

Verifying data-driven computations of Koopman spectra

Matthew Colbrook

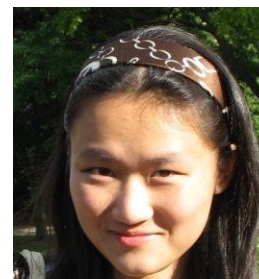
University of Cambridge

19/09/2023

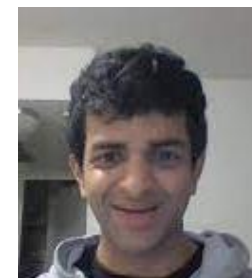
Joint work with:



Lorna Ayton



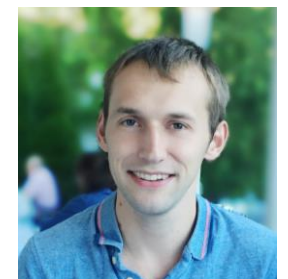
Qin Li



Ryan Raut



Matt Szőke



Alex Townsend

- 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.
- C., Li, Raut, Townsend, “*Beyond expectations: Residual Dynamic Mode Decomposition and Variance for Stochastic Dynamical Systems*,” arxiv.

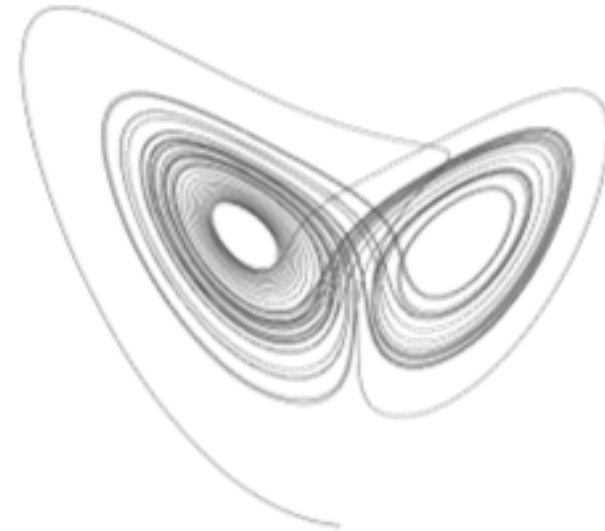
Data-driven (deterministic) dynamical systems

State $x \in \Omega \subseteq \mathbb{R}^d$.

Unknown function $F: \Omega \rightarrow \Omega$ governs dynamics: $x_{n+1} = F(x_n)$

Goal: Verified learning from data $\{x^{(m)}, y^{(m)} = F(x^{(m)})\}_{m=1}^M$.

Applications: chemistry, climatology, control, electronics, epidemiology, finance, fluids, molecular dynamics, neuroscience, plasmas, robotics, video processing, etc.



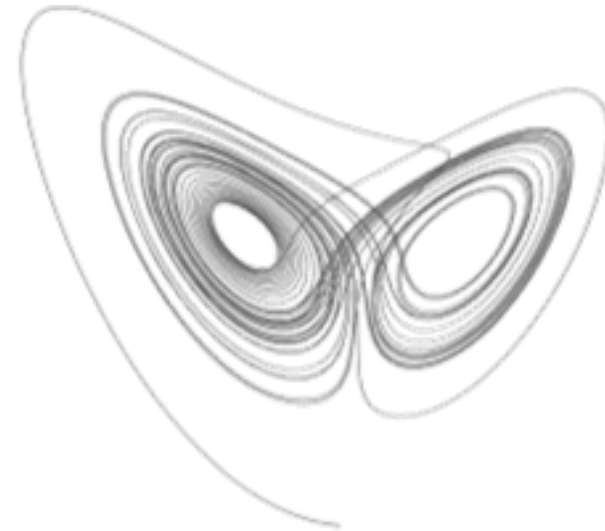
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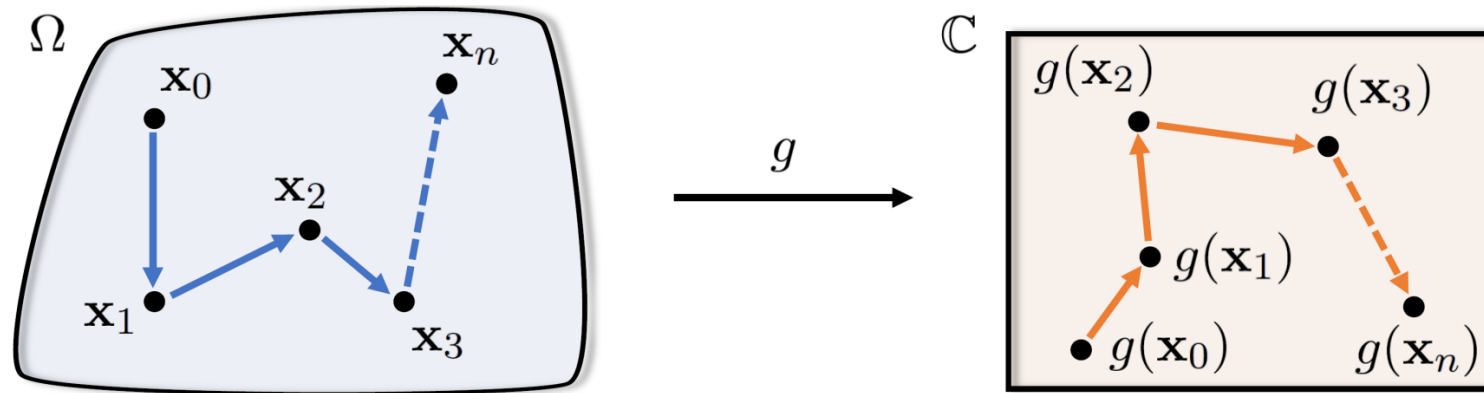
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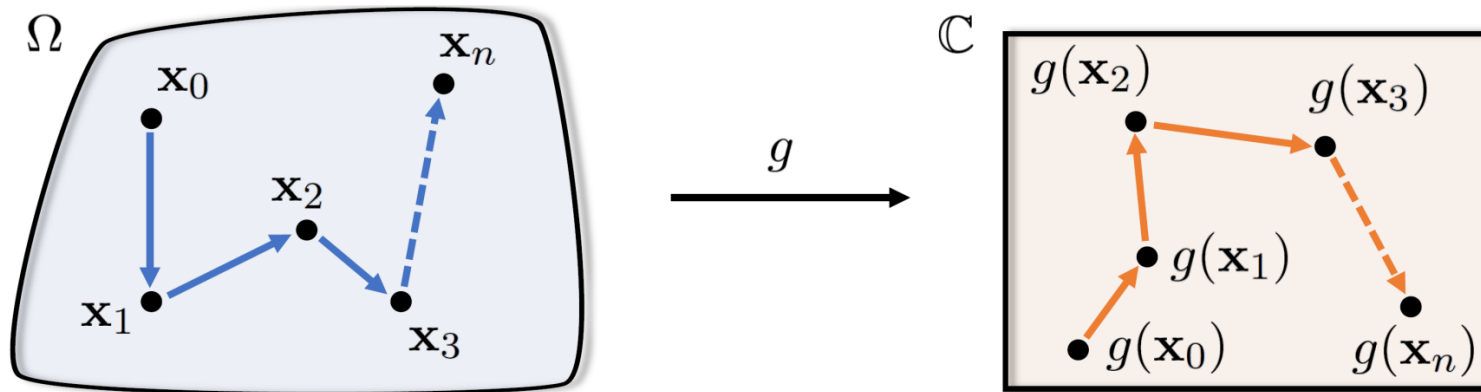
Koopman Operator $\mathcal{K}$: A global linearization



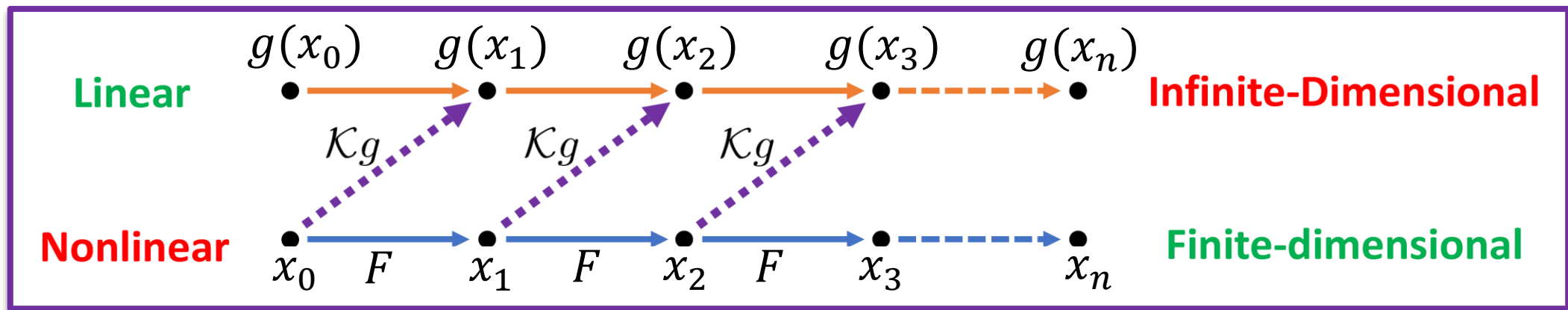
- $\mathcal{K}$ acts on functions $g: \Omega \rightarrow \mathbb{C}$, $[\mathcal{K}g](x) = g(F(x))$.
- Function space: $L^2(\Omega, \omega)$, positive measure ω , inner product $\langle \cdot, \cdot \rangle$.



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- 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.

Example 1: Why is linear much easier?

• Suppose $\Omega = \mathbb{R}^d$, $F(x) = Ax$, $A \in \mathbb{R}^{d \times d}$, $A = V\Lambda V^{-1}$.

• Set $\xi = V^{-1}x$,

$$\xi_n = V^{-1}x_n = V^{-1}A^n x_0 = \Lambda^n V^{-1}x_0 = \Lambda^n \xi_0$$

• For $w^T A = \lambda w$, set $g(x) = w^T x$,

$$[\mathcal{K}g](x) = w^T Ax = \lambda g(x)$$

Eigenfunction

Trivial dynamics!

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

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

Much more general (non-linear and even chaotic F) ...



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Trivial dynamics!

$$[\mathcal{K}g](x) = w^T Ax = \lambda g(x)$$

$$[\mathcal{K}g^n](x) = (w^T Ax)^n = \lambda^n g^n(x)$$

Eigenfunction

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

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

Much more general (non-linear and even chaotic F) ...



Example 2: Koopman mode decomposition

confirm
prove
justify
check
inspect
verify
attest
clarify
authenticate

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

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

eigenfunction of $\mathcal{K}$

generalized eigenfunction of $\mathcal{K}$

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

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

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

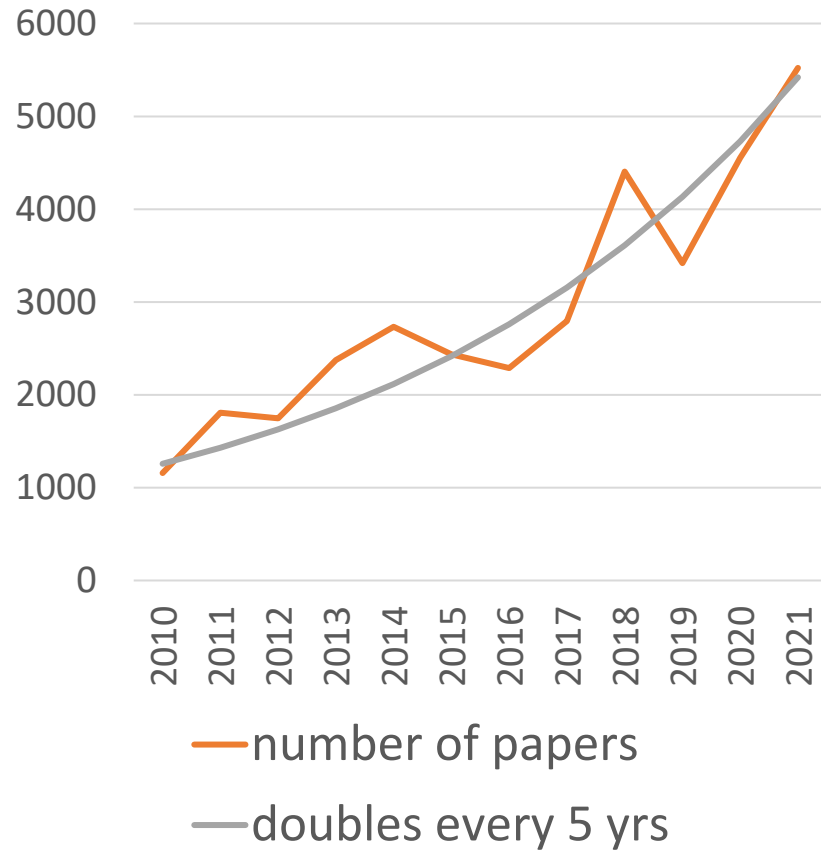
Focus on computing spectral properties of $\mathcal{K}$...

