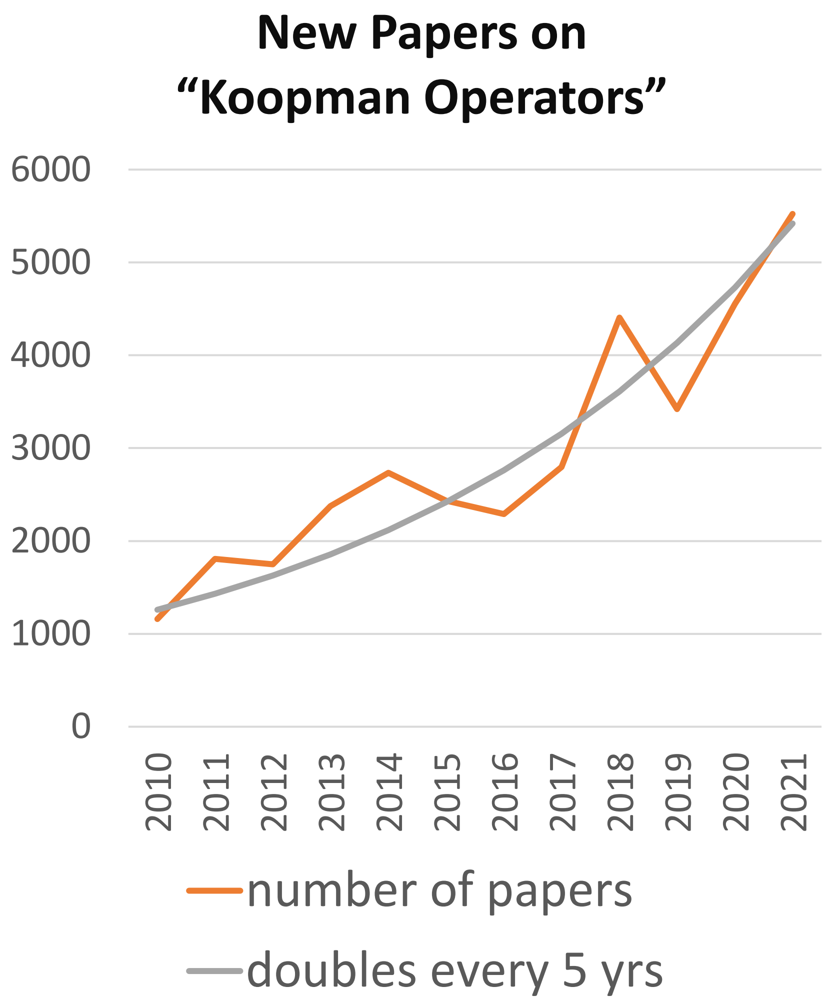
Koopmania*: a revolution in the big data era

≈35,000 papers over last decade!

***Very* little on convergence guarantees or verification.**

Why is this lacking?

- Koopman operators have so far been quite distinct from both analysis and computational communities.
- Dealing with infinite dim is notoriously hard …



**Wikipedia*: *"its wild surge in popularity is sometimes jokingly called 'Koopmania'"*

Can we compute spectral properties in inf. dim.?

$$\mathrm{Spec}(\mathcal{K}) = \{\lambda \in \mathbb{C} : \mathcal{K} - \lambda I \ \text{ is not invertible}\}$$

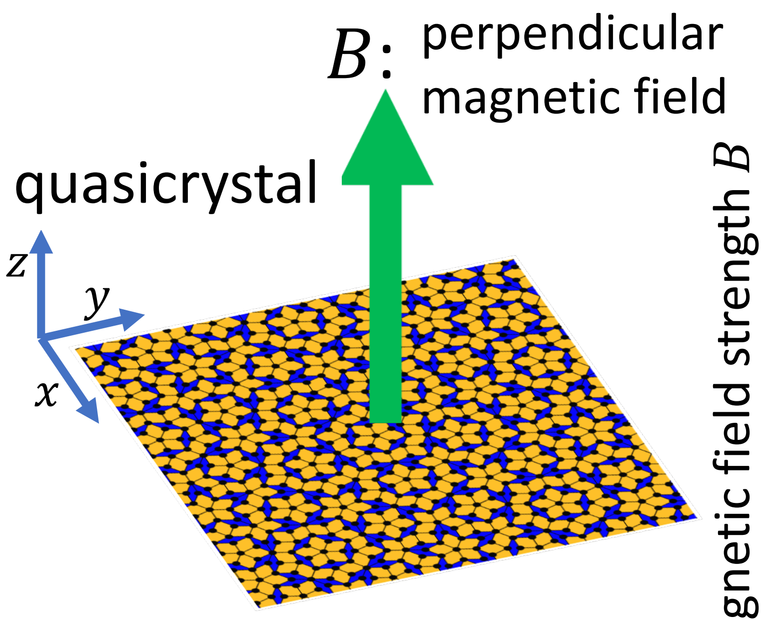
*"Operators that arise in practice are not **diagonalized**, and it is often very hard to locate the spectrum. Thus, one has to settle for numerical approximations. Unfortunately, there are **no proven <u>general</u> techniques**."* W. Arveson, Berkeley (1994)

Naïve: $\mathcal{K}$ ⟶ $\mathbb{K} \in \mathbb{C}^{N\times N}$ + compute e-values, **problems:**

1) **"Too much":** Approximate spurious modes $\lambda \notin \mathrm{Spec}(\mathcal{K})$ - "spectral pollution"
2) **"Too little":** Miss parts of $\mathrm{Spec}(\mathcal{K})$
3) **Continuous spectra**
4) **Verification:** Which part of an approximation can we trust?

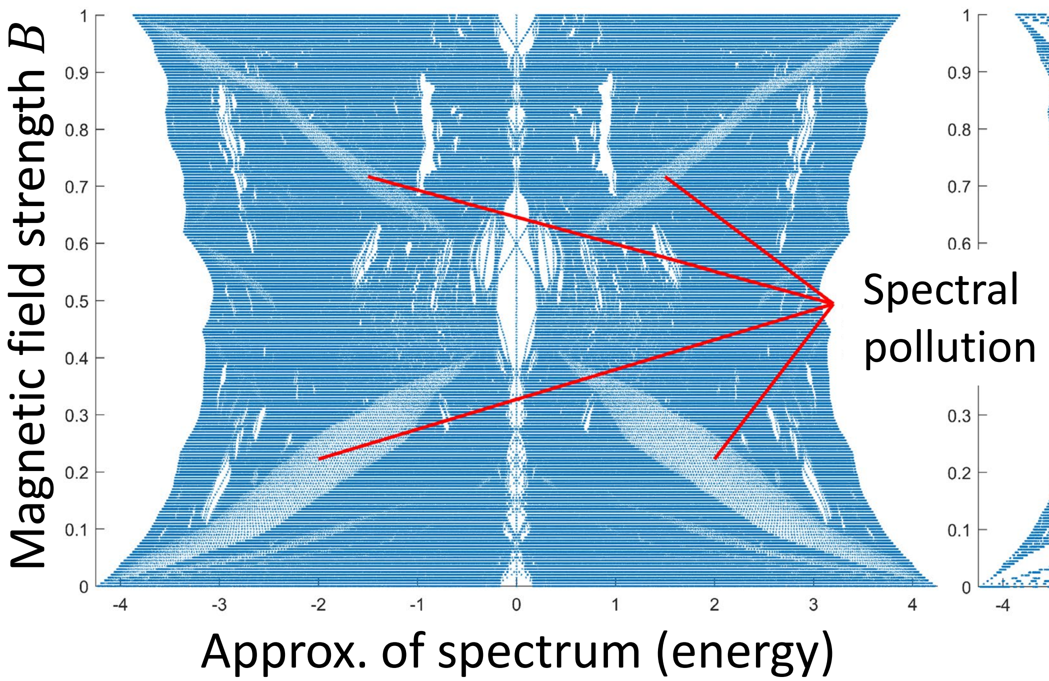
- Arveson, *"The role of C^*-algebras in infinite dimensional numerical linear algebra,"* **Contemp. Math.**, 1994.
- Davies, *"Linear operators and their spectra,"* **CUP**, 2007.
- Brunton, Kutz, *"Data-driven Science and Engineering: Machine learning, Dynamical systems, and Control,"* **CUP**, 2019.

Example of "too much" (spectral pollution)



Infinite matrix: discrete Schrödinger operator

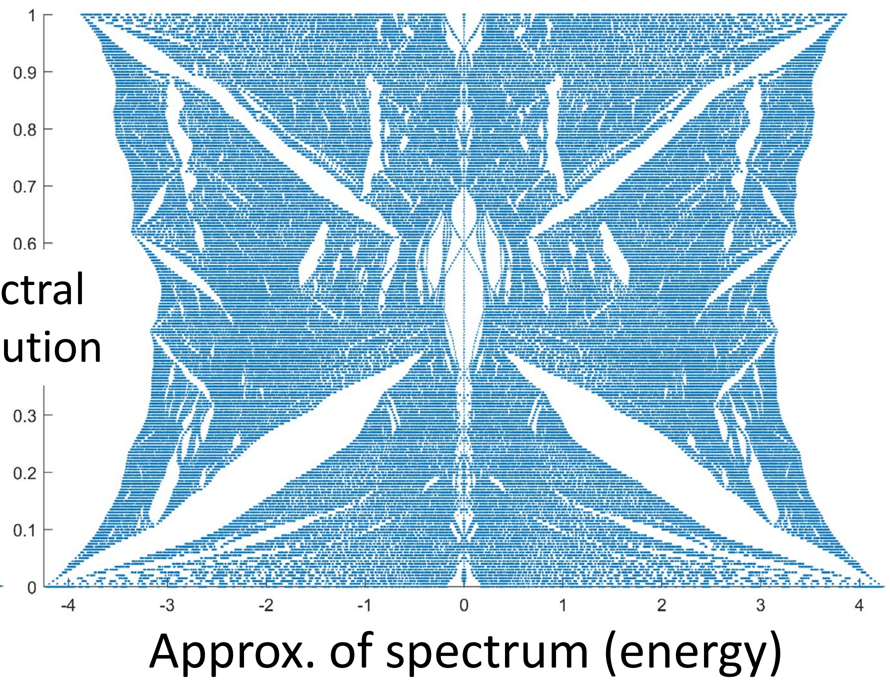
Naïve method



Spectral pollution

No error control

"Infinite-dimensional" method



Convergent computation

Error control

- C., Roman, Hansen, *"How to compute spectra with error control,"* **Physical Review Letters**, 2019.
- C., Horning, Townsend, *"Computing spectral measures of self-adjoint operators,"* **SIAM Review**, 2021.
- Johnstone, C., Nielsen, Öhberg, Duncan, *"Bulk Localised Transport States in Infinite and Finite Quasicrystals via Magnetic Aperiodicity,"* **PRB**, 2022.

Example of “too much” (spec

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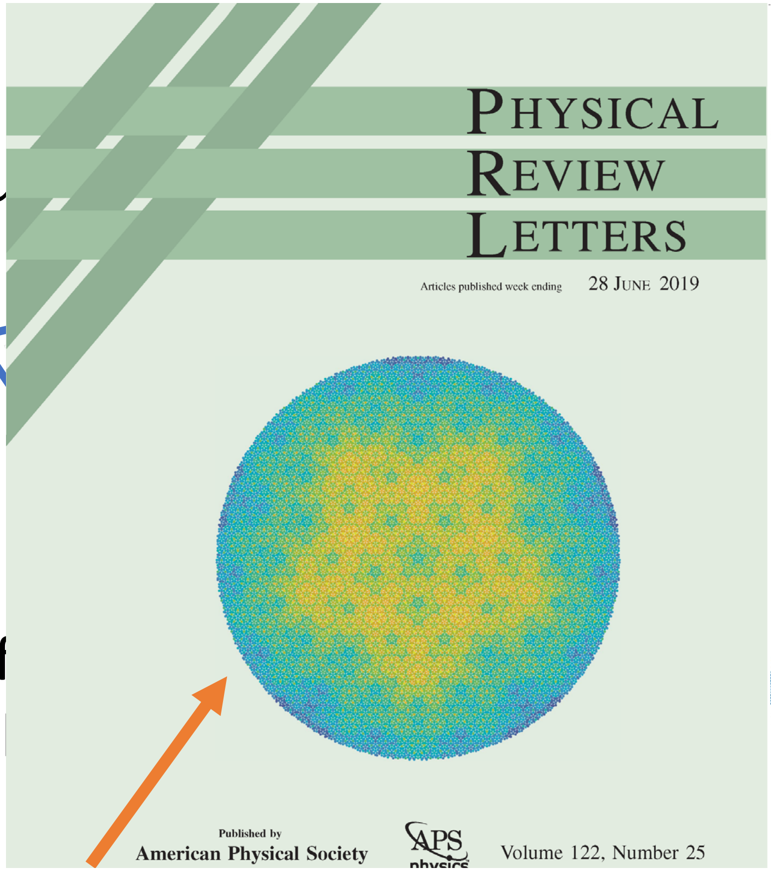
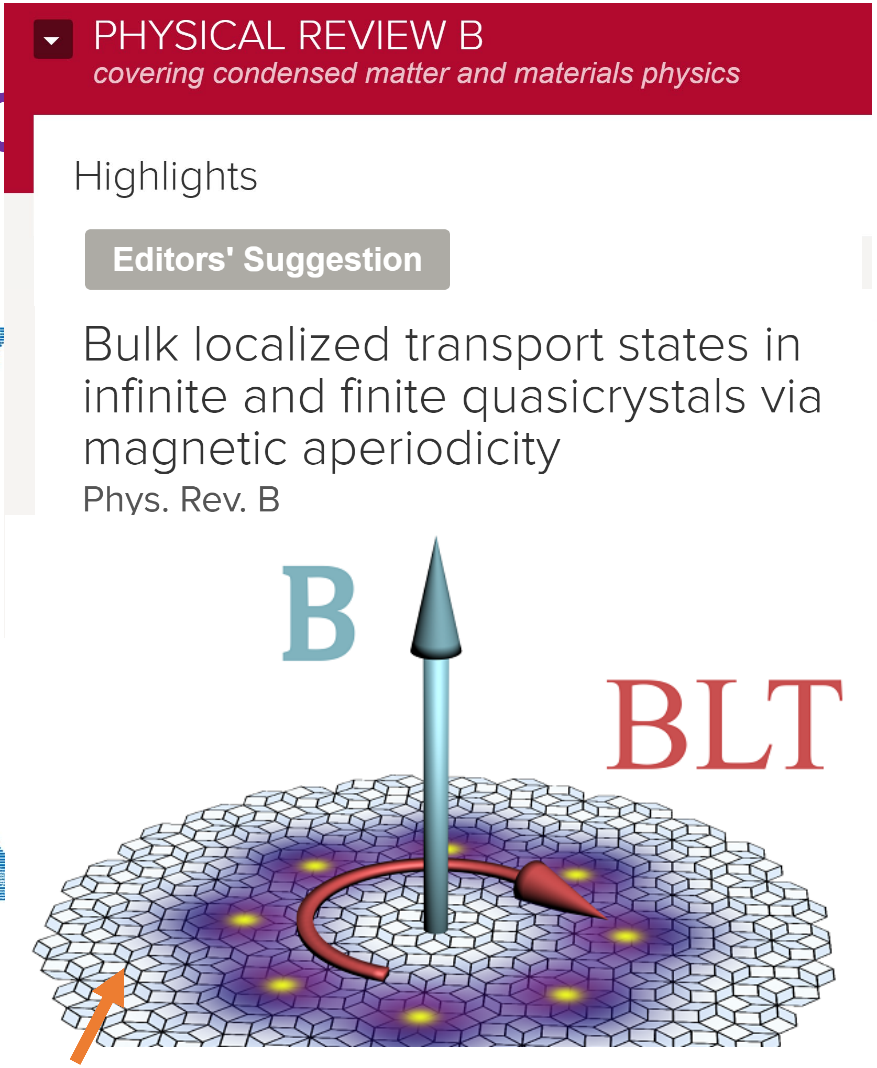


