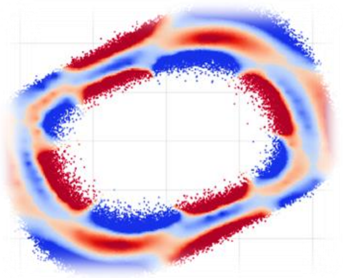
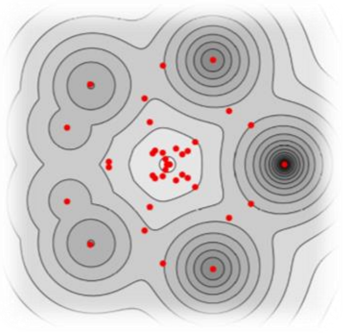
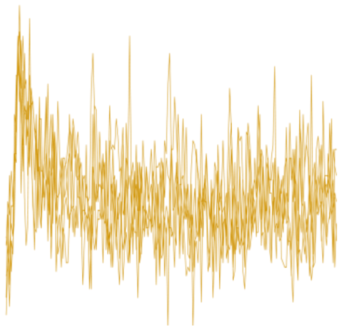
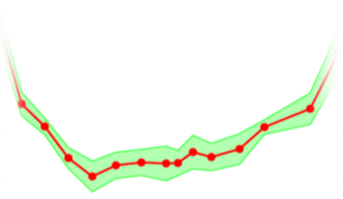








Residual Dynamic Mode Decomposition for Stochastic Systems

Matthew Colbrook

University of Cambridge

21/08/2024

Qin Li

Ryan Raut

Alex Townsend

C., Li, Raut, Townsend, *"Beyond expectations: Residual Dynamic Mode Decomposition and Variance for Stochastic Dynamical Systems,"* **Nonlinear Dynamics**, 2024.

Stochastic Dynamical System

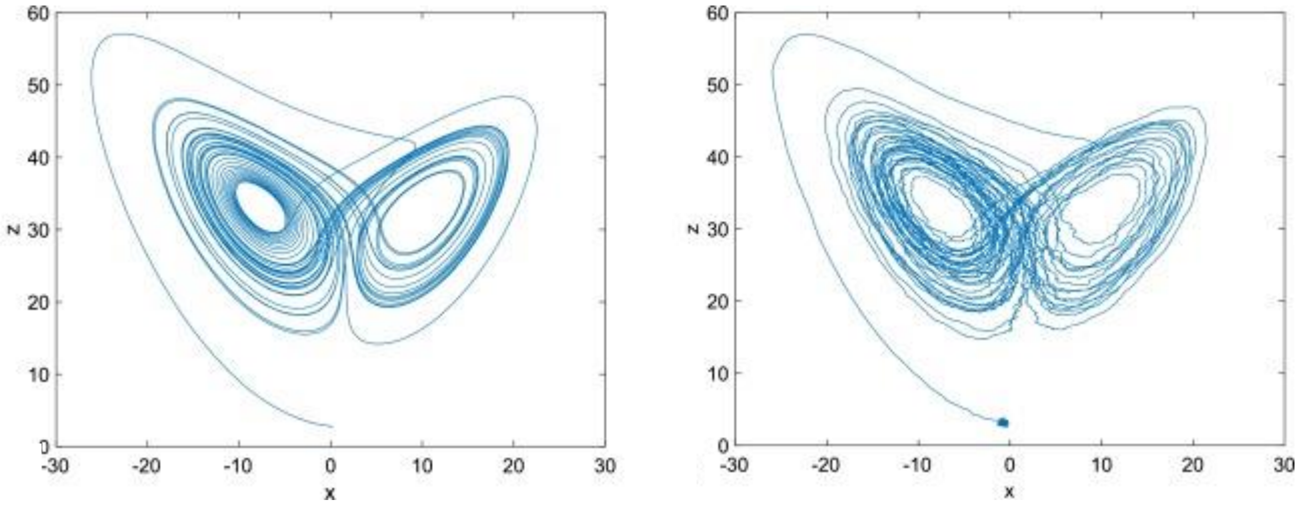
State $x \in \Omega \subseteq \mathbb{R}^d$, i.i.d. random variables $\tau_1, \tau_2, \ldots$