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



Koopmania! $\approx 35,000$ papers in last decade!

New Papers on
"Koopman Operators"



Few works on convergence guarantees or verification.

Why?

- Perhaps a different community with different focus?
- Dealing with infinite dimensions is notoriously hard ...



Challenges of computing

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

Truncate/discretize: $\mathcal{K} \longrightarrow \mathbb{K} \in \mathbb{C}^{N \times N}$

- 1) **Too much:** Spurious modes $\lambda \notin \text{Spec}(\mathcal{K})$
- 2) **Too little:** Miss parts of $\text{Spec}(\mathcal{K})$
- 3) **Continuous spectra**
- 4) **Verification**
- 5) **Instability**



Caution



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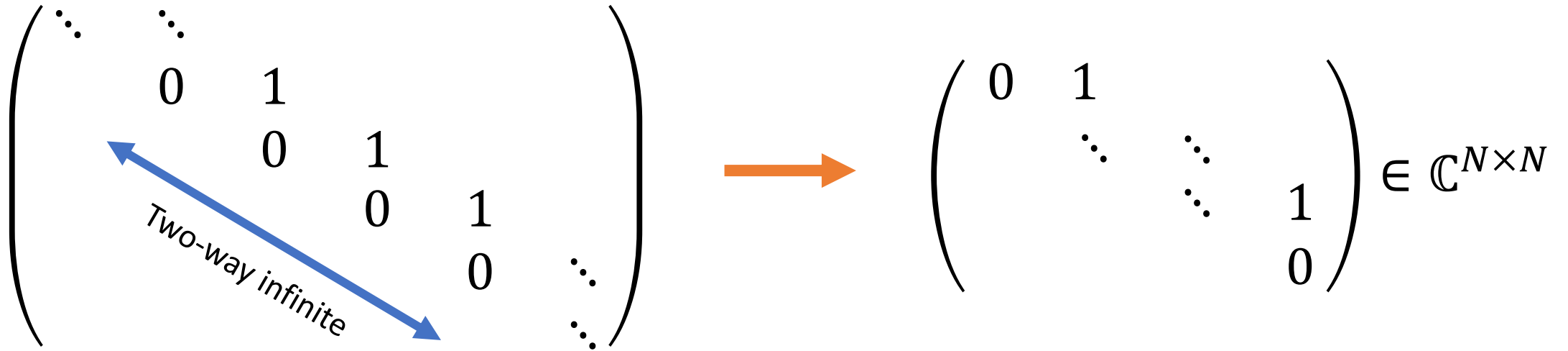
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Caution

Some inf-dim comp. spec. problems cannot be solved, regardless of computational power, time or model.

A simple example on $\ell^2(\mathbb{Z})$



The diagram illustrates the relationship between a two-way infinite operator and its finite truncation. On the left, a large matrix is shown with a blue double-headed arrow labeled "Two-way infinite" passing through it. The matrix has a tridiagonal structure with 0s on the main diagonal and 1s on the diagonals immediately above and below. Ellipses at the top and bottom indicate the infinite extent of the matrix. An orange arrow points from this matrix to a finite $N \times N$ matrix on the right. This finite matrix is also tridiagonal, with 0s on the main diagonal and 1s on the diagonals immediately above and below, and it is labeled as belonging to $\mathbb{C}^{N \times N}$.

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

- Spectrum is unit circle.
- Spectrum is stable.
- Continuous spectra.

- Spectrum is $\{0\}$.
- Spectrum is unstable.
- Discrete spectra.

Example might look silly, but lots of Koopman operators are built up from operators like these!

Dynamic Mode Decomposition (DMD)

Given dictionary $\{\psi_1, \dots, \psi_N\}$ of functions $\psi_j: \Omega \rightarrow \mathbb{C}$,

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

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

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

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

Challenges: too much, too little, continuous spectra, verification, instability.

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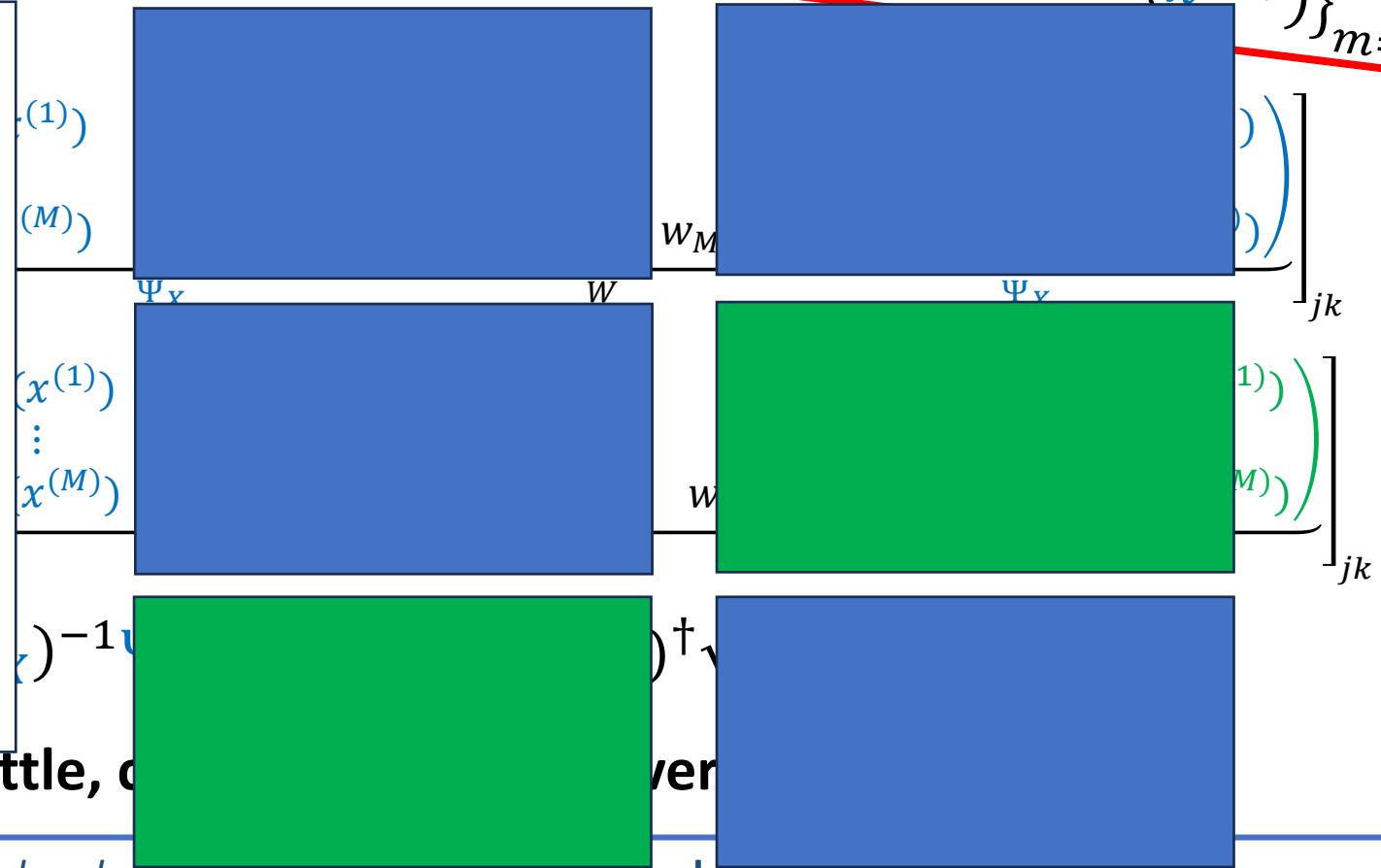
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Residual DMD (ResDMD): $\mathcal{K}$ and $\mathcal{K}^* \mathcal{K}$

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

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

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ResDMD: avoiding “too much”

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

eigenvectors eigenvalues

Algorithm 1:

1. Compute $G, K_1, K_2 \in \mathbb{C}^{N \times N}$ and eigendecomposition $K_1 V = G V \Lambda$.
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 $\text{res}(\lambda, \mathbf{v}) \leq \varepsilon$ ($\varepsilon = \text{input tol}$).

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

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



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



ResDMD: avoiding “too little”

$$\text{Sp}_\varepsilon(\mathcal{K}) = \bigcup_{\|\mathcal{B}\| \leq \varepsilon} \text{Sp}(\mathcal{K} + \mathcal{B}), \quad \lim_{\varepsilon \downarrow 0} \text{Sp}_\varepsilon(\mathcal{K}) = \text{Sp}(\mathcal{K})$$

Algorithm 2:

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

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

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

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



Quadrature with trajectory data

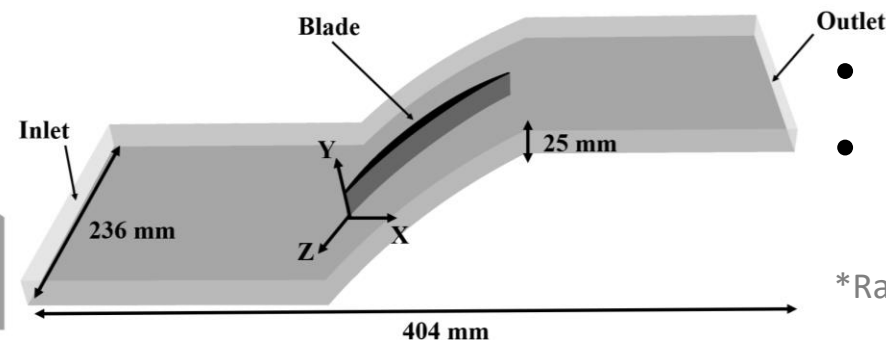
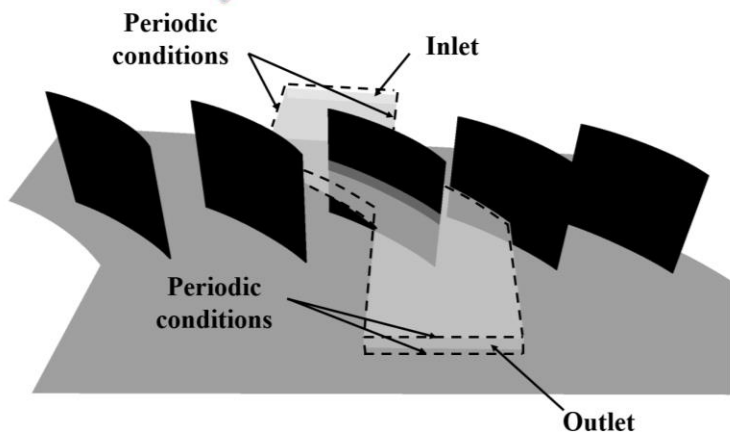
$$\text{E.g., } \langle \mathcal{K}\psi_k, \psi_j \rangle = \lim_{M \rightarrow \infty} \sum_{m=1}^M w_m \overline{\psi_j(x^{(m)})} \underbrace{\psi_k(y^{(m)})}_{[\mathcal{K}\psi_k](x^{(m)})}$$