E.g., ground state of quasicrystal

Spectral methods for continuous spectra

E.g., cts spec of graphene



E.g., new states and phenomena: **bulk localised transport** states

- C., Roman, Hansen, “*How to compute spectra with error control,*” **Physical Review Letters**, 2019.
- C., Horning, Townsend, “*Computing spectral measures of self-adjoint operators,*” **SIAM Review**, 2021.
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Example of “too much” (spec

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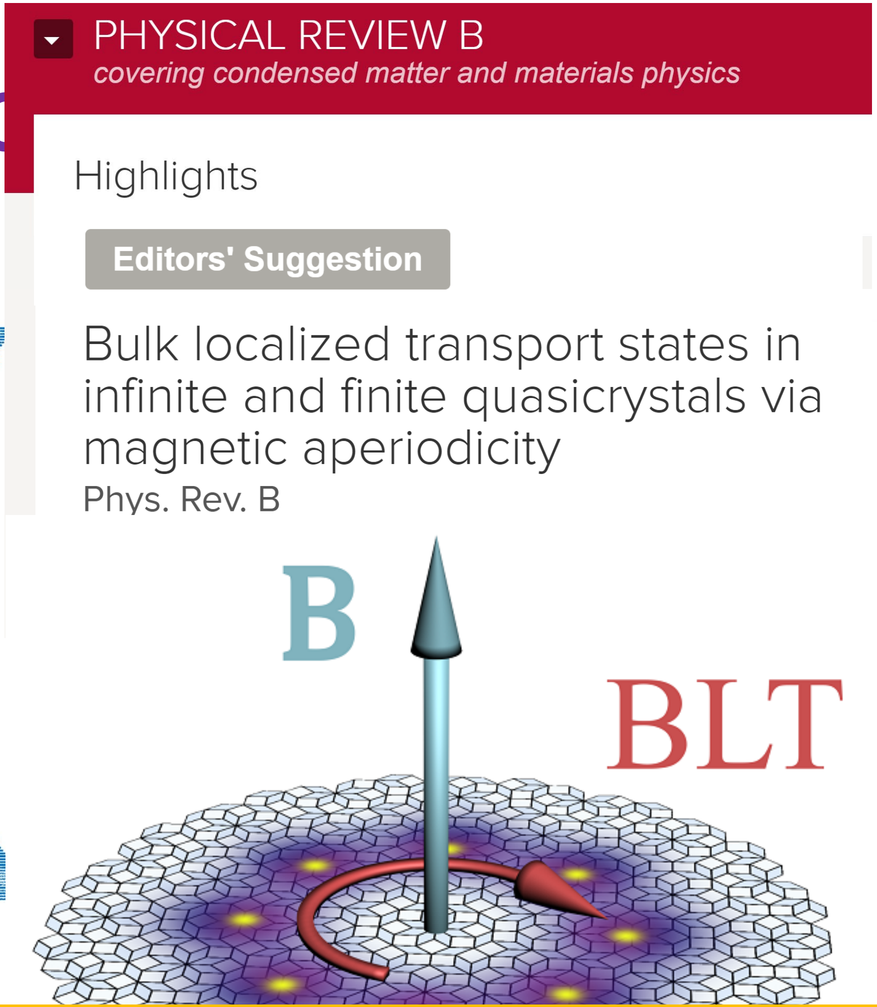

Need new tools for data-driven dynamical systems …

- C., Roman, Hansen, “*How to compute spectra with error control,*” **Physical Review Letters**, 2019.
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Build the matrix: Dynamic Mode Decomposition (DMD)

Given dictionary $\{\psi_1, \ldots, \psi_{N_K}\}$ of functions $\psi_j : \Omega \to \mathbb{C}$

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

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

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

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

Recall open problems: 1) "too much", 2) "too little", 3) continuous spectra, 4) verification.

- Schmid, "*Dynamic mode decomposition of numerical and experimental data,*" **Journal of fluid mechanics**, 2010.
- Kutz, Brunton, Brunton, Proctor, "*Dynamic mode decomposition: data-driven modeling of complex systems,*" **SIAM**, 2016.
- Williams, Kevrekidis, Rowley "*A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition,*" **Journal of Nonlinear Science**, 2015.

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

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

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

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

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

- C., Townsend, *"Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems,"* **Communications on Pure and Applied Mathematics**, under review.
- Code: https://github.com/MColbrook/Residual-Dynamic-Mode-Decomposition

ResDMD: avoiding "too much"

$$\mathrm{res}(\lambda, \mathbf{g})^2 = \frac{\mathbf{g}^*\left[K_2 - \lambda {K_1}^* - \bar{\lambda} K_1 + |\lambda|^2 G\right]\mathbf{g}}{\mathbf{g}^* G \mathbf{g}}$$

Algorithm 1:

1. Compute $G, K_1, K_2 \in \mathbb{C}^{N_K \times N_K}$ and eigendecomposition $K_1 V = G V \Lambda$.
2. For each eigenpair $(\lambda, \mathbf{v})$, compute $\mathrm{res}(\lambda, \mathbf{v})$.
3. **Output:** subset of e-vectors $V_{(\varepsilon)}$ & e-vals $\Lambda_{(\varepsilon)}$ with $\mathrm{res}(\lambda, \mathbf{v}) \leq \varepsilon$ ($\varepsilon =$ input tol).

Theorem (no spectral pollution): Suppose quad. rule converges. Then

$$\limsup_{M \to \infty} \max_{\lambda \in \Lambda^{(\varepsilon)}} \|(\mathcal{K} - \lambda)^{-1}\|^{-1} \leq \varepsilon$$

ResDMD: avoiding "too much"

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$$\limsup_{M \to \infty} \max_{\lambda \in \Lambda^{(\varepsilon)}} \|(\mathcal{K} - \lambda)^{-1}\|^{-1} \leq \varepsilon$$

BUT: Typically, does not capture all of spectrum! ("too little")

ResDMD: avoiding "too little"

$$\mathrm{Spec}_\varepsilon(\mathcal{K}) = \bigcup_{\|\mathcal{B}\|\leq\varepsilon} \mathrm{Spec}(\mathcal{K}+\mathcal{B}), \qquad \lim_{\varepsilon\downarrow 0} \mathrm{Spec}_\varepsilon(\mathcal{K}) = \mathrm{Spec}(\mathcal{K})$$

Algorithm 2:

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

1. Compute $G, K_1, K_2 \in \mathbb{C}^{N_K \times N_K}$.
2. For z_k in comp. grid, compute $\tau_k = \min_{g=\sum_{j=1}^{N_K} \mathbf{g}_j \psi_j} \mathrm{res}(z_k, g)$, corresponding g_k (gen. SVD).
3. **Output:** $\{z_k : \tau_k < \varepsilon\}$ (approx. of $\mathrm{Spec}_\varepsilon(\mathcal{K})$), $\{g_k : \tau_k < \varepsilon\}$ (ε-pseudo-eigenfunctions).

Theorem (full convergence): Suppose the quadrature rule converges.

- **Error control:** $\{z_k : \tau_k < \varepsilon\} \subseteq \mathrm{Spec}_\varepsilon(\mathcal{K})$ (as $M \to \infty$)
- **Convergence:** Converges locally uniformly to $\mathrm{Spec}_\varepsilon(\mathcal{K})$ (as $N_K \to \infty$)

Setup for continuous spectra

Suppose system is measure preserving (e.g., Hamiltonian, ergodic, …)

$$\Leftrightarrow \mathcal{K}^*\mathcal{K} = I \text{ (isometry)}$$

$$\Longrightarrow \mathrm{Spec}(\mathcal{K}) \subseteq \{z : |z| \leq 1\}$$

(For those interested: we consider canonical unitary extensions.)

Spectral measures → diagonalisation

- **Fin.-dim.:** $B \in \mathbb{C}^{n\times n}$, $B^*B = BB^*$, o.n. basis of e-vectors $\{v_j\}_{j=1}^n$

$$v = \left[\sum_{j=1}^n v_j {v_j}^*\right] v, \qquad Bv = \left[\sum_{j=1}^n \lambda_j v_j {v_j}^*\right] v, \qquad \forall v \in \mathbb{C}^n$$

- **Inf.-dim.:** Operator $\mathcal{L}: \mathcal{D}(\mathcal{L}) \to \mathcal{H}$. Typically, no basis of e-vectors! *Spectral theorem*: (projection-valued) spectral measure E

$$g = \left[\int_{\mathrm{Spec}(\mathcal{L})} 1 \, \mathrm{d}E(\lambda)\right] g, \qquad \mathcal{L}g = \left[\int_{\mathrm{Spec}(\mathcal{L})} \lambda \, \mathrm{d}E(\lambda)\right] g, \qquad \forall g \in \mathcal{H}$$

- **Spectral measures:** $\nu_g(U) = \langle E(U)g, g\rangle$ ($\|g\| = 1$) prob. measure.

Koopman mode decomposition (again!)

ν_g probability measures on $[-\pi,\pi]_{\text{per}}$

Leb. decomp: $$d\nu_g(y) = \underbrace{\sum_{\text{eigenvalues } \lambda_j = \exp(i\theta_j)} \langle P_{\lambda_j} g, g \rangle \, \delta(y-\theta_j)}_{\text{discrete}} + \underbrace{\rho_g(y)dy + d\nu_g^{sc}(y)}_{\text{continuous}}$$

eigenfunction of $\mathcal{K}$

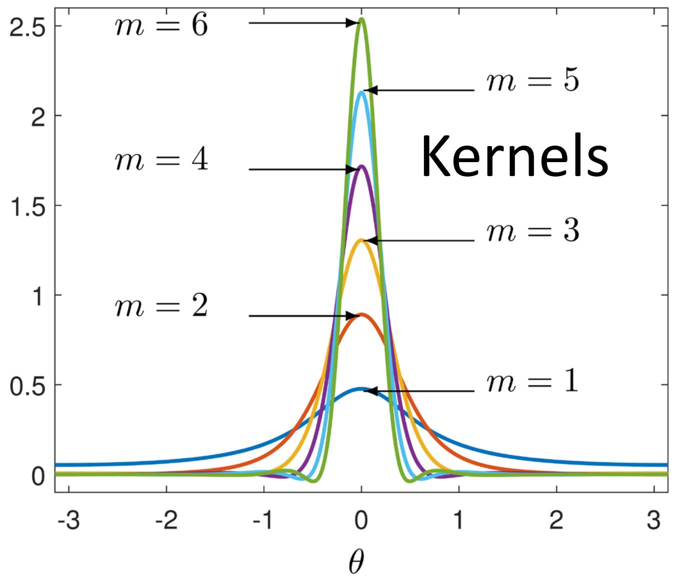
generalised eigenfunction of $\mathcal{K}$

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

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

Computing ν_g diagonalises non-linear dynamical system!

mth order Plemelj formula



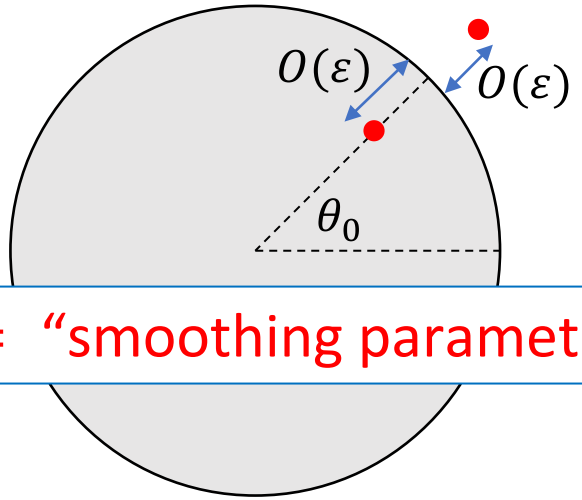
$$\mathcal{C}_g(z) = \int_{-\pi}^{\pi} \frac{e^{i\theta}\mathrm{d}\nu_g(\theta)}{e^{i\theta}-z} = \begin{cases} \langle(\mathcal{K}-zI)^{-1}g, \mathcal{K}^*g\rangle, \text{if } |z|>1 \\ -z^{-1}\langle g, (\mathcal{K}-\bar{z}^{-1}I)^{-1}g\rangle, \text{if } 0<|z|<1 \end{cases}$$