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, uncertainty, random process…



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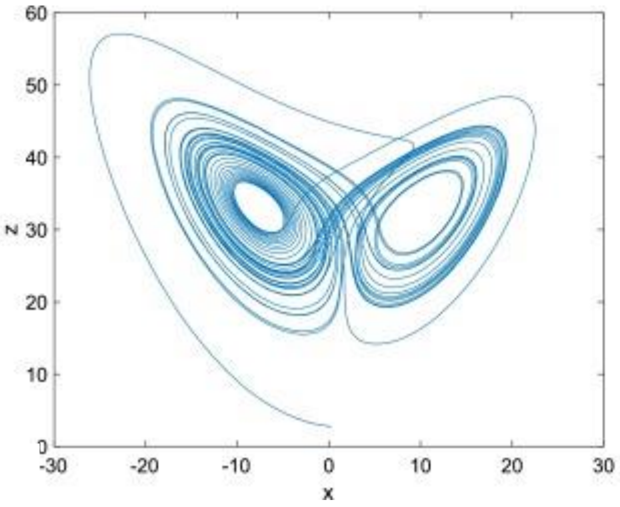
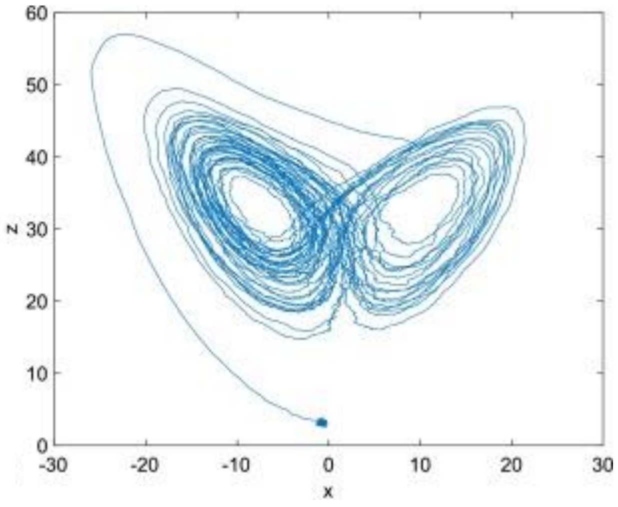
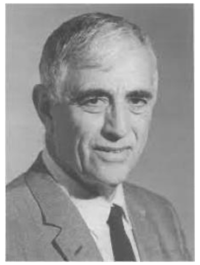




Goal: Verified learning from data $\left\{x^{(m)}, y^{(m)} = F_{\tau_m}(x^{(m)})\right\}_{m=1}^{M}$.

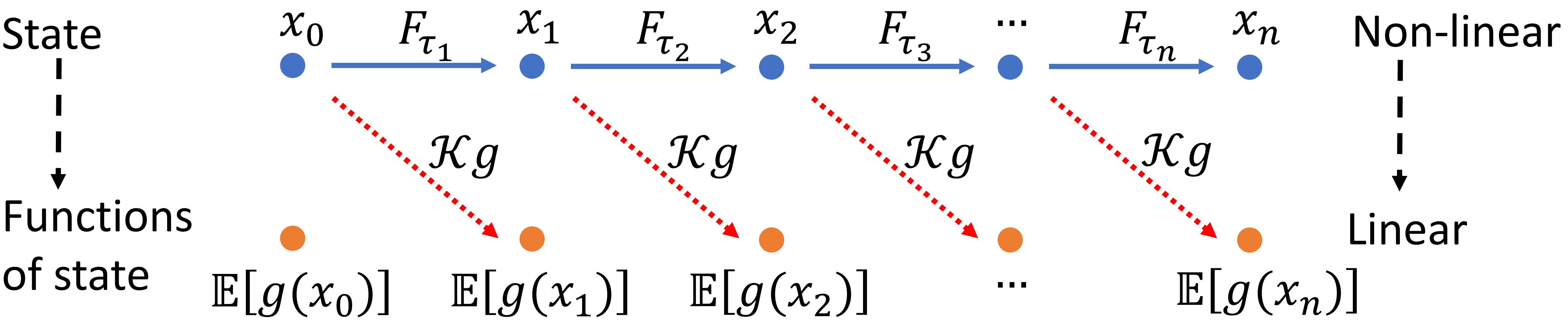
Koopman Operator

Koopman



von Neumann

$\mathcal{K}$ acts on functions $g: \Omega \to \mathbb{C}$: $[\mathcal{K}g](x) = \mathbb{E}\left[g\left(F_\tau(x)\right)\right]$



Nonlinearity.