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

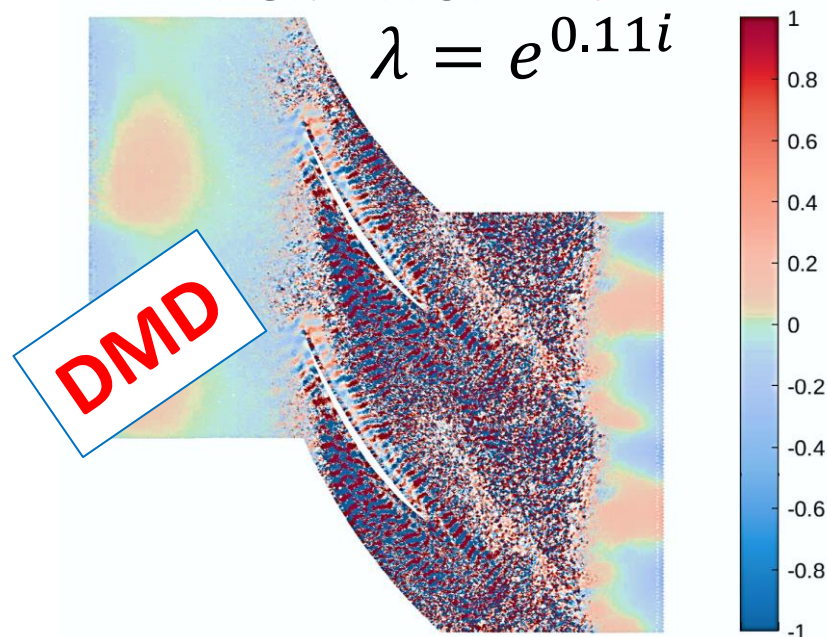
Example: Verified modes



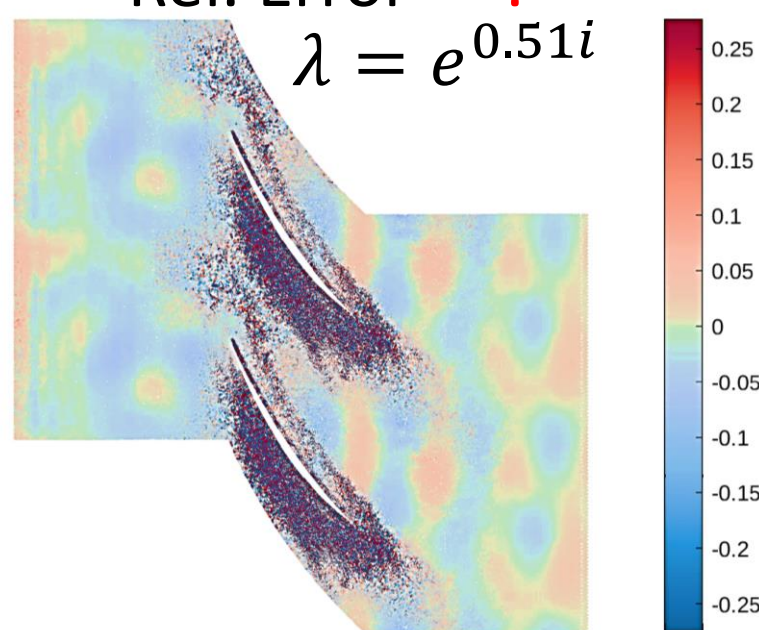
- Reynolds number $\approx 3.9 \times 10^5$
- Ambient dimension (d) $\approx 300,000$ (number of measurement points)

*Raw measurements provided by Stephane Moreau (Sherbrooke)

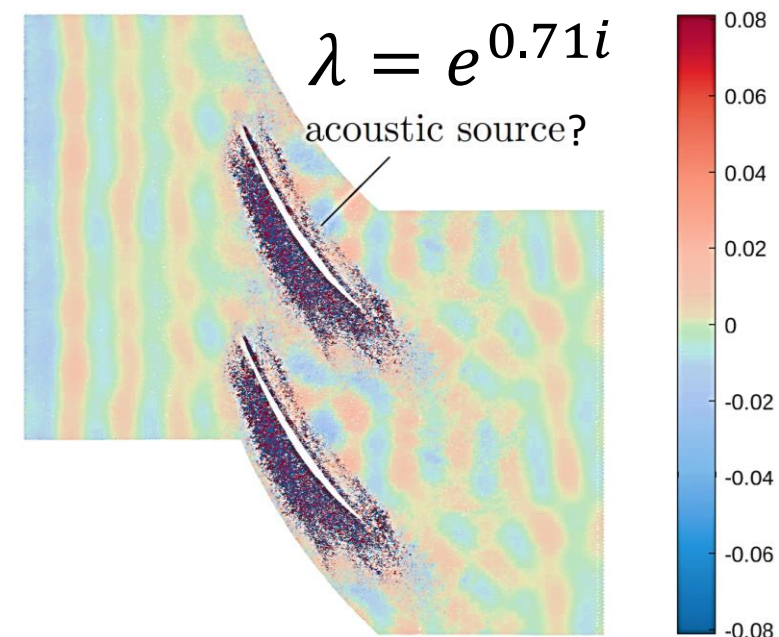
Rel. Error = ?
 $\lambda = e^{0.11i}$



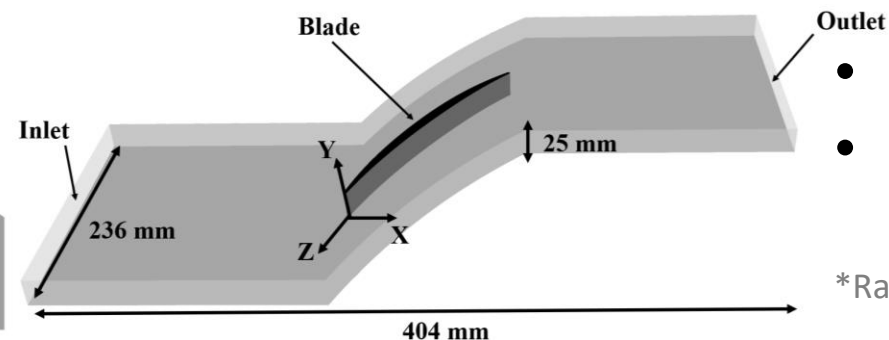
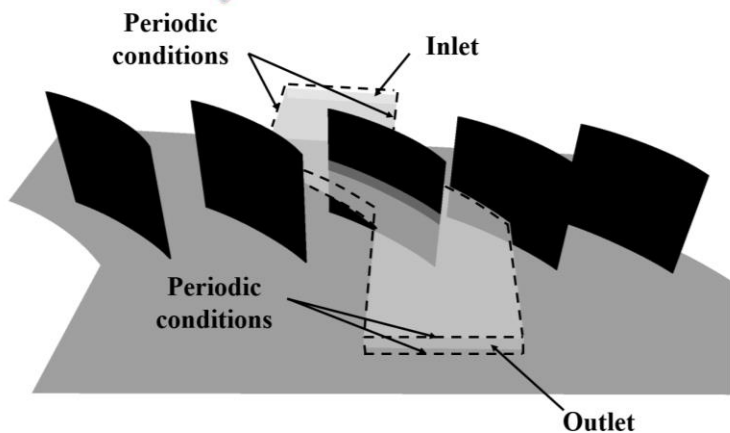
Rel. Error = ?
 $\lambda = e^{0.51i}$



Rel. Error = ?
 $\lambda = e^{0.71i}$



Example: Verified modes



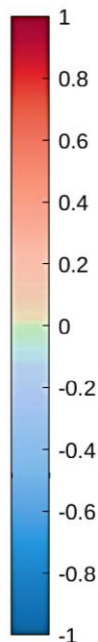
- Reynolds number $\approx 3.9 \times 10^5$
- Ambient dimension (d) $\approx 300,000$ (number of measurement points)

*Raw measurements provided by Stephane Moreau (Sherbrooke)

Rel. Error ≤ 0.0054

$$\lambda = e^{0.11i}$$

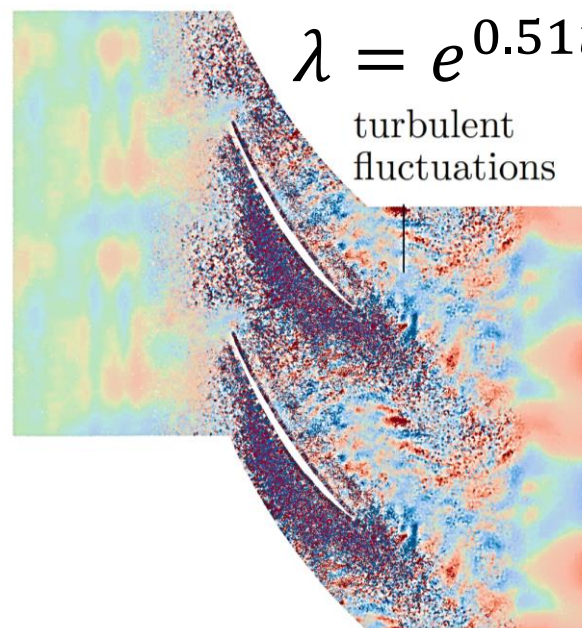
ResDMD



Rel. Error ≤ 0.0128

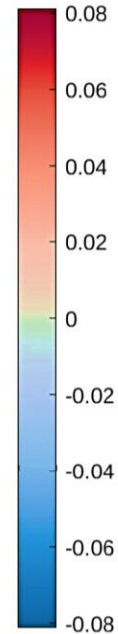
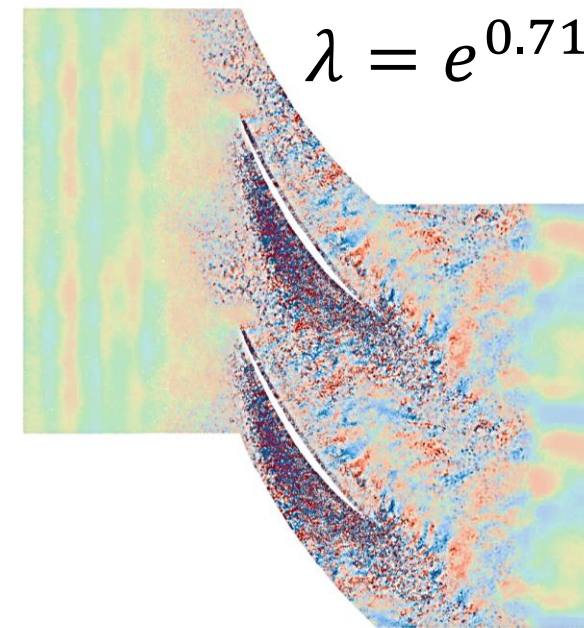
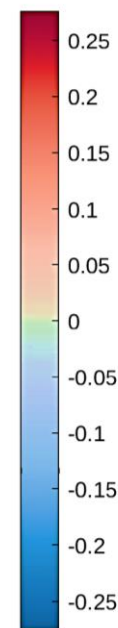
$$\lambda = e^{0.51i}$$

turbulent
fluctuations



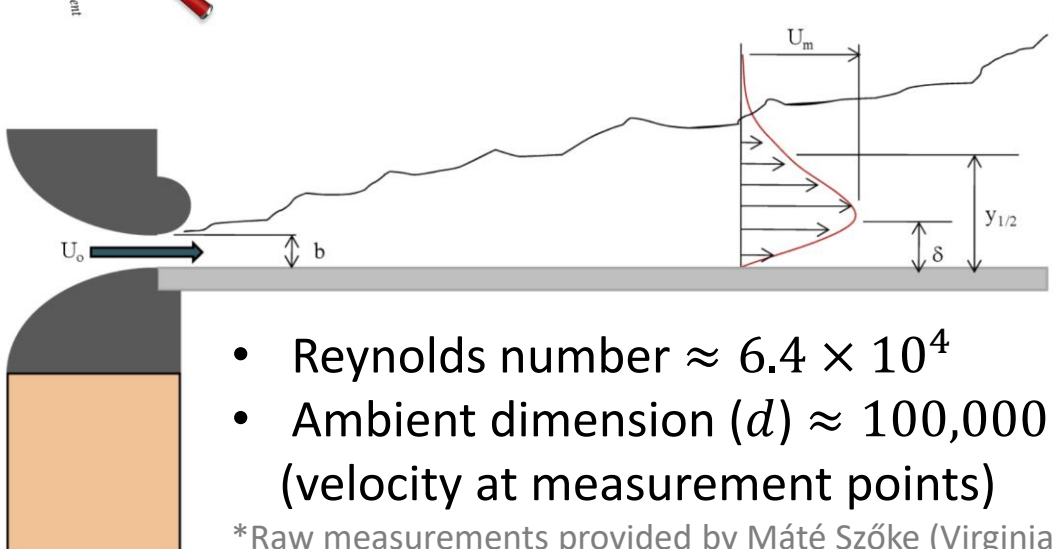
Rel. Error ≤ 0.0196

$$\lambda = e^{0.71i}$$



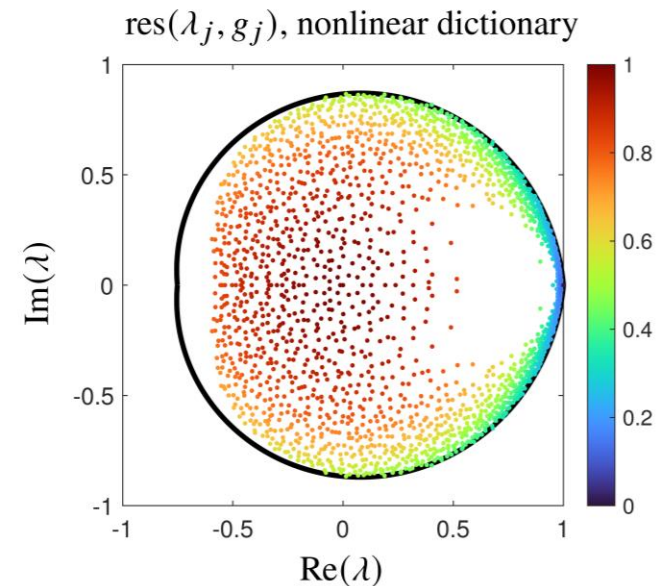
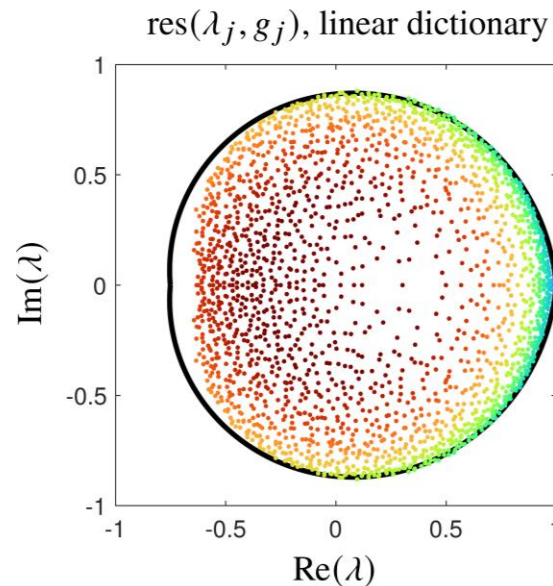
acoustic vibrations