ResDMD computes with error control

mth order rational kernels

$$K_\varepsilon(\theta) = \frac{e^{-i\theta}}{2\pi}\sum_{j=1}^{m}\left[\frac{c_j}{e^{-i\theta}-(1+\varepsilon\bar{z_j})^{-1}} - \frac{d_j}{e^{-i\theta}-(1+\varepsilon z_j)}\right]$$

$$[K_\varepsilon * \nu_g](\theta_0) = \sum_{j=1}^{m}\left[c_j\mathcal{C}_g\left(e^{i\theta_0}(1+\varepsilon\bar{z_j})^{-1}\right) - d_j\mathcal{C}_g\left(e^{i\theta_0}(1+\varepsilon z_j)\right)\right]$$



$\varepsilon =$ "smoothing parameter"

$O(PN_K)$ cost for evaluation at P values of θ

Convergence

Theorem: *Automatic* selection of $N_K(\varepsilon)$ with $O(\varepsilon^m \log(1/\varepsilon))$ convergence:

- Density of continuous spectrum ρ_g. (pointwise and L^p)
- Integration against test functions. (weak convergence)

$$\int_{-\pi}^{\pi} h(\theta)\, [K_\varepsilon * \nu_g](\theta)\, \mathrm{d}\theta = \int_{-\pi}^{\pi} h(\theta)\ \mathrm{d}\nu_g(\theta) + O(\varepsilon^m \log(1/\varepsilon))$$

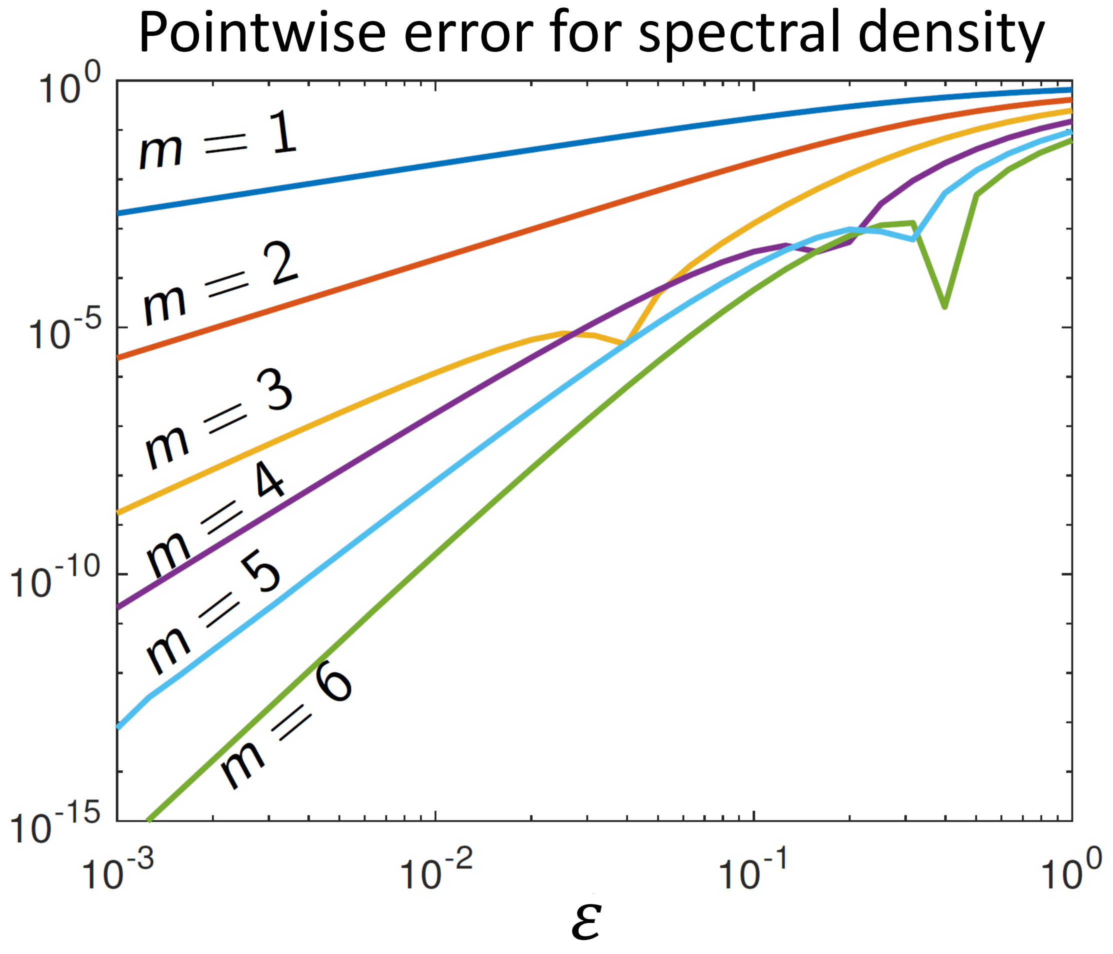
- Also recover discrete spectrum.

Example

$$\mathcal{K} = \begin{pmatrix} \overline{\alpha_0} & \overline{\alpha_1}\rho_0 & \rho_0\rho_1 & & & \\ \rho_0 & -\overline{\alpha_1}\alpha_0 & -\alpha_0\rho_1 & & & \\ & \overline{\alpha_2}\rho_1 & -\overline{\alpha_2}\alpha_1 & \overline{\alpha_3}\rho_2 & \rho_3\rho_2 & \\ & \rho_2\rho_1 & -\alpha_1\rho_2 & -\overline{\alpha_3}\alpha_2 & -\rho_3\alpha_2 & \ddots \\ & & & \overline{\alpha_4}\rho_3 & -\overline{\alpha_4}\alpha_3 & \ddots \\ & & & \ddots & \ddots & \ddots \end{pmatrix}$$

$$\alpha_j = (-1)^j 0.95^{(j+1)/2}, \qquad \rho_j = \sqrt{1 - |\alpha_j|^2}$$

Generalised shift, typical building block of many dynamical systems.



NB: Small N_K critical in data-driven computations.

Large d ($\Omega \subseteq \mathbb{R}^d$): *robust* and *scalable*

Popular to learn dictionary $\{\psi_1, \ldots, \psi_{N_K}\}$

E.g., DMD with truncated SVD (linear dictionary, most popular), kernel methods (this talk), neural networks, etc.

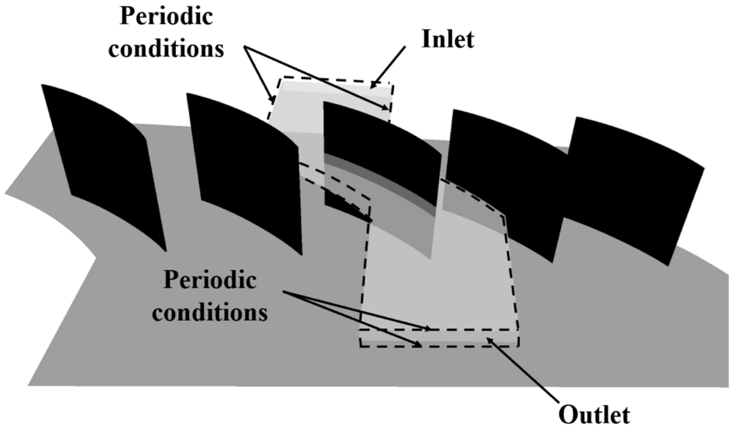
Q: Is discretisation span$\{\psi_1, \ldots, \psi_{N_K}\}$ large/rich enough?

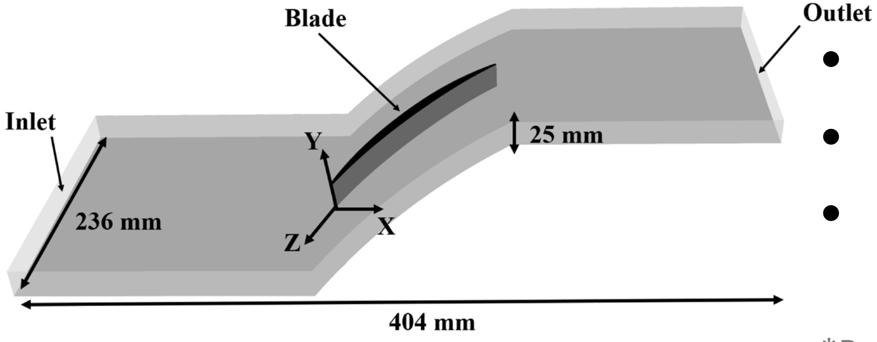
Above algorithms:

- Pseudospectra: $\{z_k : \tau_k < \varepsilon\} \subseteq \mathrm{Spec}_\varepsilon(\mathcal{K})$ **error control**
- Spectral measures: $\mathcal{C}_g(z)$ and smoothed measures **adaptive check**

$\Longrightarrow$ Rigorously ***verify*** learnt dictionary $\{\psi_1, \ldots, \psi_{N_K}\}$

Example: pressure field of turbulent flow

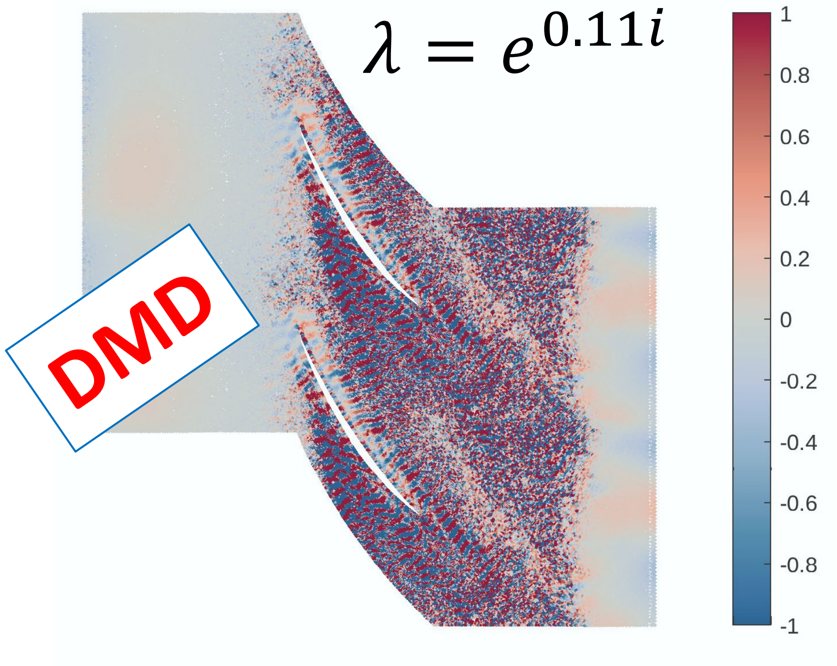




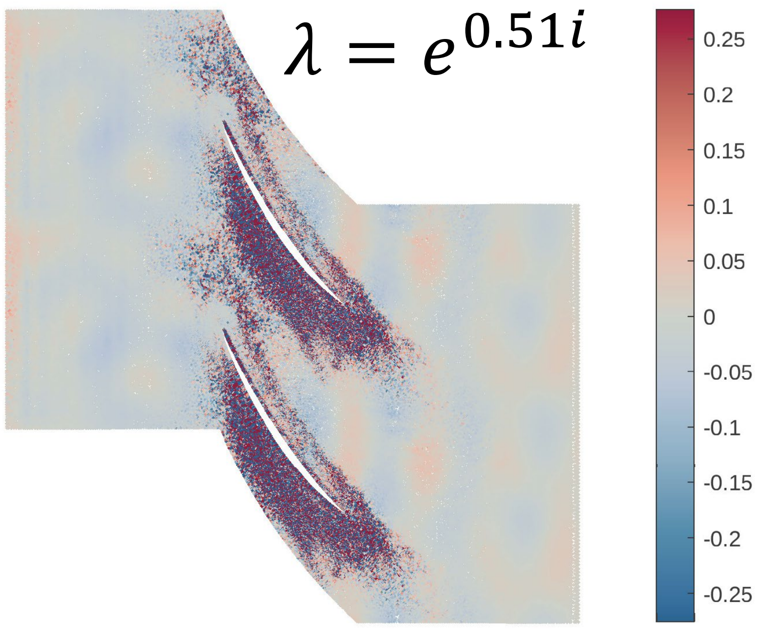
- Data collected for 2×10^{-4}s
- Reynolds number $\approx 3.9 \times 10^5$
- Ambient dimension $\approx 300{,}000$ (number of measurement points*)

*Raw measurements provided by Stephane Moreau (Sherbrooke)

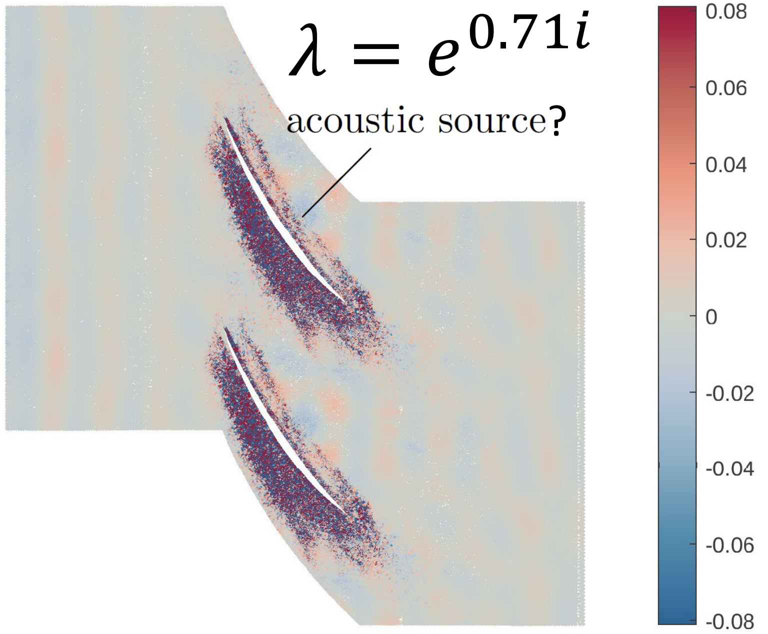
Rel. Error = ?