Infinite dimensions.

- 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.

Time for an example!

Stochastic van der Pol oscillator:

$$\mathrm{d}X_1 = X_2 \mathrm{d}t,$$
$$\mathrm{d}X_2 = [0.5(1 - X_1^2)X_2 - X_1]\mathrm{d}t + 0.2\mathrm{d}B_t$$

Sample at $\Delta t = 0.3$.

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

Semigroup property

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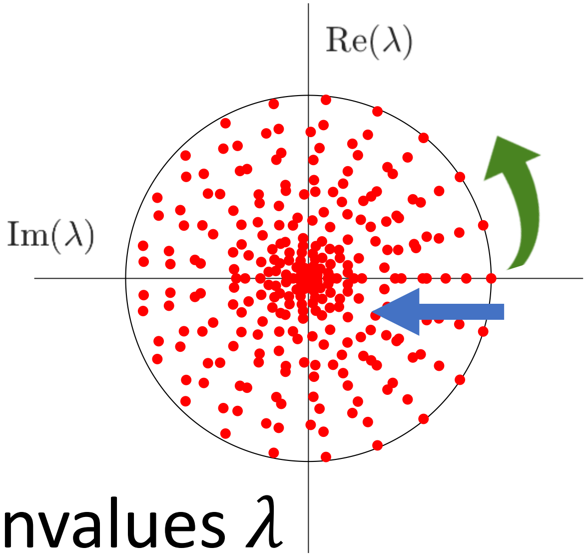

Eigenvalues λ

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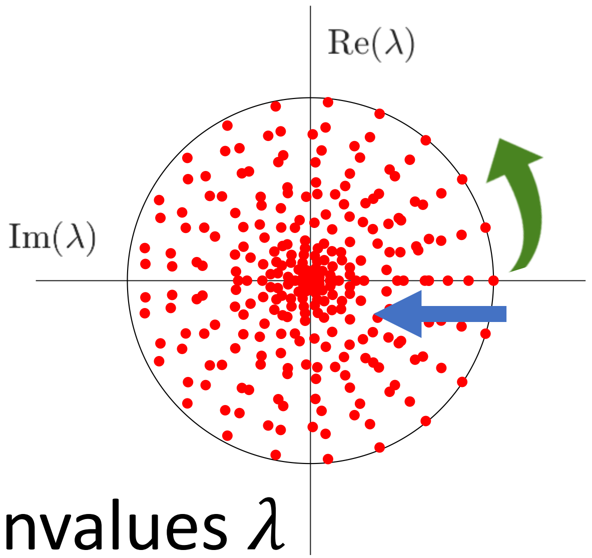