Example: Verified dictionary

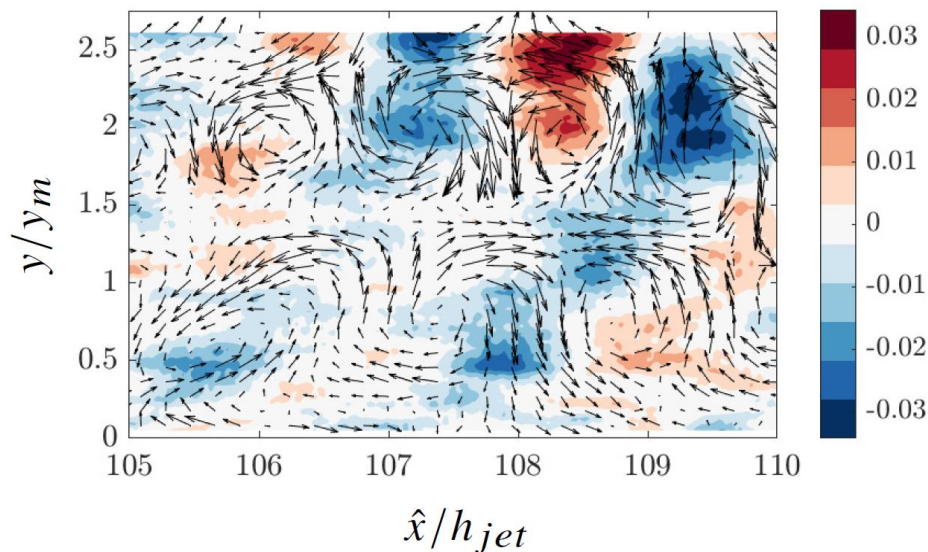


- Reynolds number $\approx 6.4 \times 10^4$
- Ambient dimension (d) $\approx 100,000$ (velocity at measurement points)

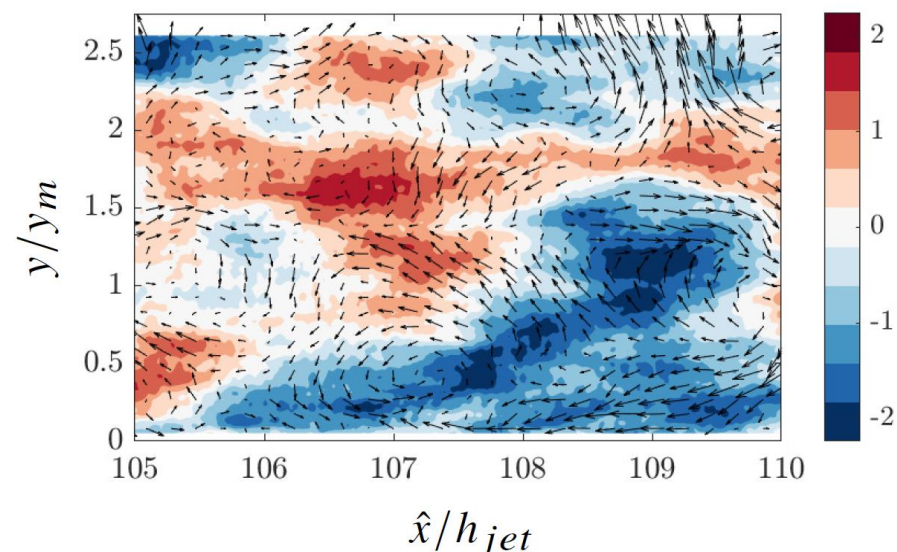
*Raw measurements provided by Máté Szőke (Virginia Tech)



$$\lambda = 0.9439 + 0.2458i, \text{ error} \leq 0.0765$$

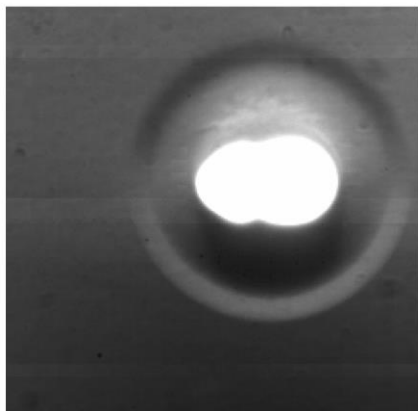


$$\lambda = 0.8948 + 0.1065i, \text{ error} \leq 0.1105$$

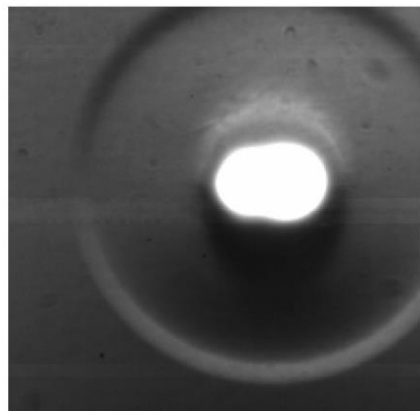




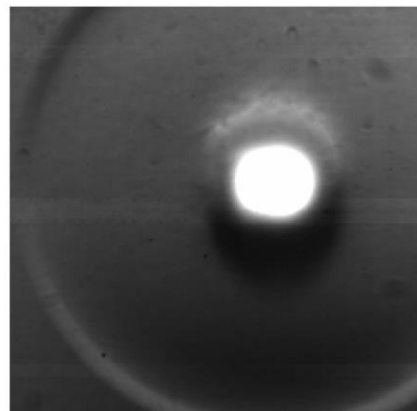
Example: Verified mode decomposition



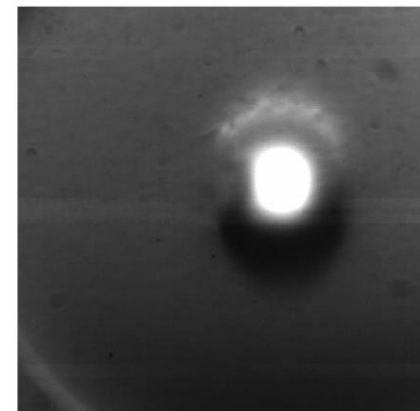
a) $t = 5 \mu\text{s}$



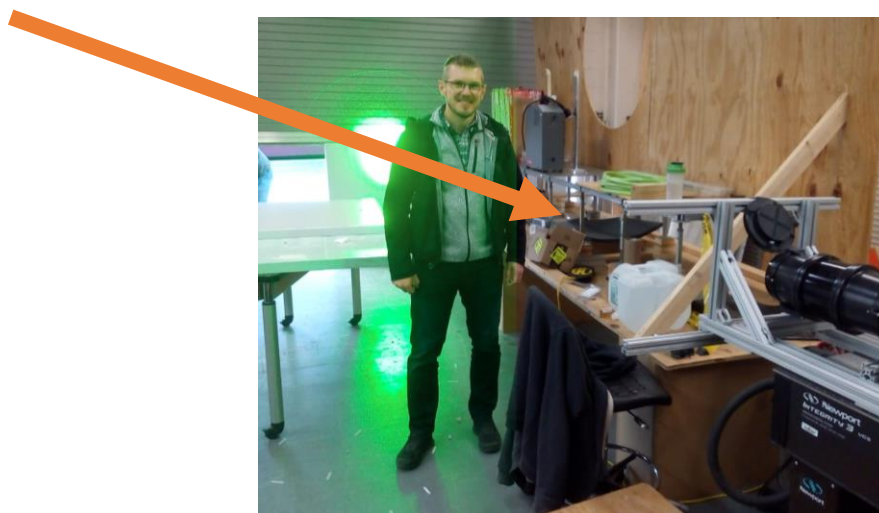
b) $t = 10 \mu\text{s}$



c) $t = 15 \mu\text{s}$

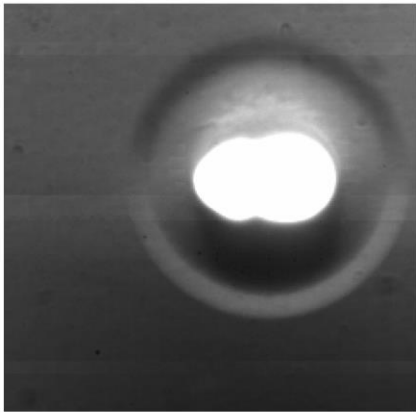


d) $t = 20 \mu\text{s}$

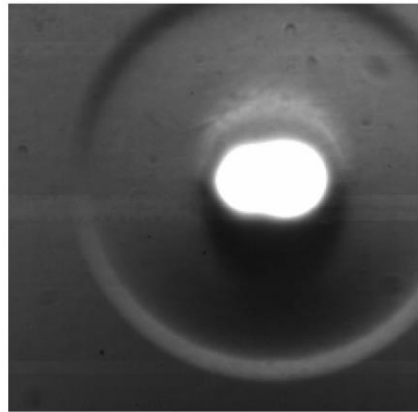


Matt Szőke showing me his laser cannon!