Rel. Error = ?



Rel. Error = ?



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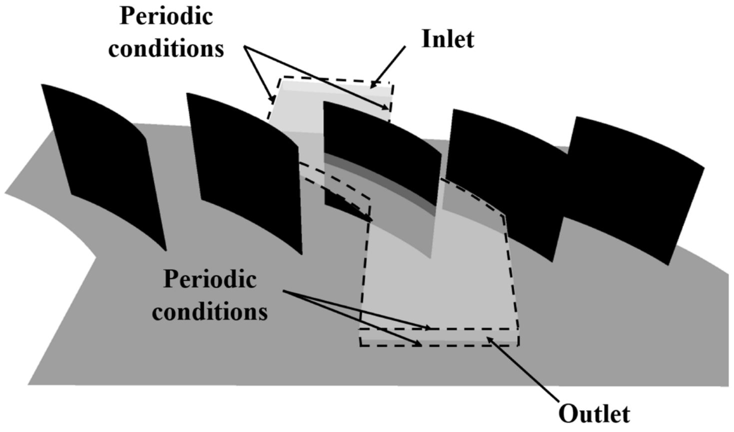
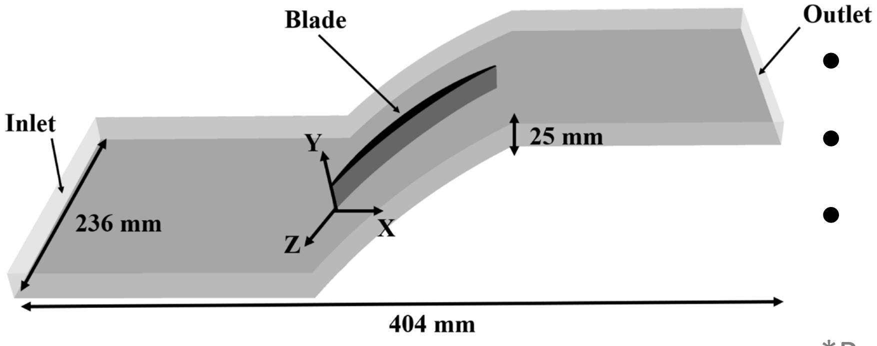
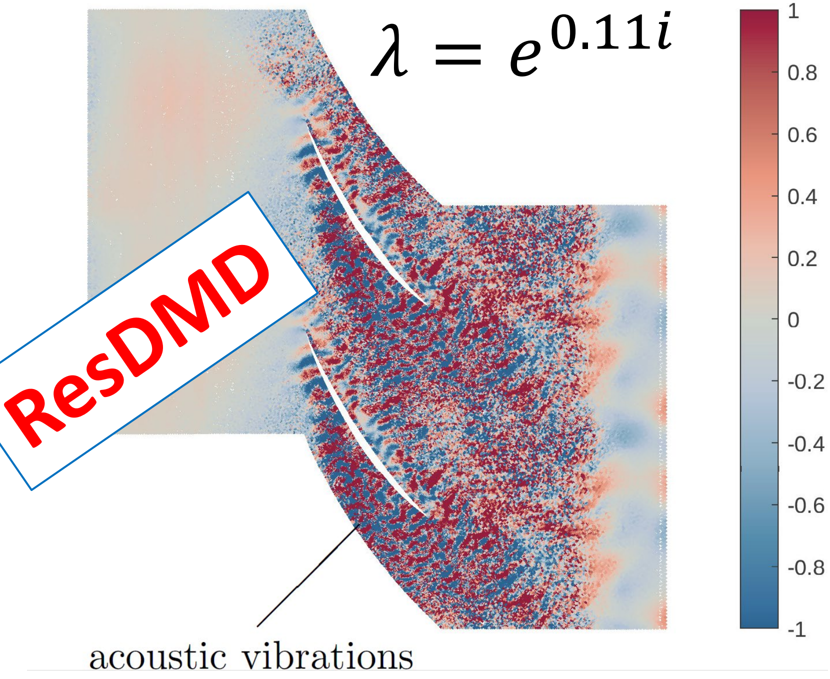




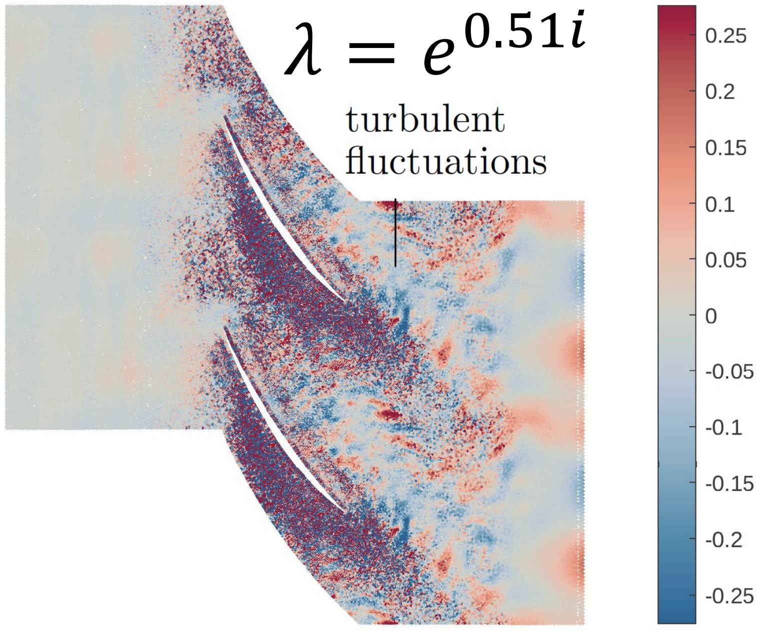
- Data collected for 2×10^{-4}s
- Reynolds number $\approx 3.9 \times 10^5$
- Ambient dimension $\approx$ 300,000 (number of measurement points*)

*Raw measurements provided by Stephane Moreau (Sherbrooke)

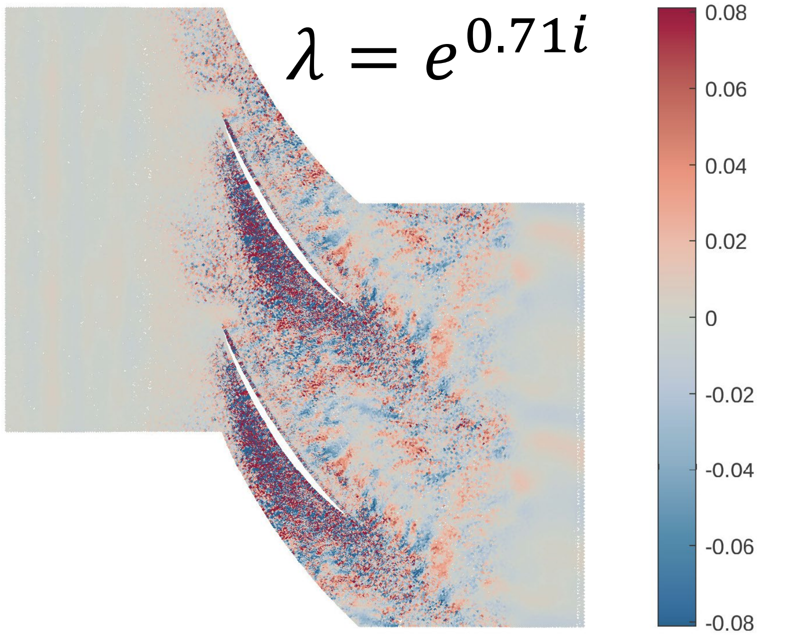
Rel. Error ≤ 0.0054



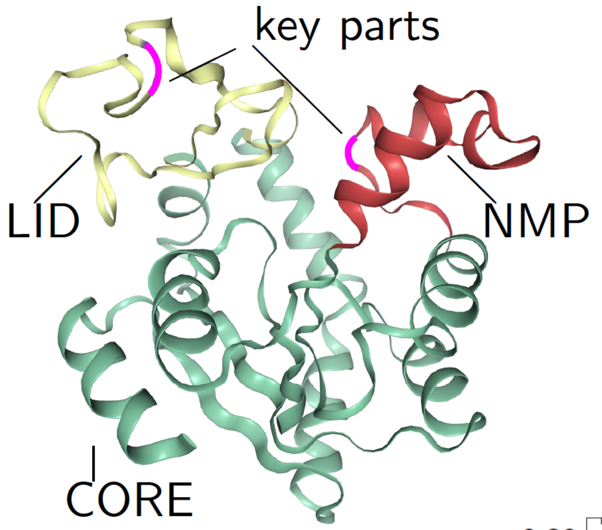
Rel. Error ≤ 0.0128

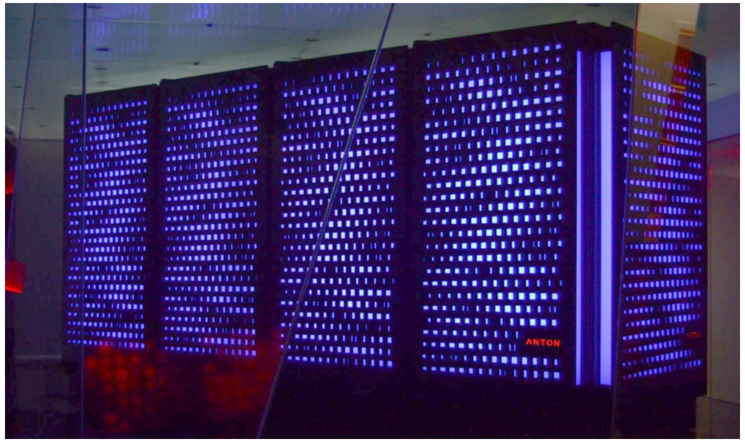


Rel. Error ≤ 0.0196



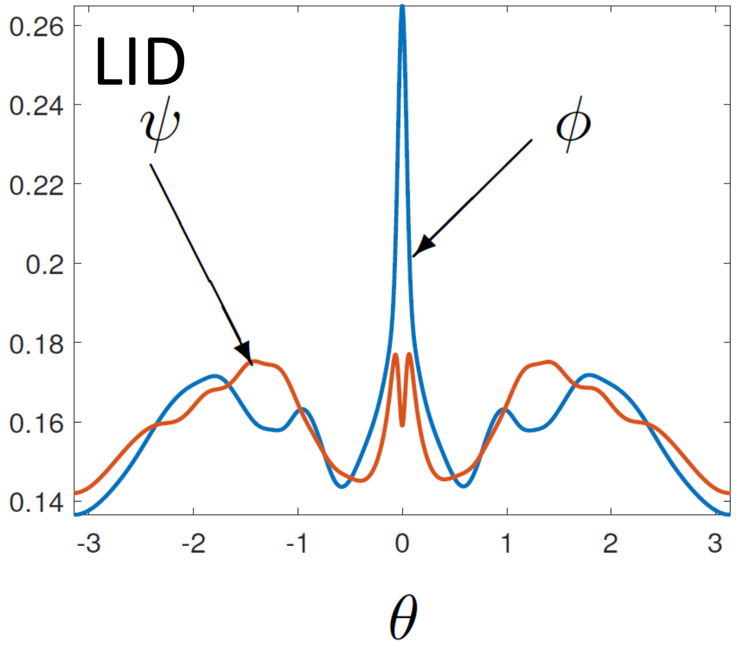
Example: molecular dynamics (Adenylate Kinase)

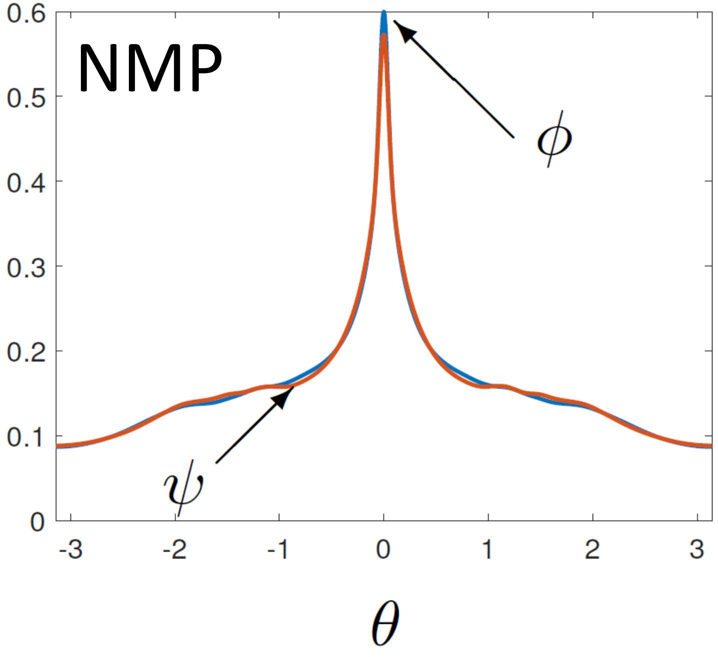




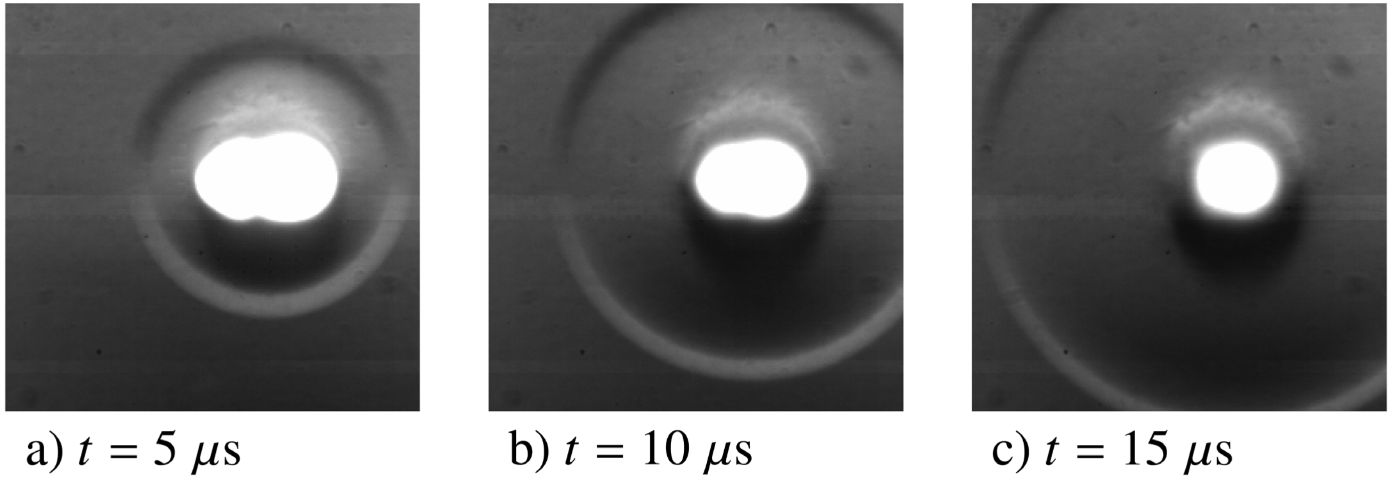
- All-atom equilibrium simulation for 1.004×10^{-6}s
- Ambient dimension ≈ 20,000 (positions and momenta of atoms)
- 6th order kernel (spec res 10^{-6})