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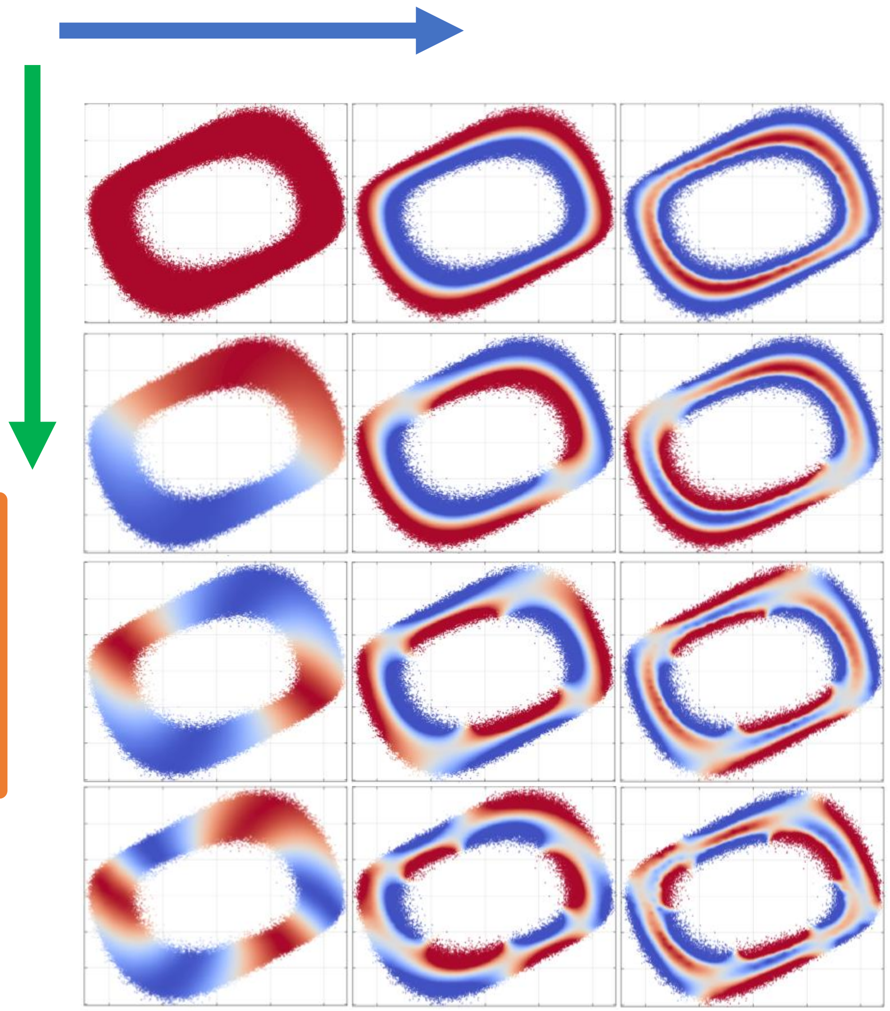
Eigenfunctions g_λ



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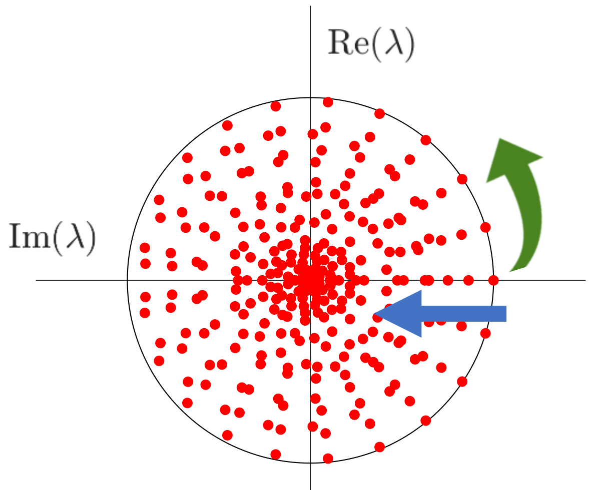