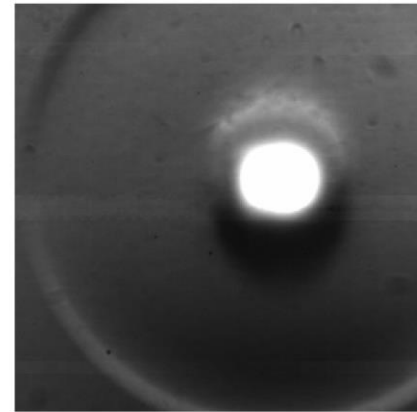
Example: Verified mode decomposition



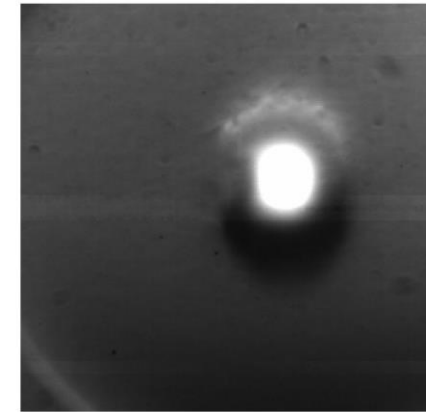
a) $t = 5 \mu\text{s}$



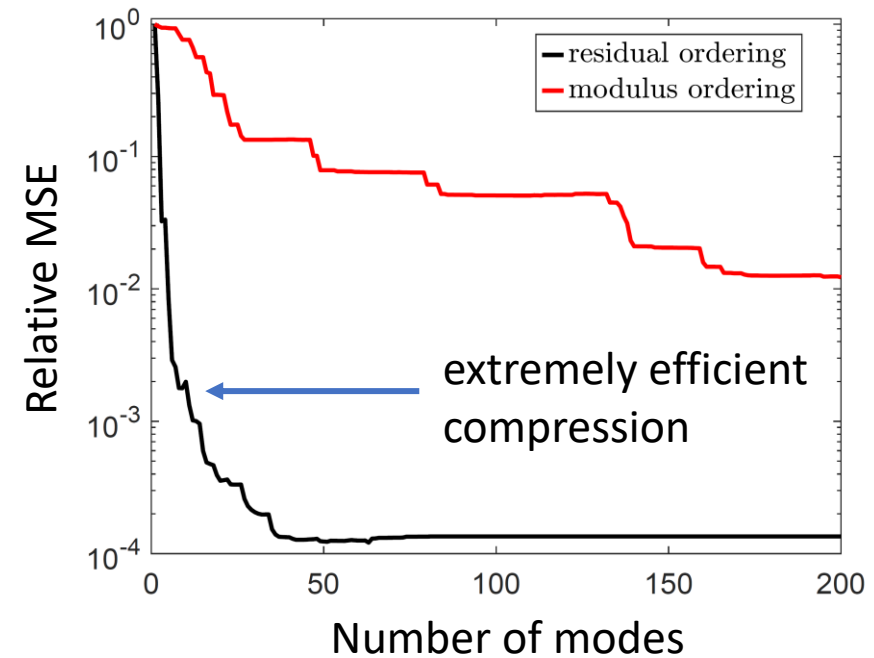
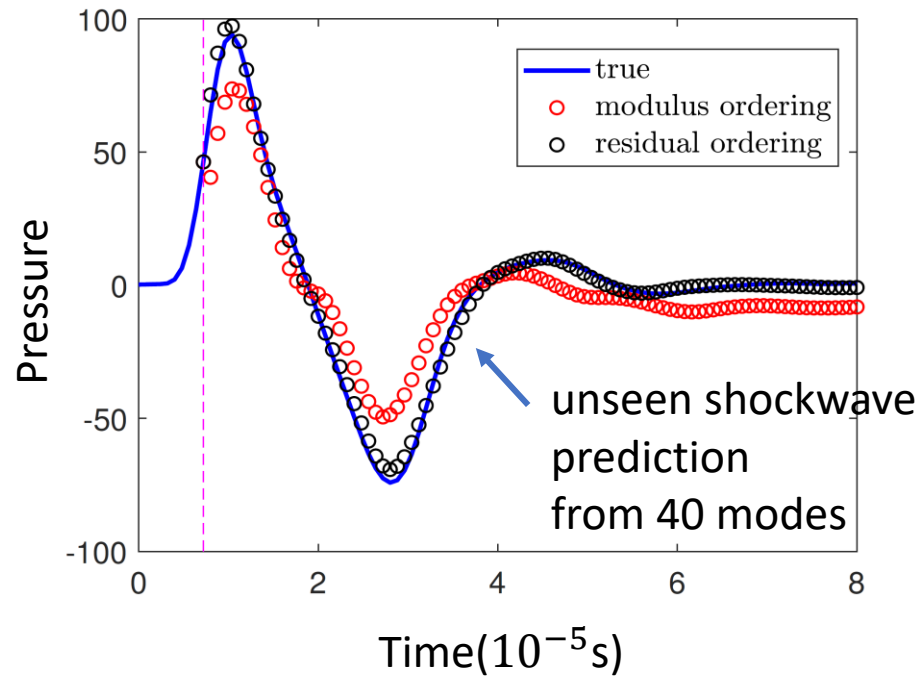
b) $t = 10 \mu\text{s}$



c) $t = 15 \mu\text{s}$



d) $t = 20 \mu\text{s}$





Stochastic Dynamical Systems

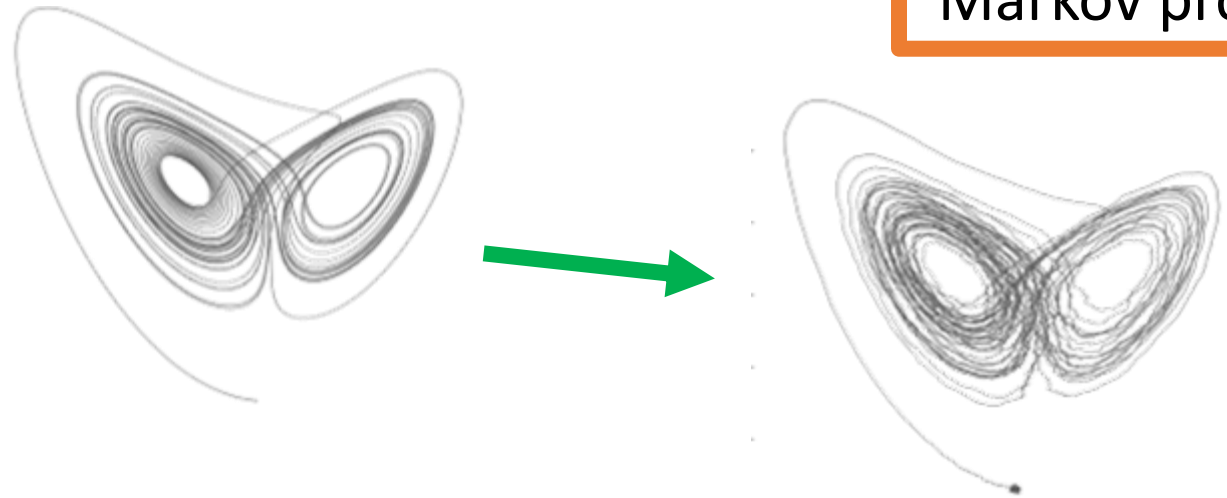
State $x \in \Omega \subseteq \mathbb{R}^d$, i.i.d. random variables $\tau_1, \tau_2, \dots$

Unknown function F governs dynamics:

$$x_n = F(x_{n-1}, \tau_n) = F_{\tau_n}(x_{n-1})$$

Discrete-time
Markov process!

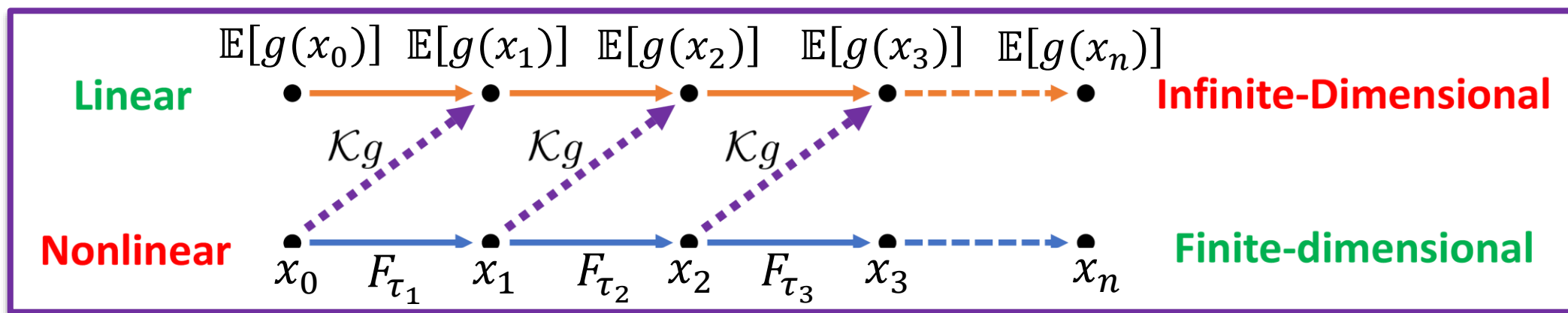
E.g., models noise or uncertainty, or truly random process.



Goal: Verified learning from data $\{x^{(m)}, y^{(m)} = F_{\tau_m}(x^{(m)})\}_{m=1}^M$.

Stochastic Koopman Operator

Now we have an expectation: $[\mathcal{K}g](x) = \mathbb{E}[g(F_\tau(x))]$



Satisfies semigroup property: $\mathbb{E}[g(\underbrace{F \circ F \circ \dots \circ F}_{n \text{ times}})] = \mathcal{K}^n g$



Time for an example!

Stochastic Van der Pol oscillator:

$$\begin{aligned}dX_1 &= X_2 dt, \\dX_2 &= [0.5(1 - X_1^2)X_2 - X_1]dt + 0.2dB_t\end{aligned}$$

Turn into discrete-time system with step 0.3.

$$\begin{aligned}\mathbb{E} \left[g_\lambda \left(F_{\tau_n} \circ \dots \circ F_{\tau_1}(x) \right) \right] \\&= [\mathcal{K}^n g_\lambda](x) \\&= \lambda^n g_\lambda(x)\end{aligned}$$

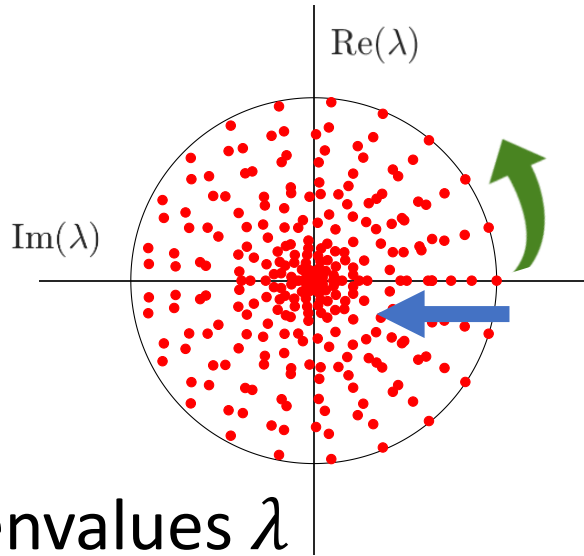


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Eigenvalues λ

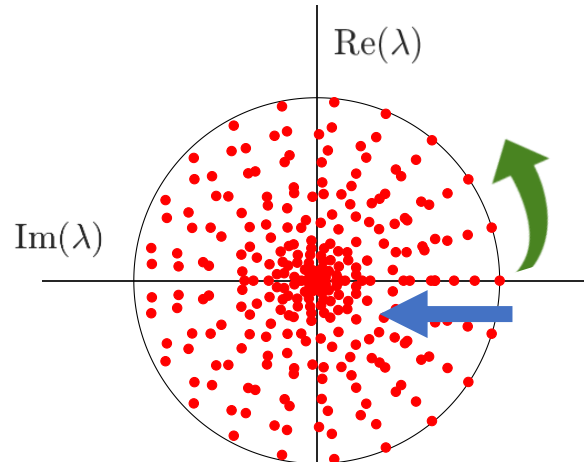


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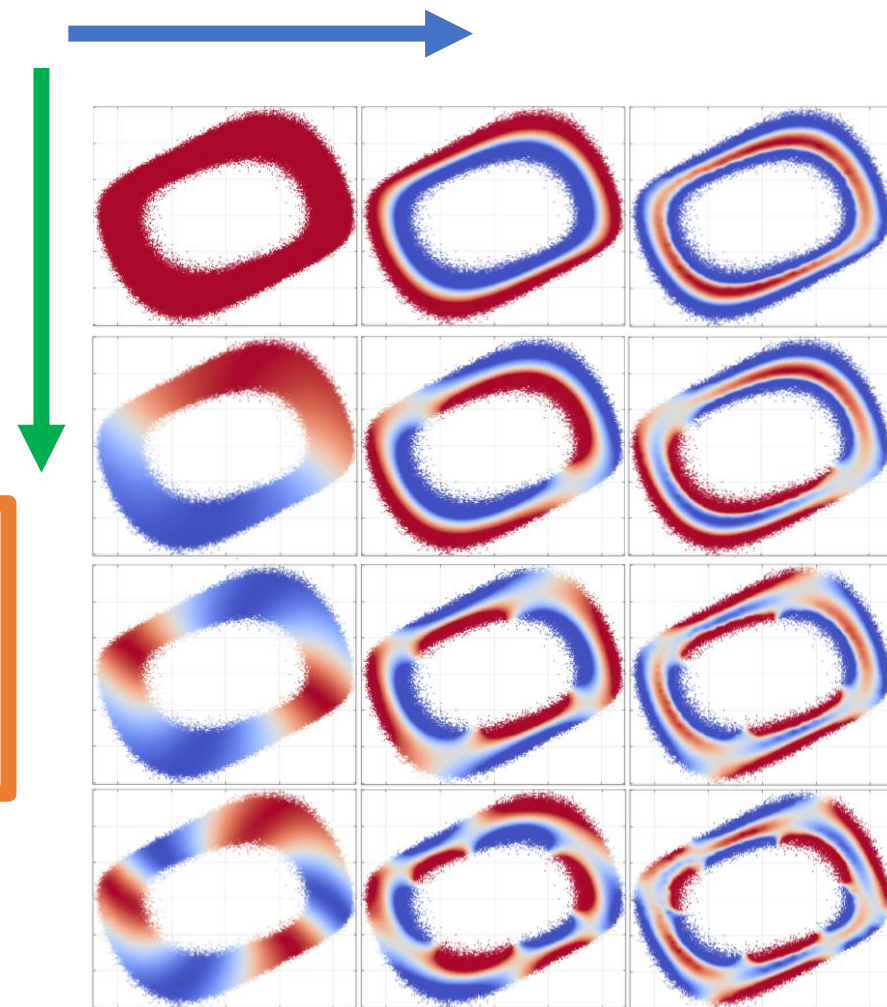
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Eigenfunctions g_λ



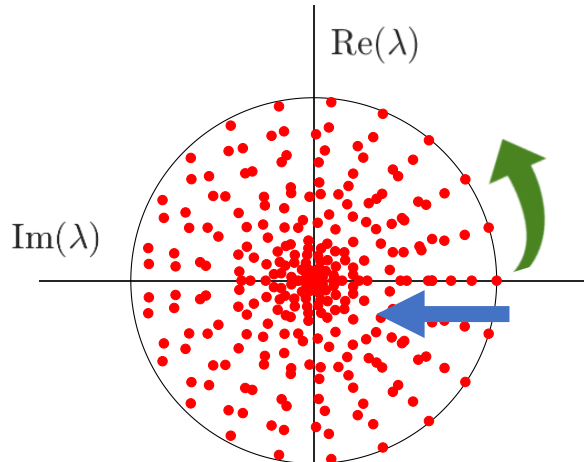


Time for an example!