*Dataset: www.mdanalysis.org/MDAnalysisData/adk_equilibrium.html



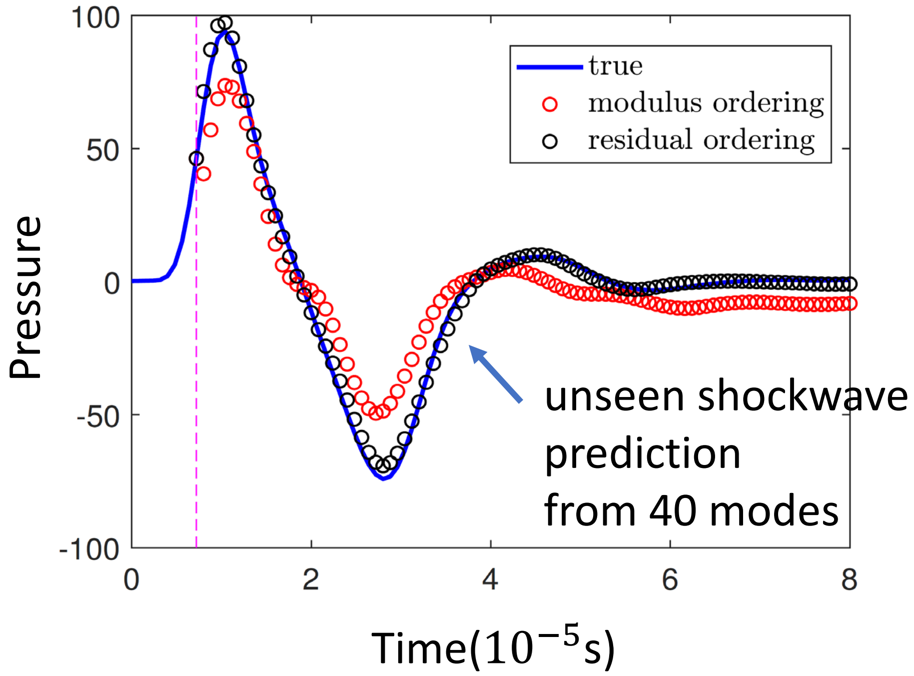


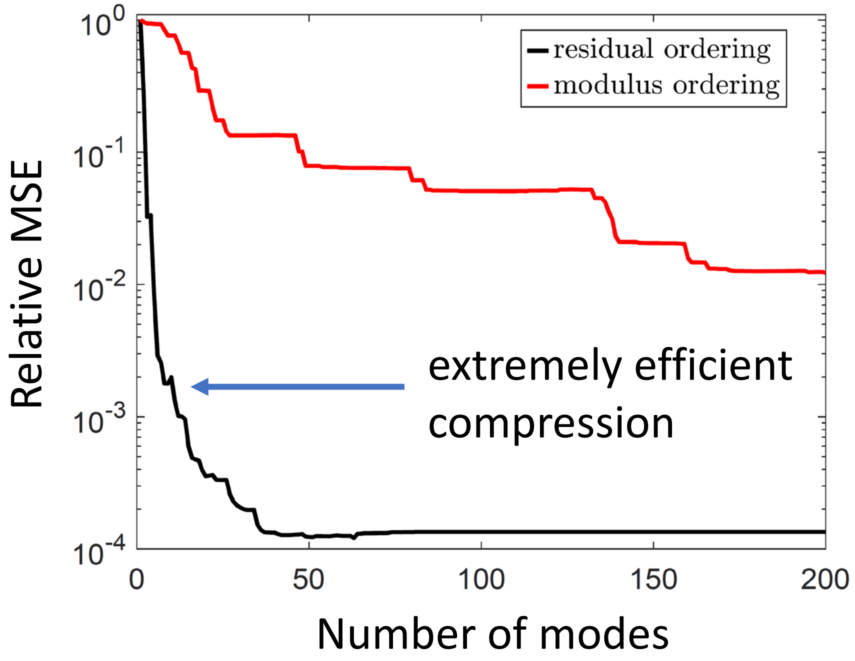
Example: laser-induced plasma



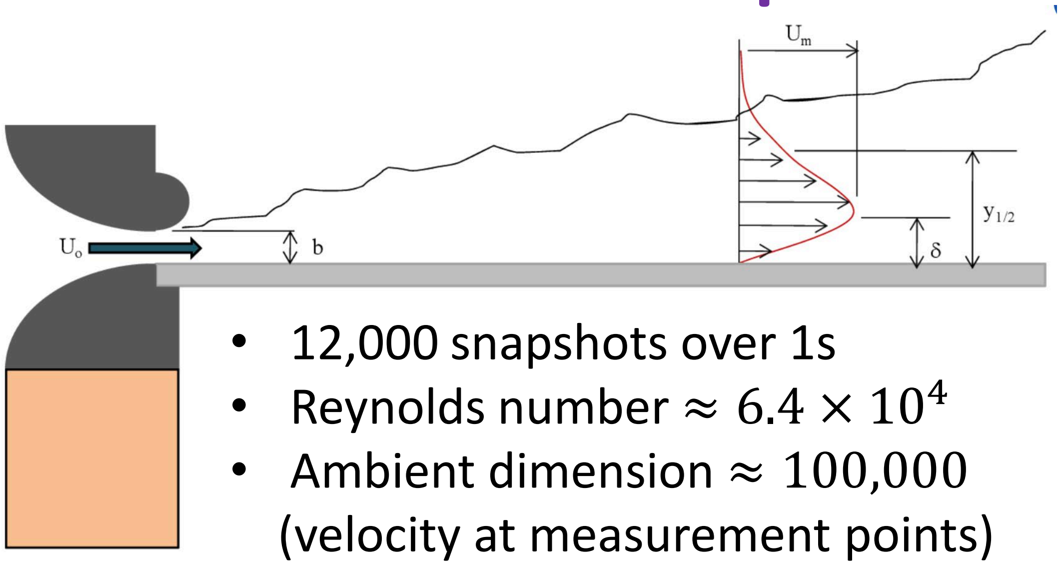
- 60 realisations ($M = 6600$)
- Ambient dimension ≈ 10 (length of initial window*)

*Raw measurements provided by Máté Szőke (Virginia Tech)



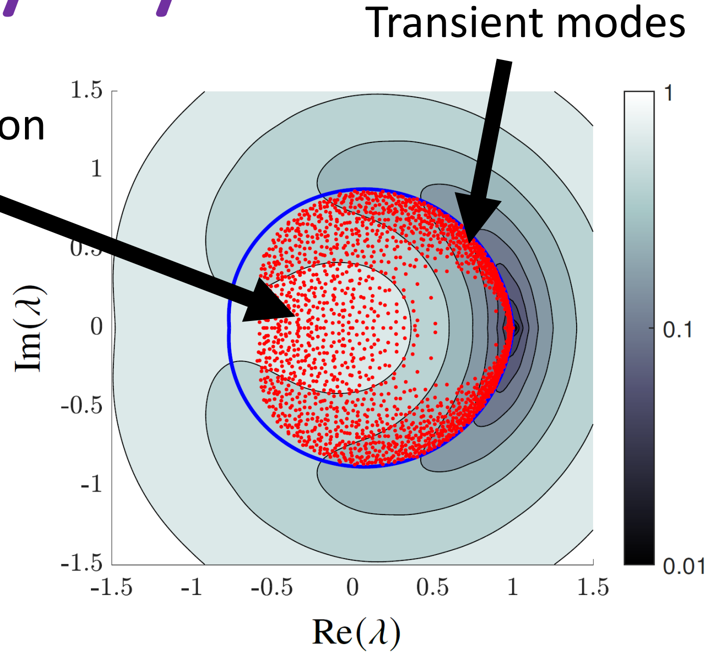


Example: wall-jet boundary layer

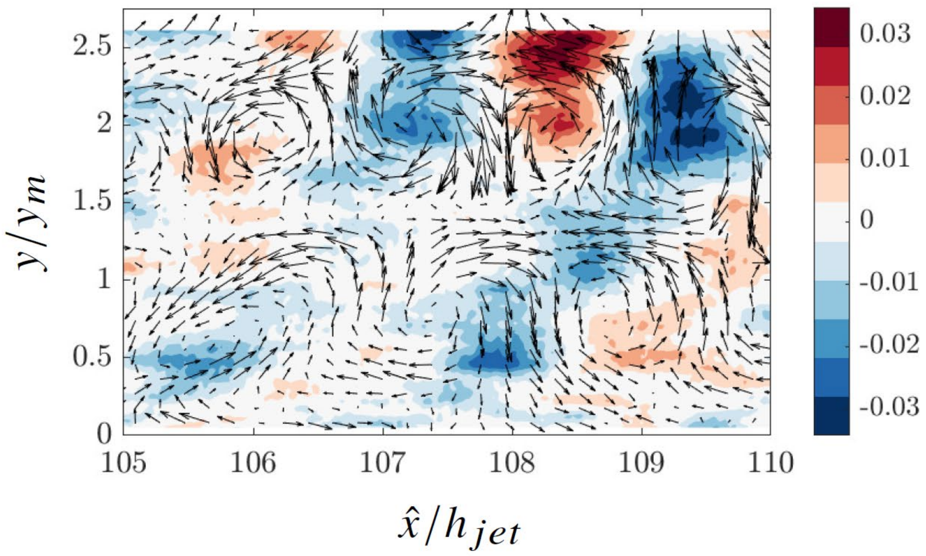


- 12,000 snapshots over 1s
- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension $\approx 100{,}000$ (velocity at measurement points)

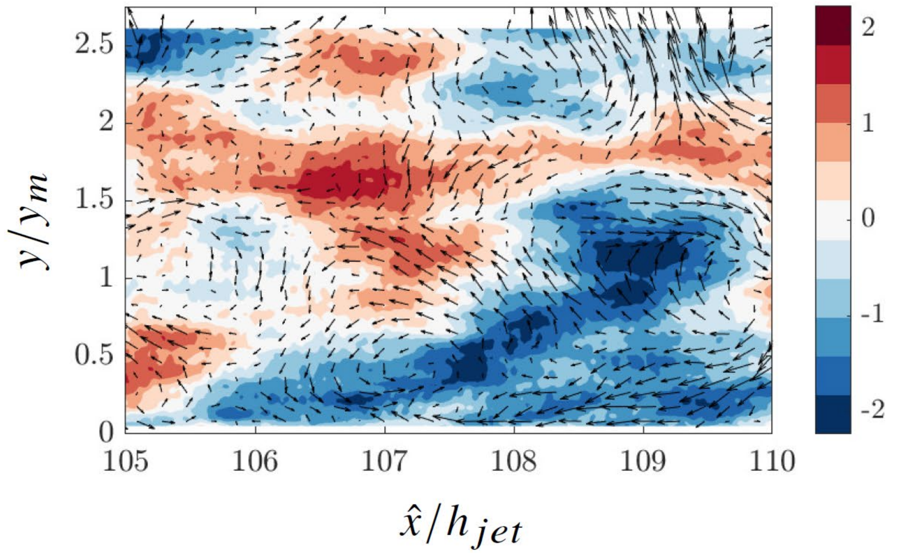
*Raw measurements provided by Máté Szőke (Virginia Tech)



$\lambda = 0.9439 + 0.2458i$, error ≤ 0.0765



$\lambda = 0.8948 + 0.1065i$, error ≤ 0.1105



Wider programme: a toolkit

- Inf.-dim. computational analysis $\Longrightarrow$ **Compute spectral properties for the first time.**
- Solvability Complexity Index hierarchy $\Longrightarrow$ **Algorithms realise the boundaries of what's possible.**
- Builds on and extends work of **Turing**, **Smale**, and **McMullen.**
- **Extends to:** Foundations of AI, PDEs (e.g., time-dep. Schrödinger eq. on $L^2(\mathbb{R}^d)$ with error control), optimisation (e.g., guarantees), computer-assisted proofs, …

- C., "*On the computation of geometric features of spectra of linear operators on Hilbert spaces*," **Found. Comput. Math.**, under revisions.
- C., "*Computing spectral measures and spectral types*," **Communications in Mathematical Physics**, 2021.
- C., Horning, Townsend "*Computing spectral measures of self-adjoint operators*," **SIAM Review**, 2021.
- C., Roman, Hansen, "*How to compute spectra with error control*," **Physical Review Letters**, 2019.
- C., Hansen, "*The foundations of spectral computations via the solvability complexity index hierarchy*," **JEMS**, 2022.
- C., Antun, 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**, 2022.
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- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "*On the solvability complexity index hierarchy and towers of algorithms*," arXiv, 2020.
- Smale, "*The fundamental theorem of algebra and complexity theory*," **Bulletin of the AMS**, 1981, *36 pp.*
- McMullen, "*Families of rational maps and iterative root-finding algorithms*," **Annals of Mathematics**, 1987, *27 pp.*

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General technique for lower bounds by embedding combinatorial problems.