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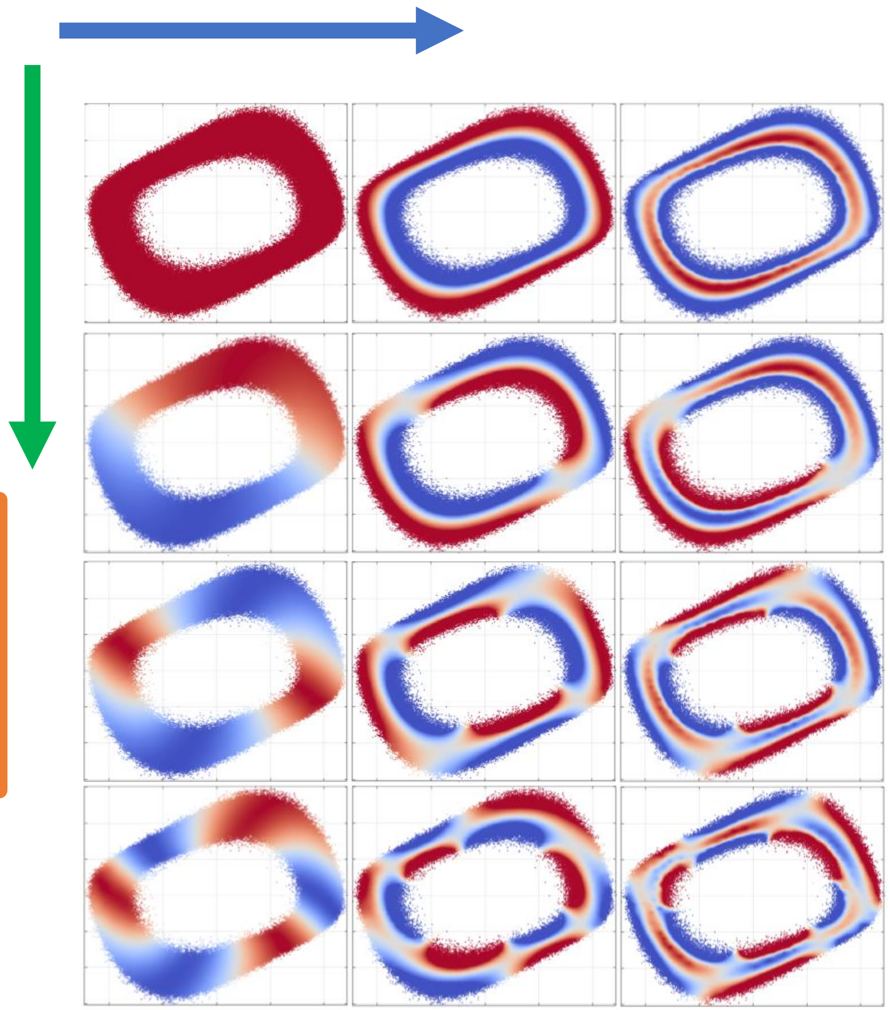
$$\mathbb{E}\left[g_\lambda\left(F_{\tau_n} \circ \cdots \circ F_{\tau_1}(x)\right)\right] = [\mathcal{K}^n g_\lambda](x) = \lambda^n g_\lambda(x)$$

Is this enough?

Eigenfunctions g_λ



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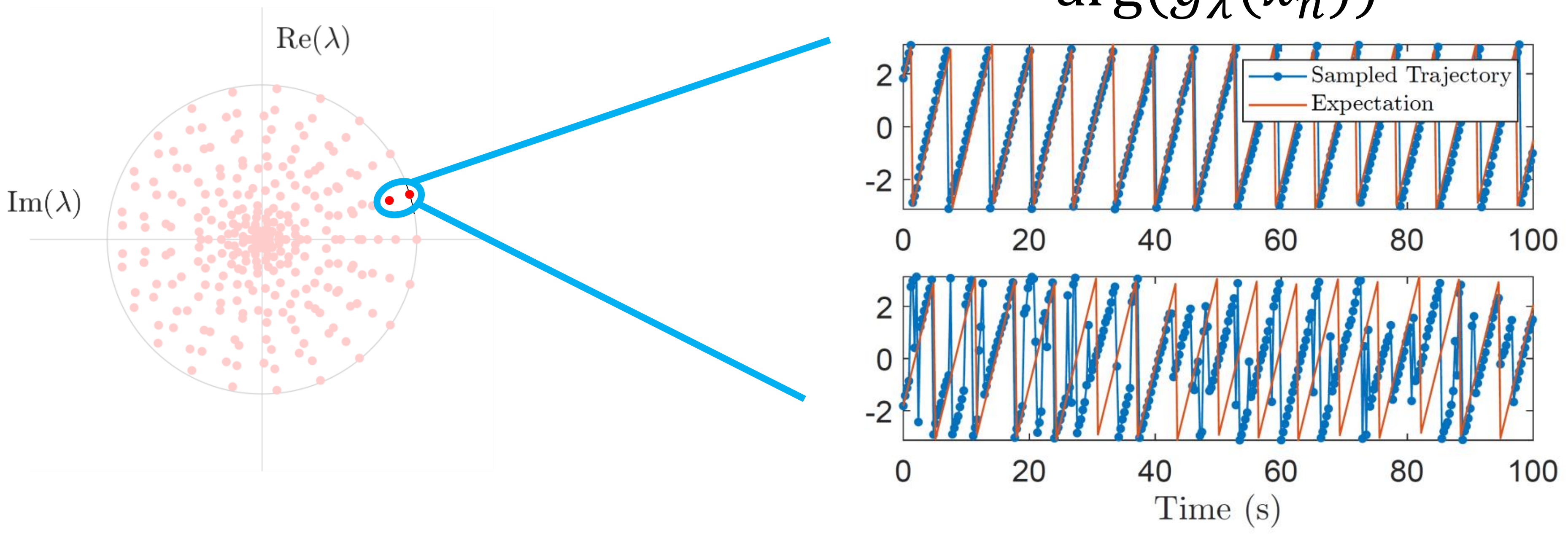
Same phase, but clearly one is more coherent than the other!