Stochastic Van der Pol oscillator:

$$\begin{aligned} dX_1 &= X_2 dt, \\ dX_2 &= [0.5(1 - X_1^2)X_2 - X_1]dt + 0.2dB_t \end{aligned}$$

Turn into discrete-time system with step 0.3.

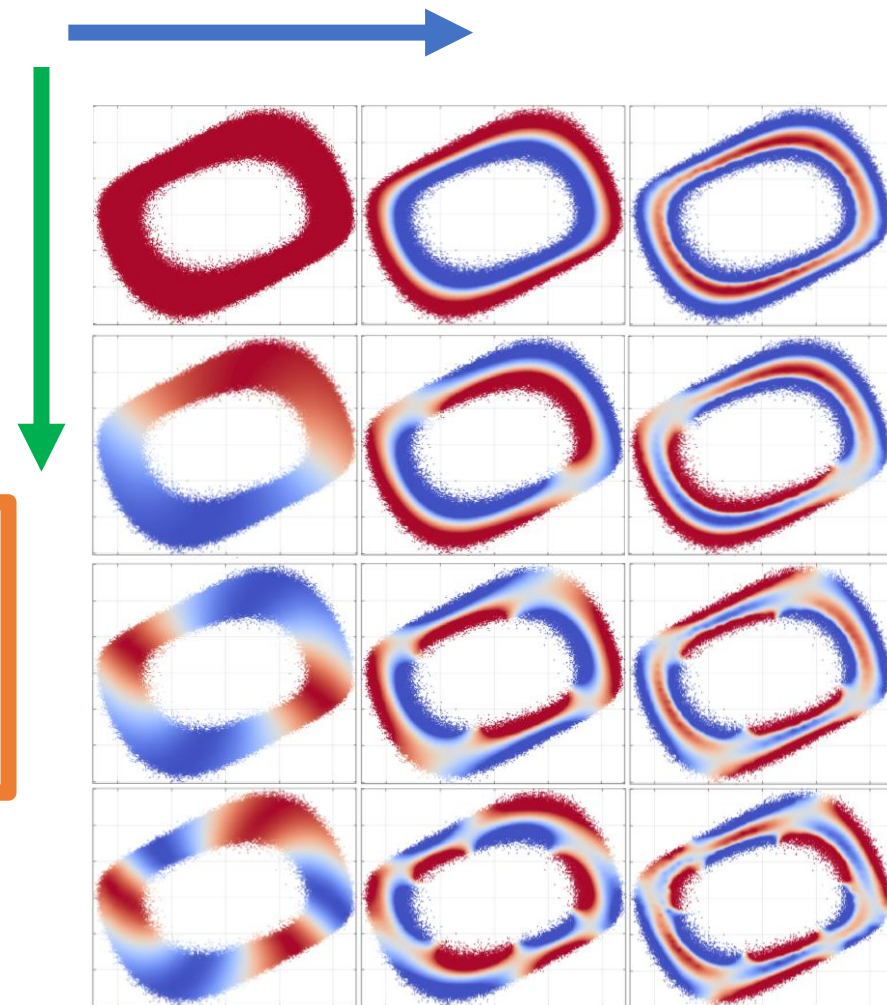


Eigenvalues λ

$$\begin{aligned} \mathbb{E} \left[g_\lambda \left(F_{\tau_n} \circ \dots \circ F_{\tau_1}(x) \right) \right] \\ = [\mathcal{K}^n g_\lambda](x) \\ = \lambda^n g_\lambda(x) \end{aligned}$$

Is this enough?

Eigenfunctions g_λ





Time for an example!

Stochastic Van der Pol oscillator:

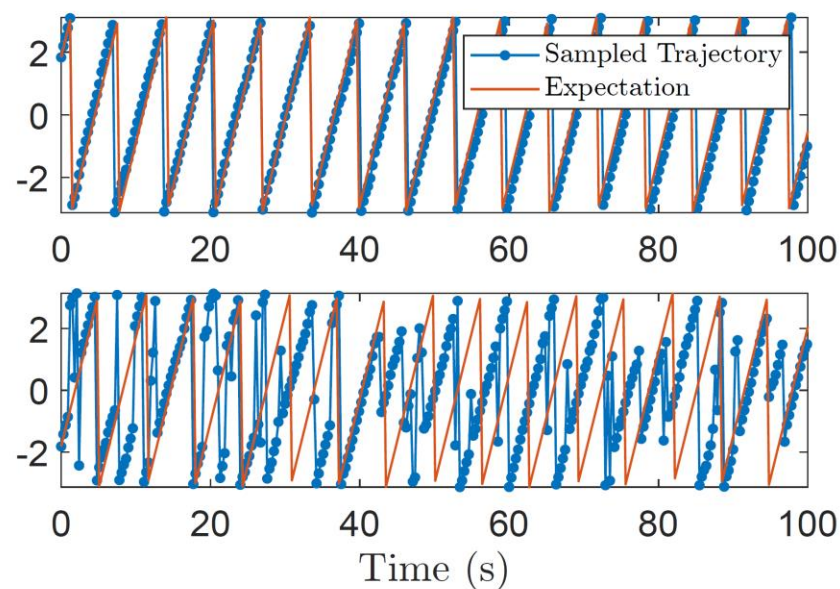
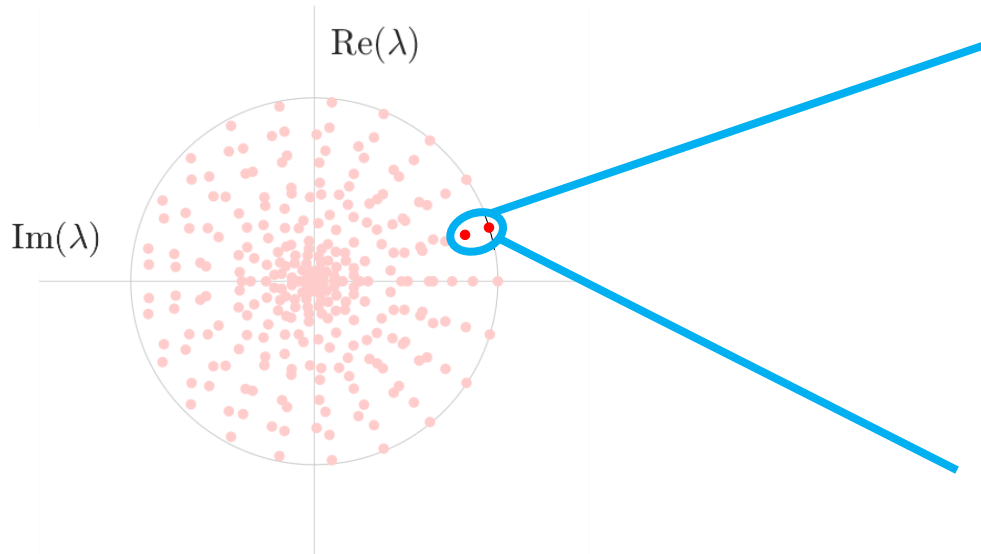
$$dX_1 = X_2 dt,$$

$$dX_2 = [0.5(1 - X_1^2)X_2 - X_1]dt + 0.2dB_t$$

Same phase, but clearly one is more coherent than the other!

Turn into discrete-time system with step 0.3.

$\arg(g_\lambda(x_n))$



$\approx 0.956 + 0.290i$

$\approx 0.825 + 0.250i$



Time for an example!

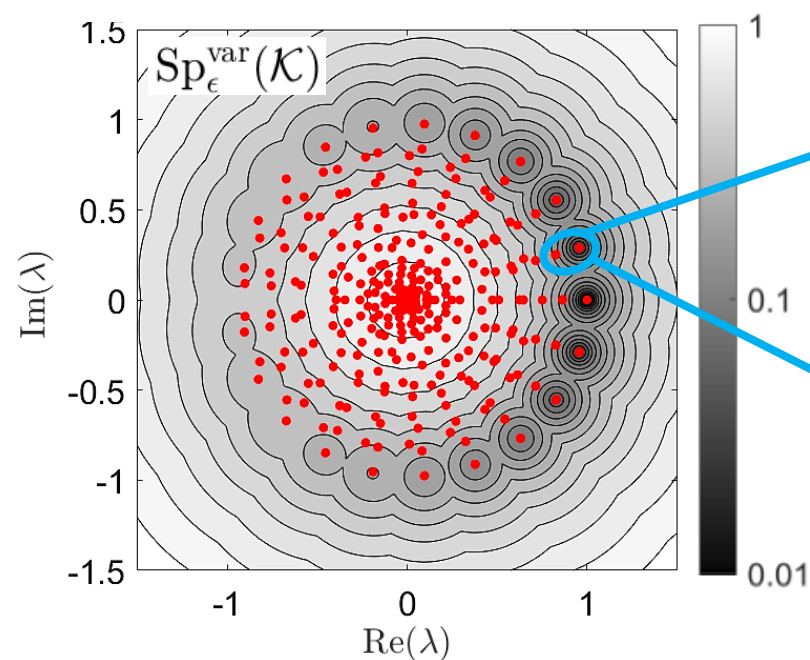
Stochastic Van der Pol oscillator:

$$dX_1 = X_2 dt,$$

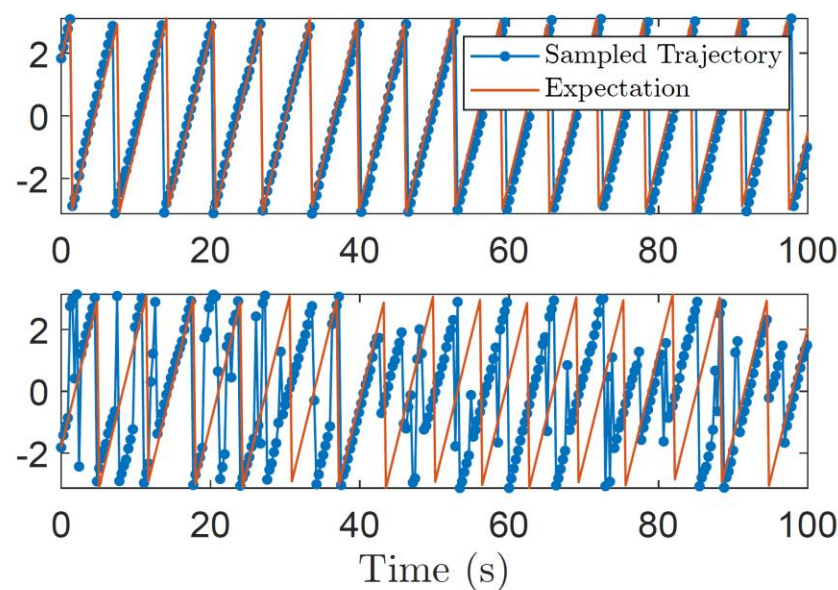
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$\arg(g_\lambda(x_n))$



$$\approx 0.956 + 0.290i$$

$$\approx 0.825 + 0.250i$$



Decomposing the residual

$$\begin{aligned}\lim_{M \rightarrow \infty} \mathbf{g}^* [K_2 - \lambda K_1^* - \bar{\lambda} K_1 + |\lambda|^2 G] \mathbf{g} \\&= \mathbb{E}[\|g \circ F_\tau - \lambda g\|^2] \\&= \|\mathcal{K}g - \lambda g\|^2 + \int_{\Omega} \text{Var}[g(F_\tau(x))] d\omega(x)\end{aligned}$$

Squared residual

Integrated variance



Decomposing the residual

$$\begin{aligned}
 \lim_{M \rightarrow \infty} \mathbf{g}^* [K_2 - \lambda K_1^* - \bar{\lambda} K_1 + |\lambda|^2 G] \mathbf{g} \\
 &= \mathbb{E}[\|g \circ F_\tau - \lambda g\|^2] \\
 &= \|\mathcal{K}g - \lambda g\|^2 + \int_{\Omega} \text{Var}[g(F_\tau(x))] \, d\omega(x)
 \end{aligned}$$

Squared residual

Integrated variance

Definition: For $\varepsilon > 0$ we define the variance- ε -pseudospectrum

$$\text{Sp}_\varepsilon^{\text{var}}(\mathcal{K}) = \{\lambda \in \mathbb{C} : \exists g \in \mathcal{D}(\mathcal{K}), \|g\| = 1, \mathbb{E}[\|g \circ F_\tau - \lambda g\|^2] < \varepsilon^2\}$$



Decomposing the residual

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Measure of statistical coherency.