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Small sample of classification theorems

Increasing difficulty

Error control

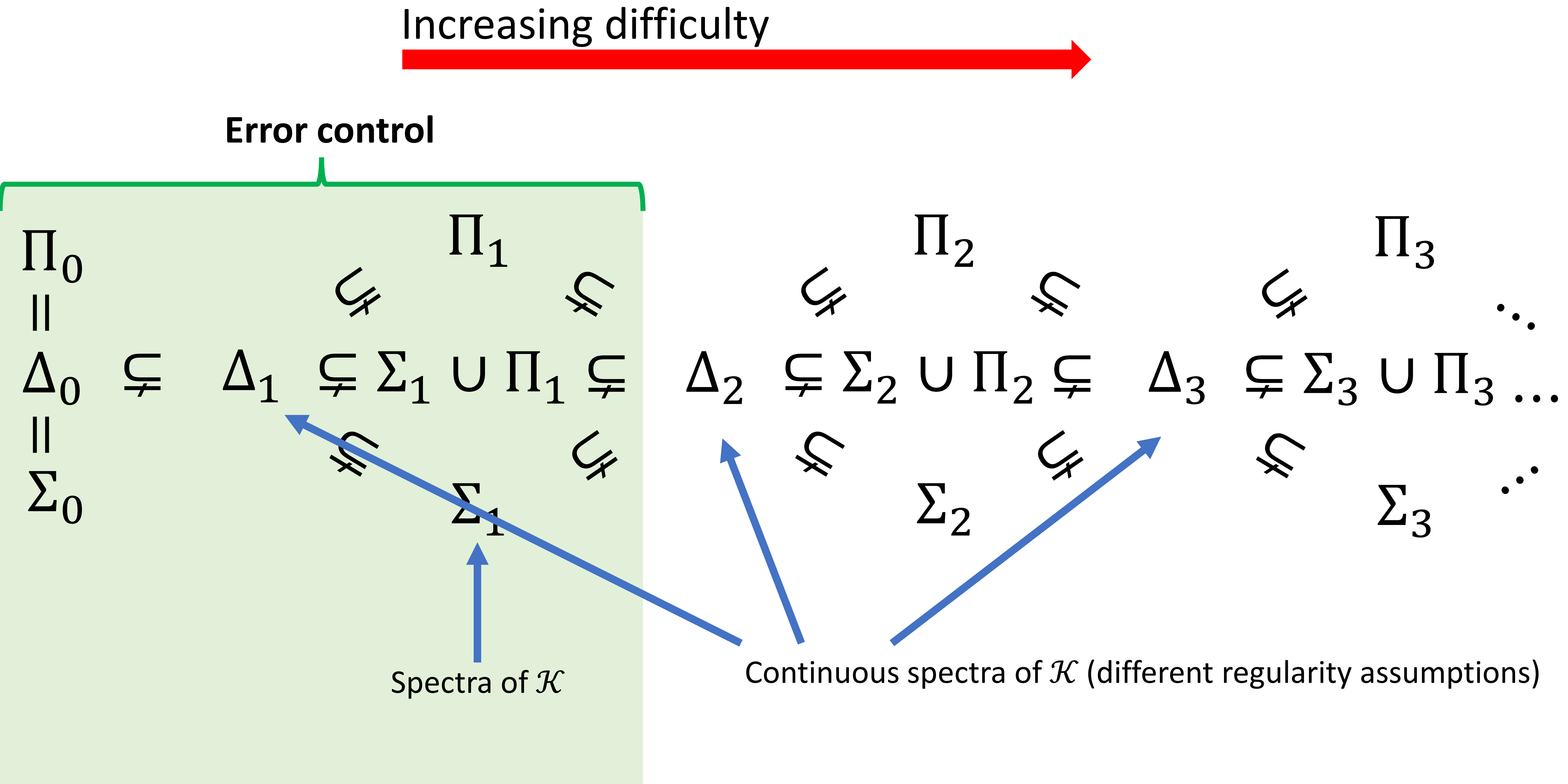
$$\Pi_0 = \Delta_0 = \Sigma_0 \subsetneq \Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \ldots$$

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

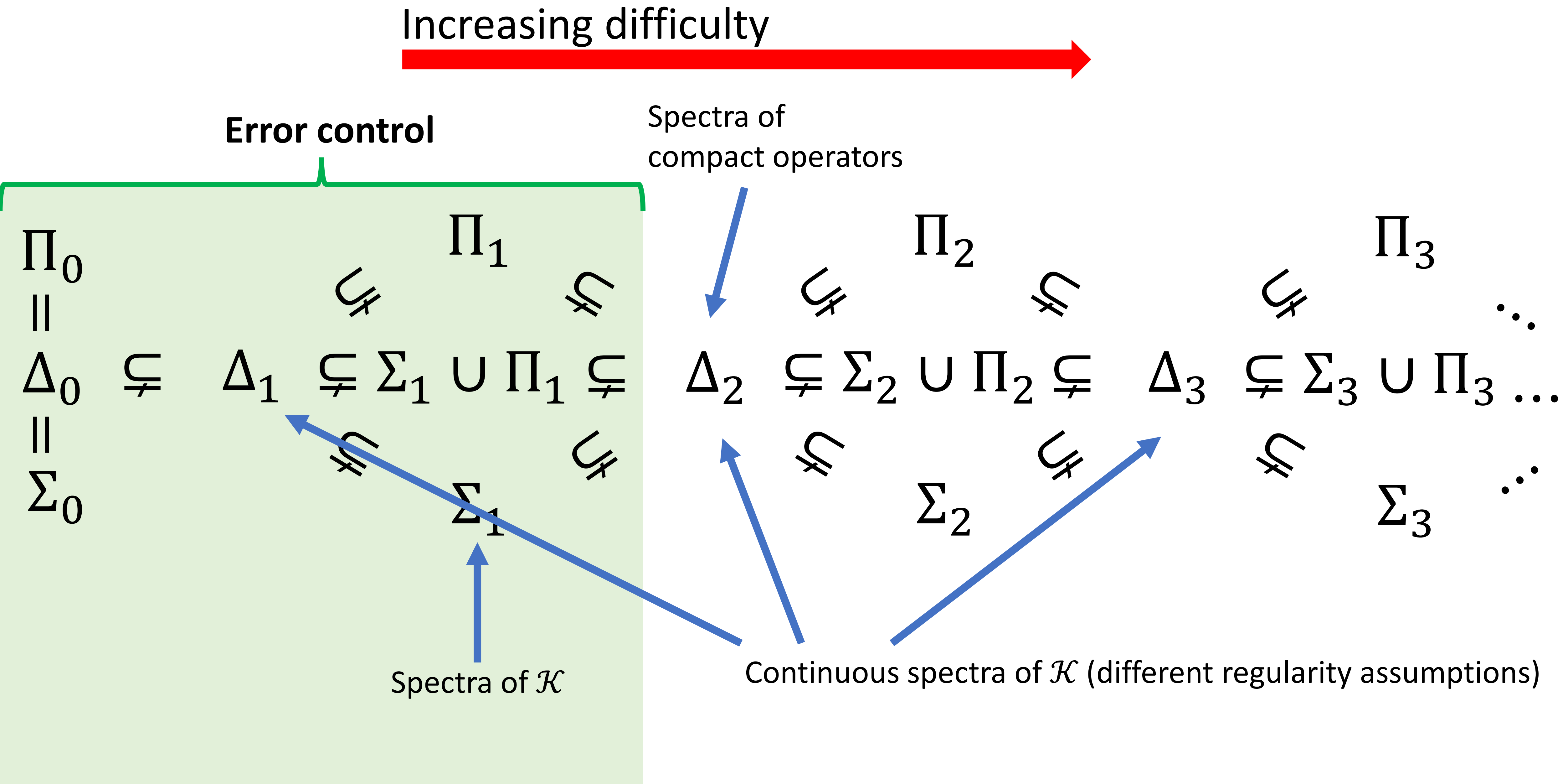
$$\Delta_2 \subsetneq \Pi_2 \subsetneq \Delta_3, \quad \Delta_2 \subsetneq \Sigma_2 \subsetneq \Delta_3$$