Sample at $\Delta t = 0.3$.

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



$\approx 0.956 + 0.290i$

$\approx 0.825 + 0.250i$

Time for an example!

Stochastic van der Pol oscillator:

$$\mathrm{d}X_1 = X_2\mathrm{d}t,$$
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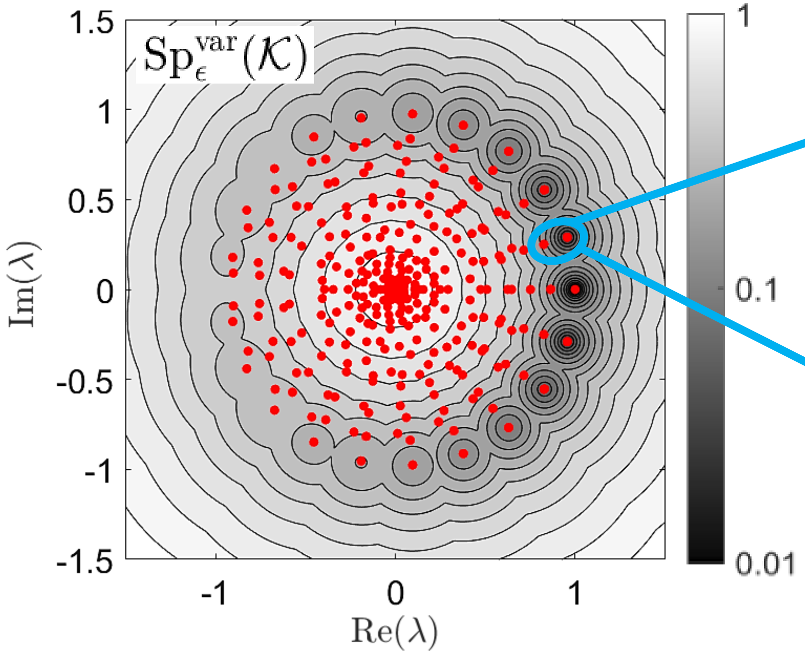