Sampler of the results we prove

Representation of higher moments via batched Koopman operators:

$$g: \Omega^r \rightarrow \mathbb{C}, \quad [\mathcal{K}_{(r)}g](x) = \mathbb{E}[g(F_\tau, \dots, F_\tau)]$$

Convergent algorithms for each of the terms in the residual decomposition.

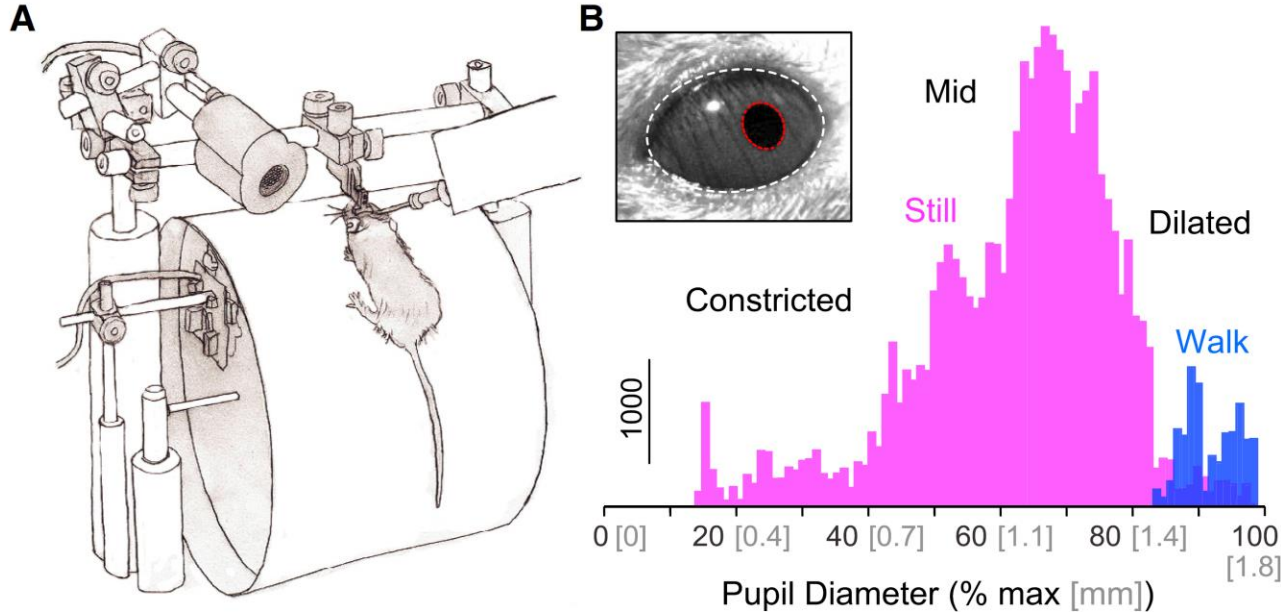
Computation of spectrum of $\mathcal{K}$ without issues such as spurious eigenvalues.

Control the error when we project to a finite-dimensional space!

Error bounds for Koopman Mode Decomposition.

Concentration bounds in terms of amount of snapshot data.

An application

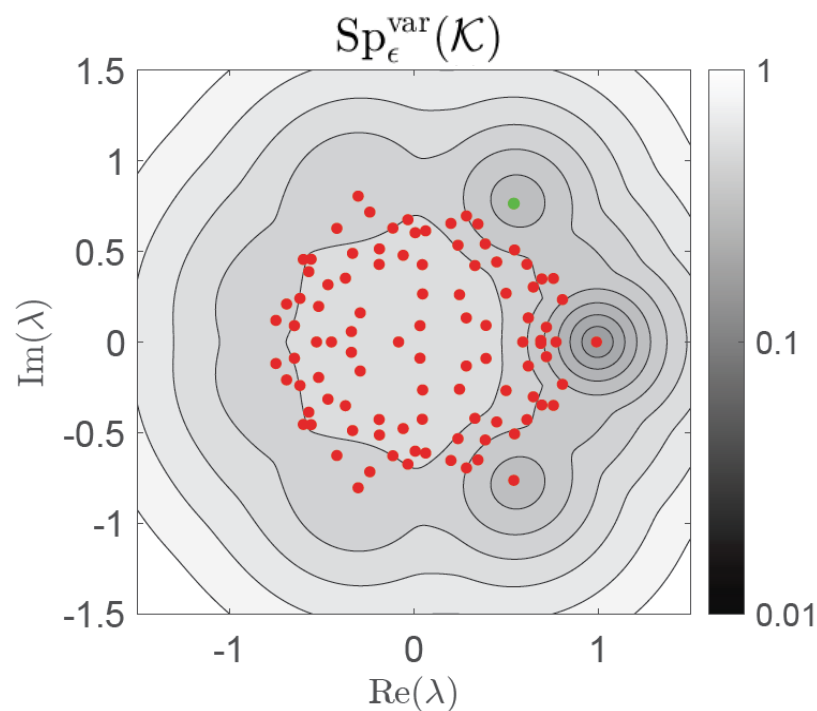


- Monitoring of large populations of neurons.
- Mice shown a drifting grating.
- Separate stochastic Koopman operators according to 15 different arousal levels (indexed by pupil diameter).

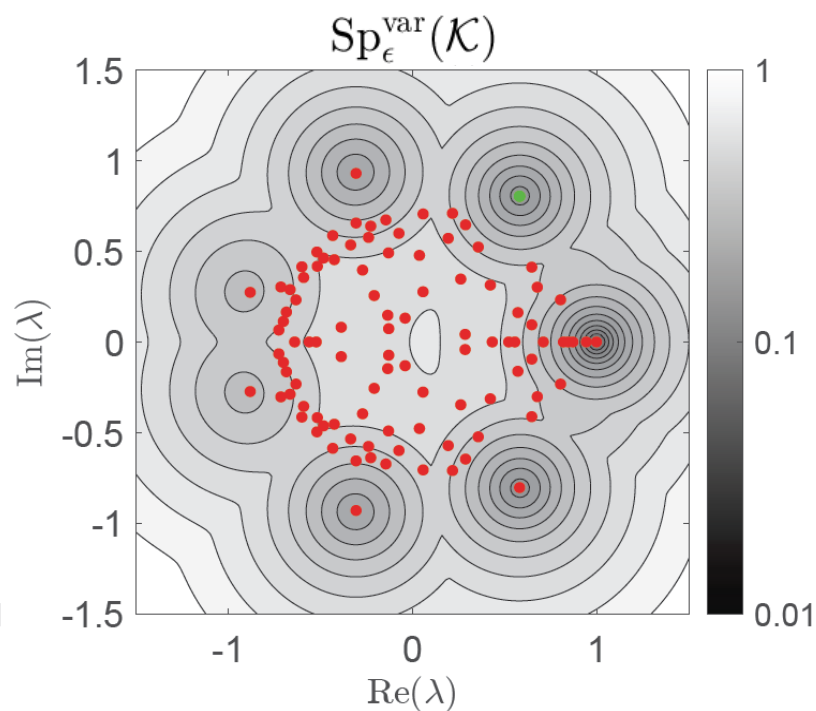
Standard DMD does not provide verification...

- Siegle, Joshua H., et al., "Survey of spiking in the mouse visual system reveals functional hierarchy," **Nature**, 2021.
- McGinley, David, McCormick, "Cortical membrane potential signature of optimal states for sensory signal detection," **Neuron**, 2015.