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

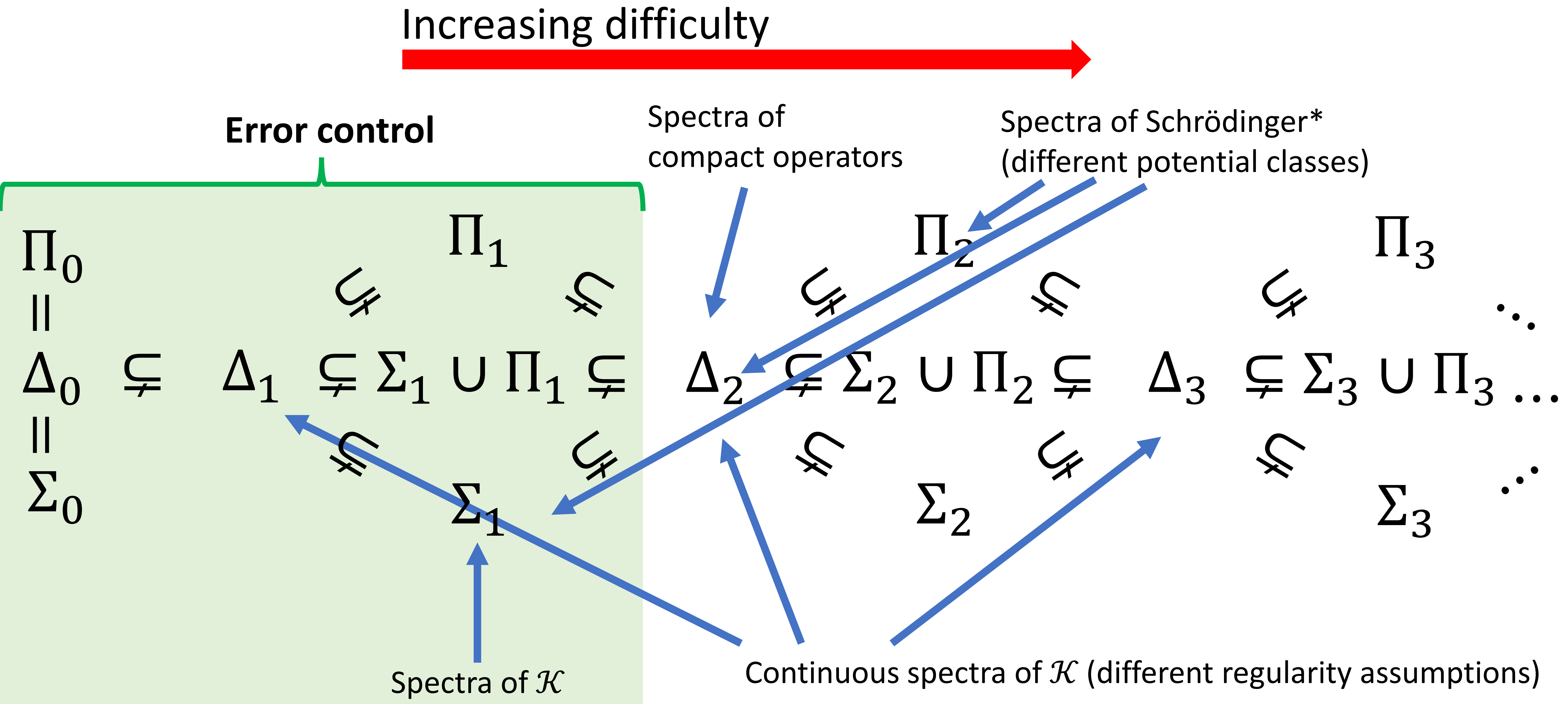
Small sample of classification theorems



Small sample of classification theorems

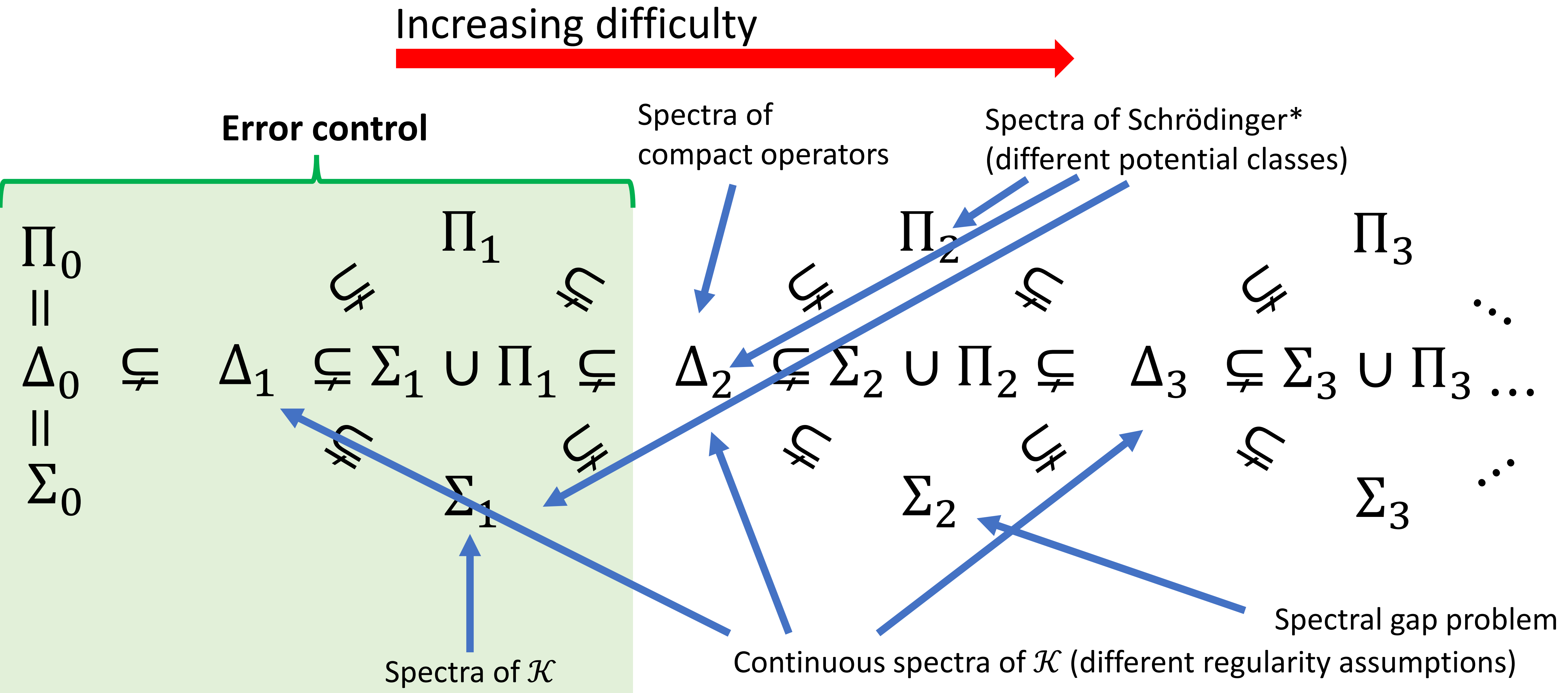


Small sample of classification theorems



**Open problem of Schwinger*: "The special canonical group," "Unitary operator bases," PNAS, 1960.

Small sample of classification theorems



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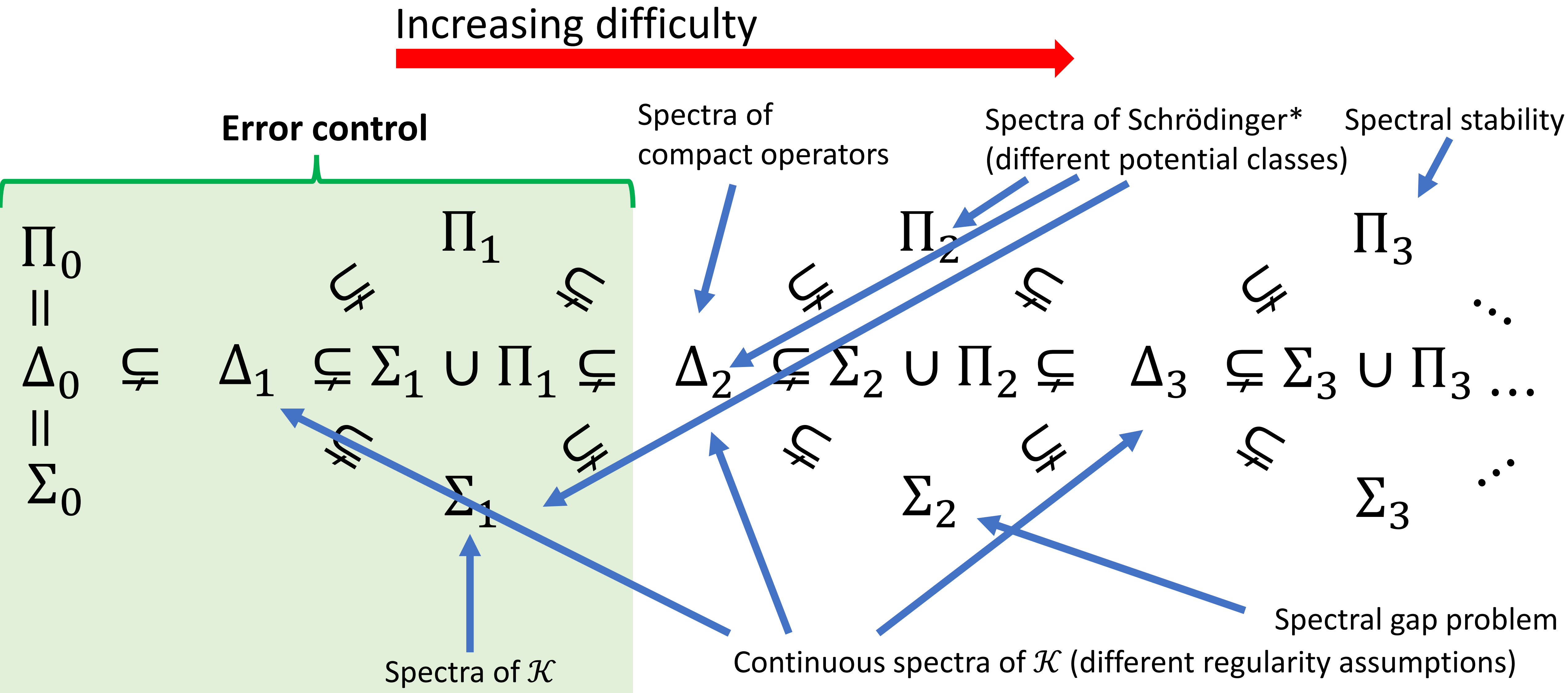
Small sample of classification theorems



**Open problem of Schwinger*: "The special canonical group," "Unitary operator bases," PNAS, 1960.

Summary

Overcame: **1) "too much", 2) "too little", 3) continuous spectra, 4) verification.**

- Spectra, pseudospectra, residuals of general Koopman operators (error control).
    - **Idea:** New matrix for residual ⇒ ResDMD.
- Spectral measures of measure-preserving systems with high-order convergence.
    - **Idea:** Convolution with rational kernels via resolvent and ResDMD.
- Dealt with high-dimensional dynamical systems.
    - **Idea:** Use ResDMD to verify learned dictionaries.

First general methods with convergence guarantees!

⟶ Opens the door to rigorous data-driven Koopmania!

Convergence of quadrature

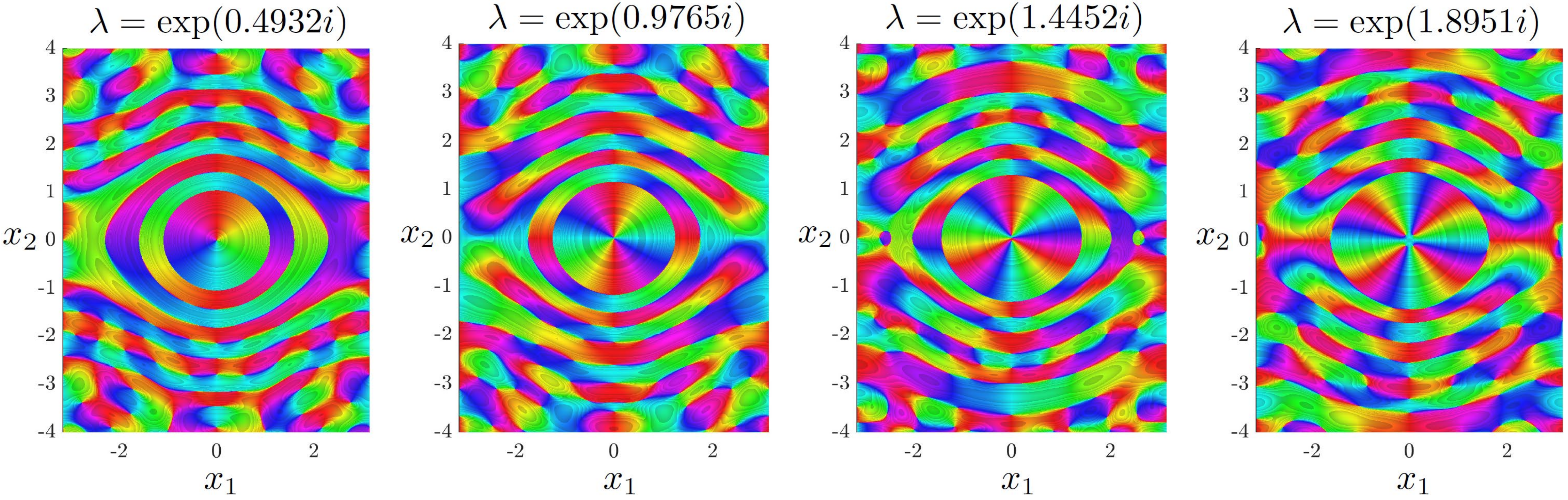
E.g., $\langle \mathcal{K}\psi_k, \psi_j \rangle = \lim_{M\to\infty} \sum_{m=1}^{M} w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})}$

Three examples:

- **High-order quadrature:** $\{x^{(m)}, w_m\}_{m=1}^{M}$ M-point quadrature rule.
  Rapid convergence. Requires free choice of $\{x^{(m)}\}_{m=1}^{M}$ and small d.
- **Random sampling:** $\{x^{(m)}\}_{m=1}^{M}$ selected at random.
  Large d. Slow Monte Carlo $O(M^{-1/2})$ rate of convergence.
- **Ergodic sampling:** $x^{(m+1)} = F(x^{(m)})$.
  Single trajectory, large d. Requires ergodicity, convergence can be slow.

Most common

Example: non-linear pendulum



Colour represents complex argument, constant modulus shown as shadowed steps.
All residuals smaller than $\varepsilon = 0.05$ (made smaller by increasing N_K).

Koopman mode decomposition ($\mathbb{K}V = V\Lambda$)

Standard Koopman mode decomposition (order modes by $|\Lambda|$):

$$g(x) \approx \underbrace{[\psi_1(x) \quad \cdots \quad \psi_{N_K}(x)]V}_{\text{approx Koopman e-functions}} \underbrace{\left(V\sqrt{W}\Psi_X\right)^{\dagger}\sqrt{W}[g(x^{(1)}) \quad \cdots \quad g(x^{(M)})]^{\mathrm{T}}}_{\text{Koopman modes}}$$

$$\overset{?}{\Rightarrow} g(x_n) \approx \underbrace{[\psi_1(x) \quad \cdots \quad \psi_{N_K}(x)]V}_{\text{approx Koopman e-functions}} \Lambda^n \underbrace{\left(V\sqrt{W}\Psi_X\right)^{\dagger}\sqrt{W}[g(x^{(1)}) \quad \cdots \quad g(x^{(M)})]^{\mathrm{T}}}_{\text{Koopman modes}}$$

Residual Koopman mode decomposition (order modes by $\mathrm{res}(\lambda, \mathbf{v})$):

Controllable error

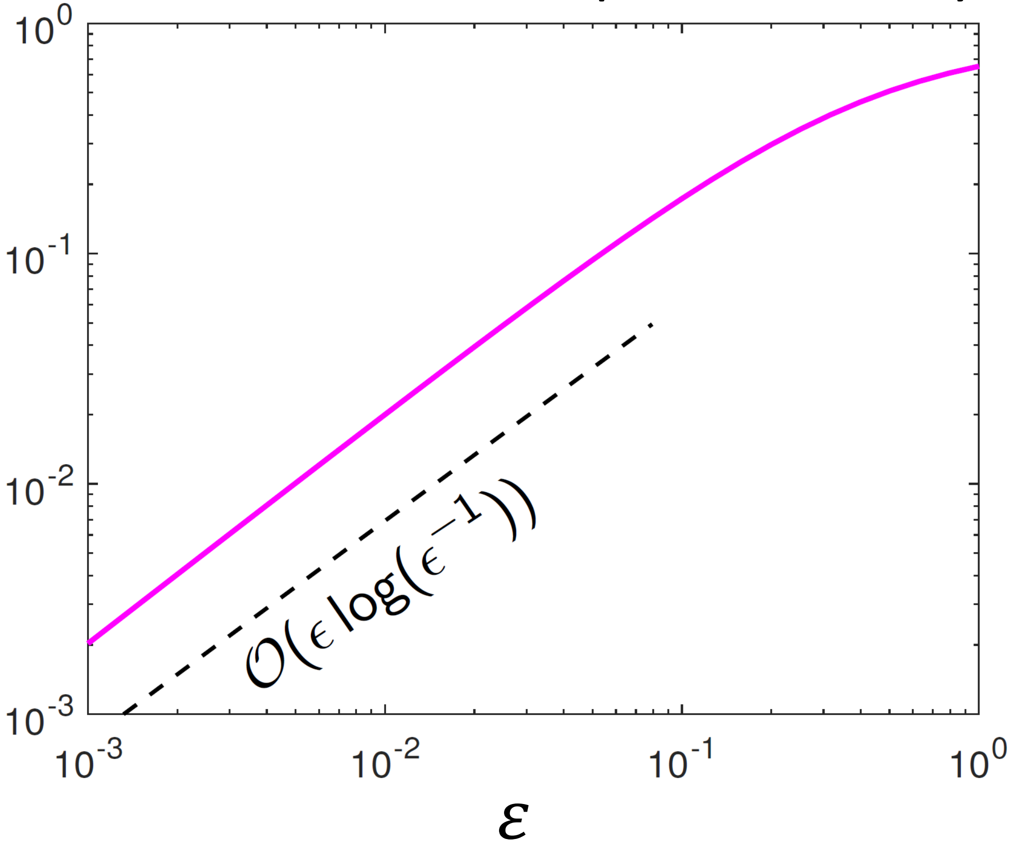
$$g(x) \approx \underbrace{[\psi_1(x) \quad \cdots \quad \psi_{N_K}(x)]V_{(\varepsilon)}}_{\text{approx Koopman e-functions}} \underbrace{\left(V_{(\varepsilon)}\sqrt{W}\Psi_X\right)^{\dagger}\sqrt{W}[g(x^{(1)}) \quad \cdots \quad g(x^{(M)})]^{\mathrm{T}}}_{\text{Koopman modes}}$$

$$g(x_n) \approx \underbrace{[\psi_1(x_0) \quad \cdots \quad \psi_{N_K}(x_0)]V_{(\varepsilon)}}_{\text{approx Koopman e-functions}} \Lambda_{(\varepsilon)}^n \underbrace{\left(V_{(\varepsilon)}\sqrt{W}\Psi_X\right)^{\dagger}\sqrt{W}[g(x^{(1)}) \quad \cdots \quad g(x^{(M)})]^{\mathrm{T}}}_{\text{Koopman modes}}$$

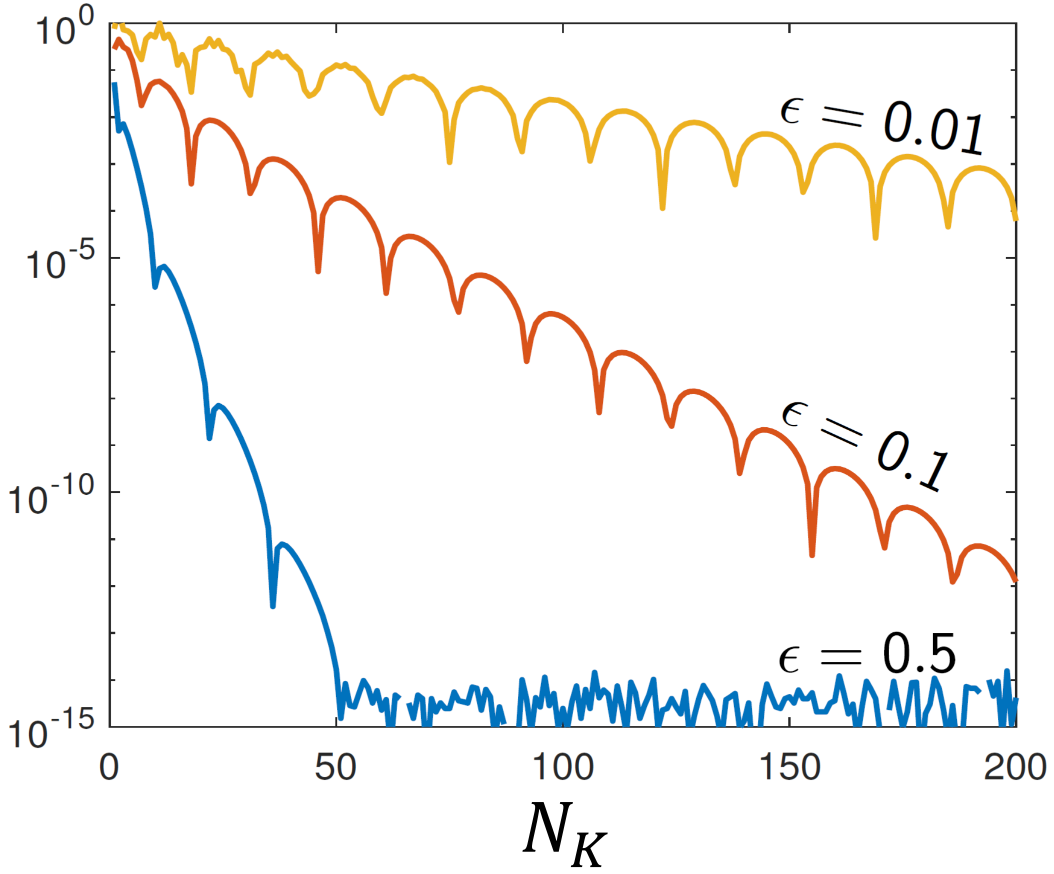
But … slow convergence

Problem: As $\varepsilon \downarrow 0$, error is $O(\varepsilon \cdot \log(1/\varepsilon))$ and $N_K(\varepsilon) \to \infty$.

Pointwise error for spectral density



Error due to discretisation



Small N_K critical in <u>data-driven</u> computations. Can we improve convergence rate?

Kernel method

Algorithm 4 A computational framework for kernelized versions of Algorithms 1 to 3.

Input: Snapshot data $\{\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)}\}_{m=1}^{M'}$ and $\{\hat{\boldsymbol{x}}^{(m)}, \hat{\boldsymbol{y}}^{(m)}\}_{m=1}^{M''}$, positive-definite kernel function $\mathcal{S} : \Omega \times \Omega \to \mathbb{R}$, and positive integer $N_K'' \leq M'$.

1: Apply kernel EDMD to $\{\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)}\}_{m=1}^{M'}$ with kernel $\mathcal{S}$ to compute the matrices $\sqrt{W}\Psi_X\Psi_X^*\sqrt{W}$ and $\sqrt{W}\Psi_Y\Psi_X^*\sqrt{W}$ using the kernel trick.

2: Compute U and Σ from the eigendecomposition $\sqrt{W}\Psi_X\Psi_X^*\sqrt{W} = U\Sigma^2U^*$.

3: Compute the dominant N_K'' eigenvectors of $\widetilde{K}_{\mathrm{EDMD}} = (\Sigma^\dagger U^*)\sqrt{W}\Psi_Y\Psi_X^*\sqrt{W}(U\Sigma^\dagger)$ and stack them column-by-column into $Z \in \mathbb{C}^{M' \times N_K''}$.

4: Apply a QR decomposition to orthogonalize Z to $Q = \begin{bmatrix} Q_1 & \cdots & Q_{N_K''} \end{bmatrix} \in \mathbb{C}^{M' \times N_K''}$.

5: Apply Algorithms 1 to 3 with $\{\hat{\boldsymbol{x}}^{(m)}, \hat{\boldsymbol{y}}^{(m)}\}_{m=1}^{M''}$ and the dictionary $\{\psi_j\}_{j=1}^{N_K''}$, where

$$\psi_j(\boldsymbol{x}) = \begin{bmatrix} \mathcal{S}(\boldsymbol{x}, \boldsymbol{x}^{(1)}) & \mathcal{S}(\boldsymbol{x}, \boldsymbol{x}^{(2)}) & \cdots & \mathcal{S}(\boldsymbol{x}, \boldsymbol{x}^{(M')}) \end{bmatrix} (U\Sigma^+)Q_j, \qquad 1 \leq j \leq N_K''.$$

Output: Spectral properties of Koopman operator according to Algorithms 1 to 3.

RESEARCH ARTICLE | APPLIED MATHEMATICS | FULL ACCESS

The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem

Matthew J. Colbrook, Vegard Antun, and Anders C. Hansen Authors Info & Affiliations

March 16, 2022 | 119 (12) e2107151119 | https://doi.org/10.1073/pnas.2107151119

Significance

Instability is the Achilles' heel of modern artificial intelligence (AI) and a paradox, with training algorithms finding unstable neural networks (NNs) despite the existence of stable ones. This foundational issue relates to Smale's 18th mathematical problem for the 21st century on the limits of AI. By expanding methodologies initiated by Gödel and Turing, we demonstrate limitations on the existence of (even randomized) algorithms for computing NNs. Despite numerous existence results of NNs with great approximation properties, only in specific cases do there also exist algorithms that can compute them. We initiate a classification theory on which NNs can be trained and introduce NNs that—under suitable conditions—are robust to perturbations and exponentially accurate in the number of hidden layers.

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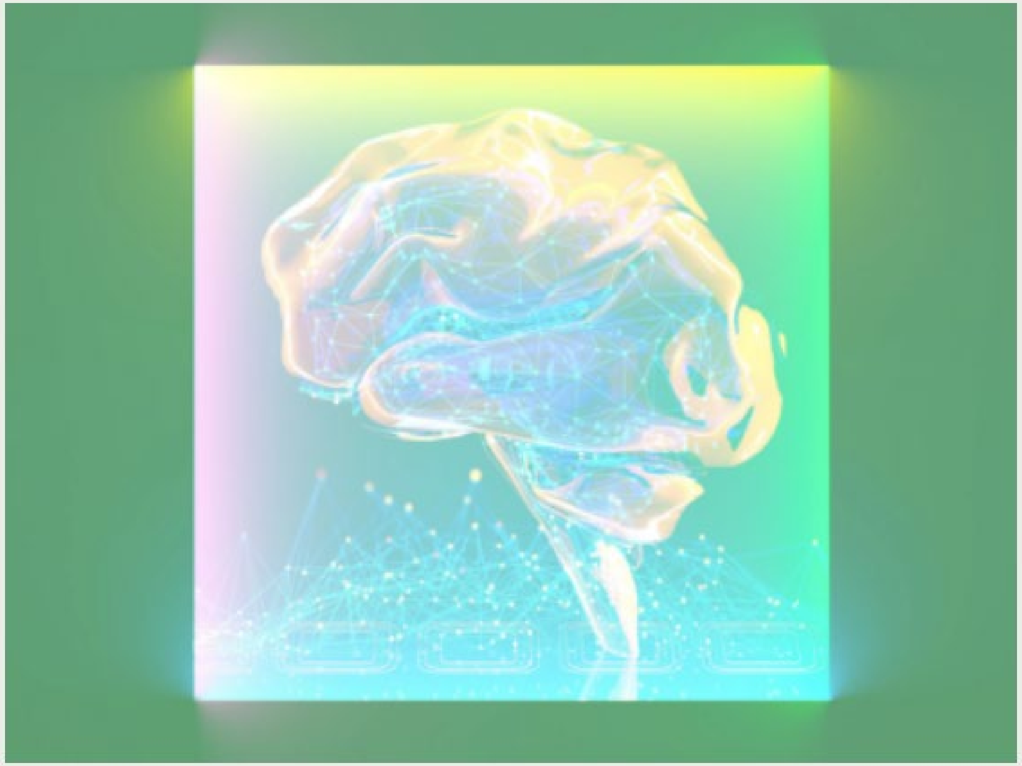

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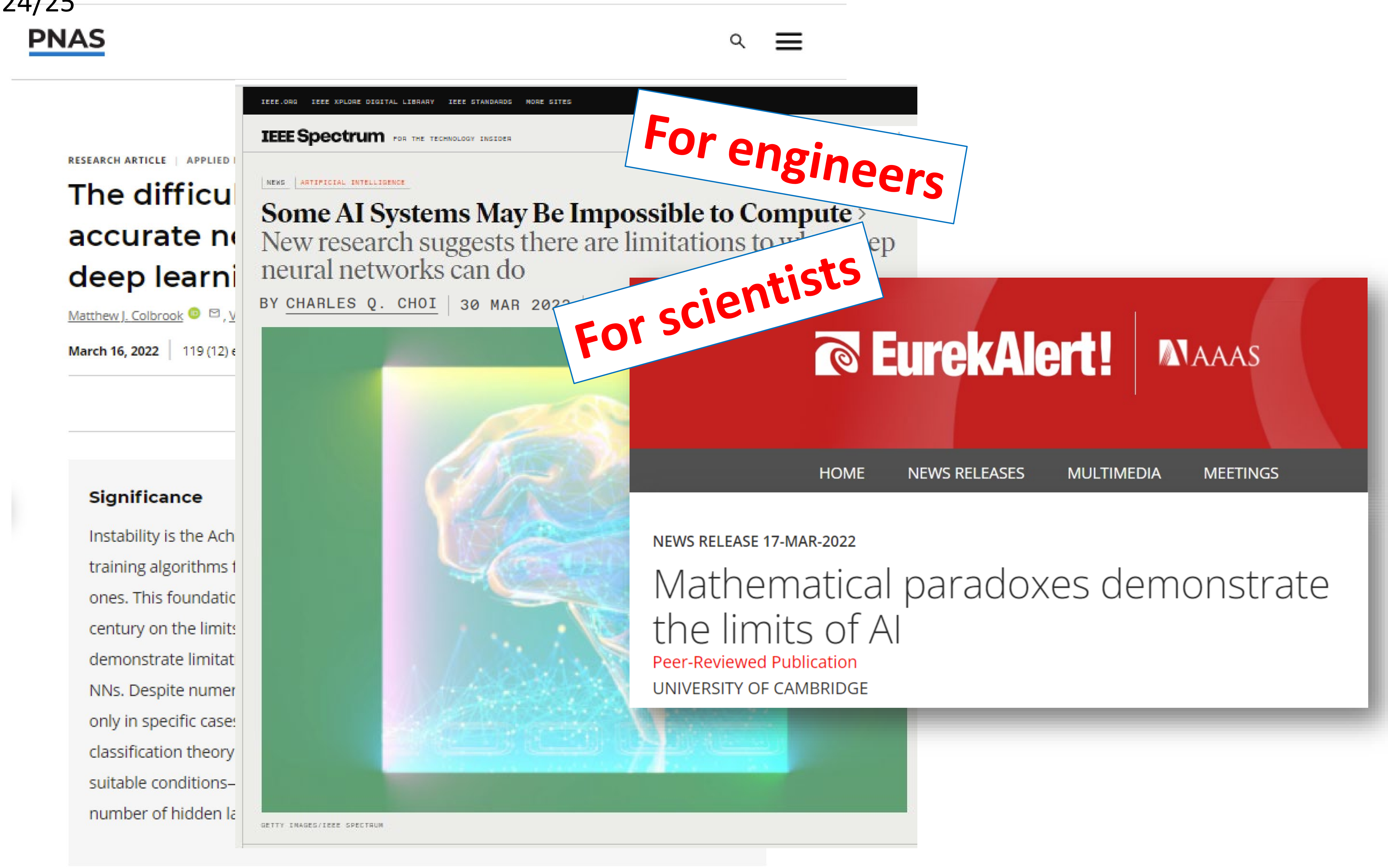
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Original image
AI reconstruction
Instabilities in medical diagnosis
Original Mole
Perturbed Mole
Benign
Malignant
Model confidence