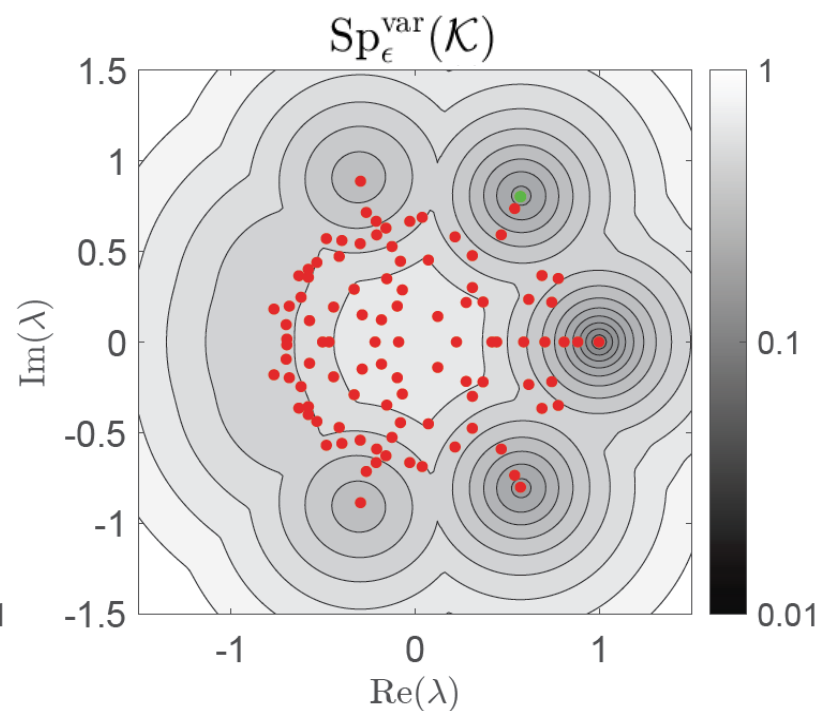
Variance pseudospectra of mouse # 11



pupil diameter 8%



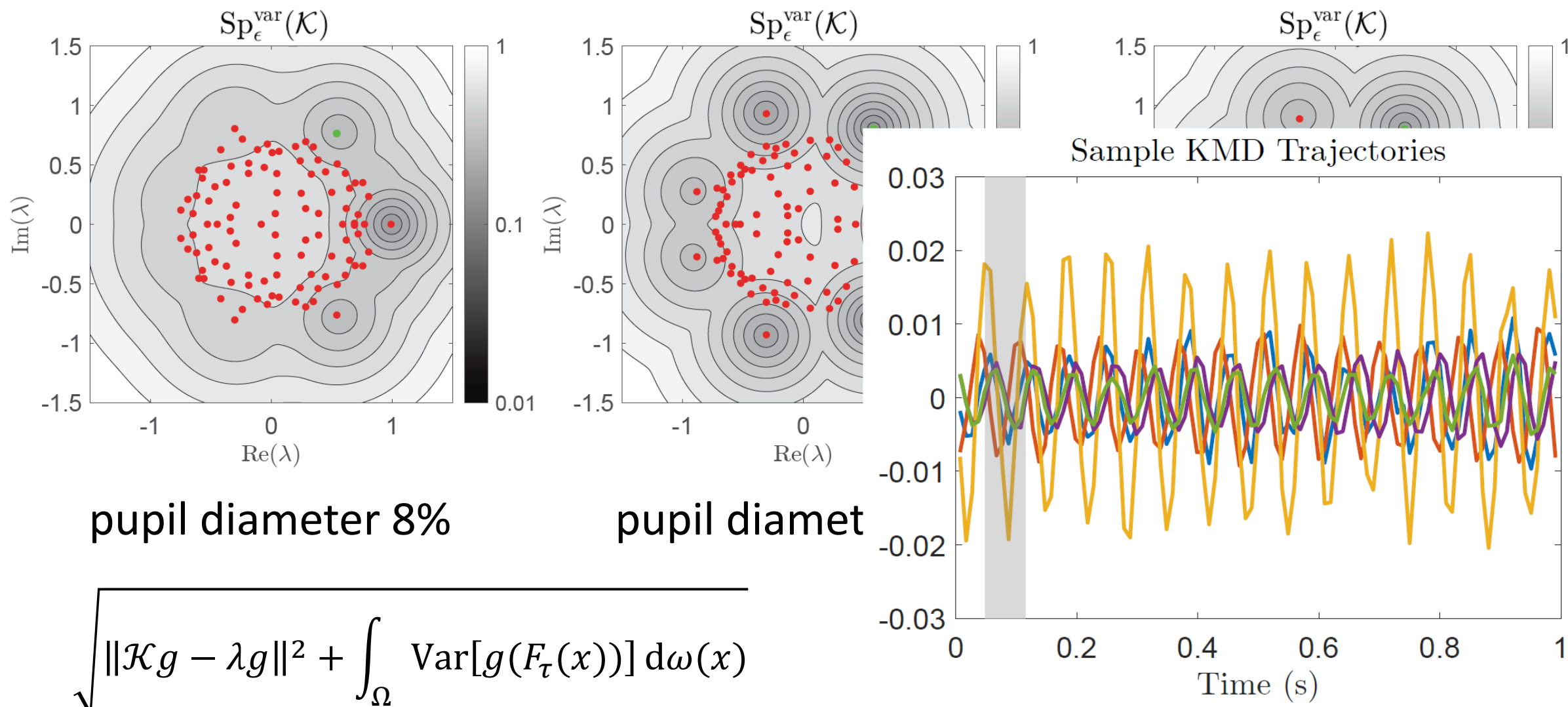
pupil diameter 28%



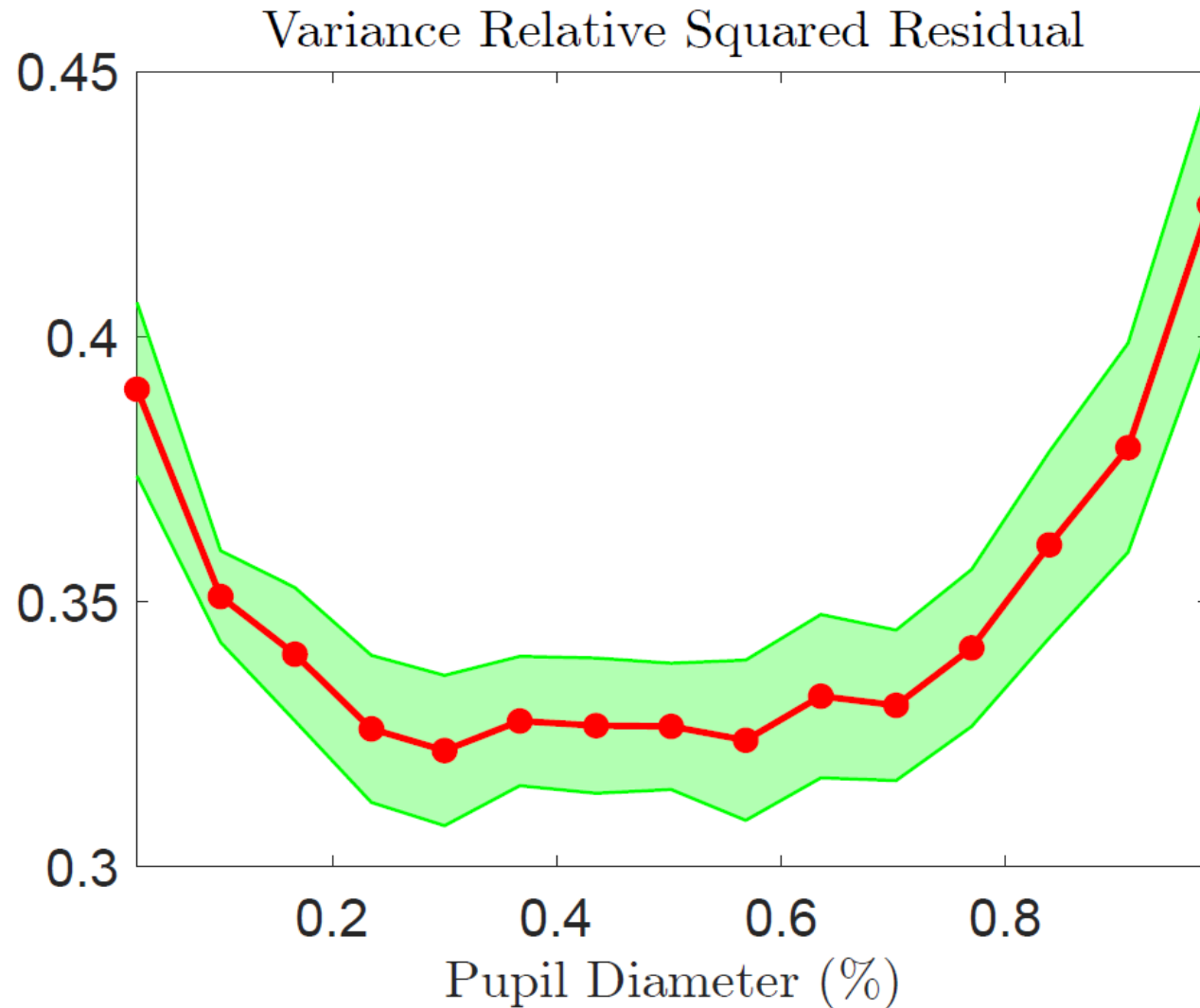
pupil diameter 43%

$$\sqrt{\|\mathcal{K}g - \lambda g\|^2 + \int_{\Omega} \text{Var}[g(F_{\tau}(x))] d\omega(x)}$$

Variance pseudospectra of mouse # 11



Yerkes-Dodson law across all mice



Yerkes-Dodson law: you reach your peak level of performance with an intermediate level of stress, or arousal. Too little or too much arousal results in poorer performance.



Wider program: Solvability Complexity Index

- Inf.-dim. computational analysis $\Rightarrow$ **Compute spectral properties rigorously, practically!**
- Continuous linear algebra $\Rightarrow$ **Avoid the woes of discretization.**
- Hierarchy $\Rightarrow$ **Classify difficulty of computational problems, prove algorithms are optimal.**

$$\begin{array}{ccccccc}
 \Pi_0^\alpha & & \Pi_1^\alpha & & \Pi_2^\alpha & & \\
 \parallel & \subsetneq & & \subsetneq & \subsetneq & \subsetneq & \subsetneq \\
 \Delta_0^\alpha & \subsetneq & \Delta_1^\alpha & \subsetneq & \Sigma_1^\alpha \cup \Pi_1^\alpha & \subsetneq & \Delta_2^\alpha & \subsetneq & \Sigma_2^\alpha \cup \Pi_2^\alpha & \subsetneq & \Delta_3^\alpha & \subsetneq & \dots \\
 \parallel & & & \subsetneq & & \subsetneq & & \subsetneq & & \subsetneq & & \subsetneq \\
 \Sigma_0^\alpha & & \Sigma_1^\alpha & & \Sigma_2^\alpha & & & & & & & &
 \end{array}$$

Extends to: Foundations of AI, optimization, computer-assisted proofs, and PDEs etc.

- C., "On the computation of geometric features of spectra of linear operators on Hilbert spaces," **Found. Comput. Math.**, 2023.
- C., Hansen, "The foundations of spectral computations via the solvability complexity index hierarchy," **J. Eur. Math. Soc.**, 2022.
- C., Antun, Hansen, "The difficulty of computing stable and accurate neural networks," **Proc. Natl. Acad. Sci. USA**, 2022.
- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "On the solvability complexity index hierarchy and towers of algorithms," arXiv, 2020.



Summary



- Koopman: **Nonlinearity**
- Presented **verified data-driven methods** for Koopman operators (deterministic and stochastic)
- Methods are **cheap, easy-to-use**, come with **convergence guarantees**.
- For **continuous spectra**, see:
 - C., Townsend, "Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems," **Commun. Pure Appl. Math.**, 2023.
 - C., "The mpEDMD algorithm for data-driven computations of measure-preserving dynamical systems." **SIAM J. Numer. Anal.**, 2023.
 - C., Horning, Townsend, "Computing spectral measures of self-adjoint operators," **SIAM Review**, 2021.

Infinite dimensions

Brief Summaries



Resilient Data-driven Dynamical Systems with Koopman: An Infinite-dimensional Numerical Analysis Perspective

By Steven L. Brunton and Matthew J. Colbrook

Dynamical systems, which describe the evolution of systems in time, are ubiquitous in modern science and engineering. They find use in a wide variety of applications, from mechanics and circuits to climatology, neuroscience, and epidemiology. Consider a discrete-time dynamical system with state x in a state space $\mathbb{X} \subset \mathbb{R}^n$ that is governed by an unknown and typically nonlinear function $F: \mathbb{X} \rightarrow \mathbb{X}$:

$$x_{n+1} = F(x_n), \quad n \geq 0. \quad (1)$$

The classical, geometric way to analyze such systems—which dates back to the seminal work of Henri Poincaré—is based

on the local analysis of fixed points, periodic orbits, stable or unstable manifolds, and so forth. Although Poincaré's framework has revolutionized our understanding of dynamical systems, this approach has at least two challenges in many modern applications: (i) Obtaining a global understanding of the nonlinear dynamics and (ii) handling systems that are either too complex to analyze or offer incomplete information about the evolution (i.e., unknown, high-dimensional, and highly nonlinear F).

Koopman operator theory, which originated with Bernard Koopman and John von Neumann [6, 7], provides a powerful alternative to the classical geometric view of dynamical systems because it addresses nonlinearity: the fundamental issue that underlies the aforementioned challenges.

We lift the nonlinear system (1) into an infinite-dimensional space of observable functions $y: \mathbb{X} \rightarrow \mathbb{C}$ via a Koopman operator K :

$$Ky(x_n) = y(F(x_n)).$$

The evolution dynamics thus become linear, allowing us to utilize generic solution techniques that are based on spectral decompositions. In recent decades, Koopman operators have captivated researchers because of emerging data-driven and numerical implementations that coincide with the rise of machine learning and high-performance computing [2].

One major goal of modern Koopman operator theory is to find a coordinate transformation with which a linear system may approximate even strongly nonlinear dynamics; this coordinate system relates to the spectrum of the Koopman operator. In 2000, Igor Mezic introduced the Koopman

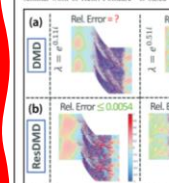


Figure 1: Koopman modes of a turbulent flow. (a) shows the real part of the Koopman modes, and (b) shows the imaginary part. The modes are visualized as 3D surfaces over a 2D domain.

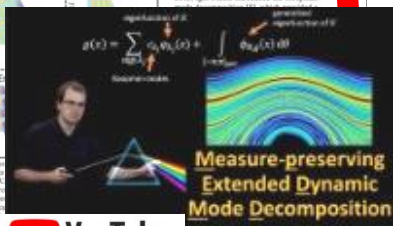


Figure 2: Measure-preserving Extended Dynamic Mode Decomposition. The figure shows a 3D visualization of the modes and a 2D plot of the modes.



Figure 3: Residual Dynamic Mode Decomposition. The figure shows a 3D visualization of the modes and a 2D plot of the modes.

References

- [1] 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).
- [2] Colbrook, Matthew J., Lorna J. Ayton, and Máté Szőke. "Residual dynamic mode decomposition: robust and verified Koopmanism." *Journal of Fluid Mechanics* 955 (2023): A21.
- [3] Colbrook, Matthew J., Qin Li, Ryan Raut, and Alex Townsend. "Beyond expectations: Residual Dynamic Mode Decomposition and Variance for Stochastic Dynamical Systems", arXiv preprint arXiv:2308.10697 (2023).
- [4] 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.
- [5] Colbrook, Matthew J., and Alex Townsend. "Avoiding discretization issues for nonlinear eigenvalue problems." arXiv preprint arXiv:2305.01691 (2023).
- [6] Colbrook, Matthew J. "Computing semigroups with error control." *SIAM Journal on Numerical Analysis* 60.1 (2022): 396-422.
- [7] 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.
- [8] Colbrook, Matthew. *The foundations of infinite-dimensional spectral computations*. Diss. University of Cambridge, 2020.
- [9] 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.
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