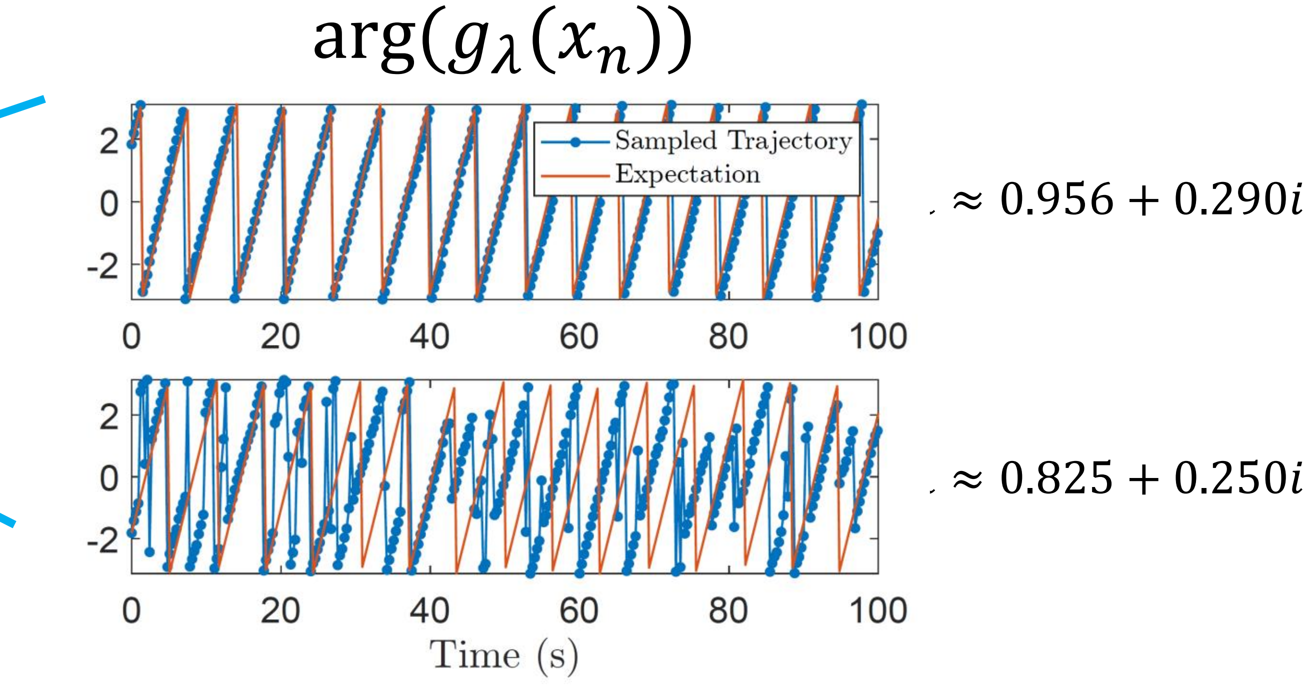

Dynamic Mode Decomposition (DMD)

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

Dictionary $\{\psi_1, \dots, \psi_N\}$ of functions $\psi_j : \Omega \to \mathbb{C}$,

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

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

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

Galerkin approximation: $\mathbb{K} = (\Psi_X^* W \Psi_X)^{-1} \Psi_X^* W \Psi_Y \in \mathbb{C}^{N \times N}$

- Schmid, *"Dynamic mode decomposition of numerical and experimental data,"* **J. Fluid Mech.**, 2010.
- Rowley, Mezić, Bagheri, Schlatter, Henningson, *"Spectral analysis of nonlinear flows,"* **J. Fluid Mech.**, 2009.
- 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,"* **J. Nonlinear Sci.**, 2015.

The missing matrix: Residual DMD

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

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

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

$$\lim_{M\to\infty} [K_2]_{jk} = \langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle + \int_{\Omega} \underbrace{\mathbb{E}\left[\left(\psi_k(F_\tau(x)) - [\mathcal{K}\psi_k](x)\right)\overline{\left(\psi_j(F_\tau(x)) - [\mathcal{K}\psi_j](x)\right)}\right]}_{\text{Covariance}} \mathrm{d}\omega(x)$$

Candidate eigenpair residuals

Function $g = \sum_{j=1}^{N} \mathbf{g}_j \psi_j$, scalar $\lambda \in \mathbb{C}$, want $g \circ F_\tau \approx \lambda g$

Statistical coherency: $\mathbb{E}[\|g \circ F_\tau - \lambda g\|^2]$

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Computation

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Computation

Squared residual

Integrated variance

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Definition: For $\varepsilon > 0$, the variance-ε-pseudospectrum is

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

Separation: *Batched* Koopman operator

Definition: For $g \in L^2(\Omega^r)$, $\left[\mathcal{K}_{(r)} g\right](x_1, \dots, x_r) = \mathbb{E}\left[g\left(F_\tau(x_1), \dots, F_\tau(x_r)\right)\right]$

Same realisation of τ used across the r arguments.

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Can approximate this with batched data. E.g., $r = 2$:

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Can separate residual & variance, extends to higher moments, etc.

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Can separate residual & variance, extends to higher moments, etc.

Concentration bounds on how much snapshot data is needed

Example formulas (with symmetrization)

$$G = \Psi_X^* W \Psi_X, \qquad K_1 = \Psi_X^* W (\Psi_{Y_1} + \Psi_{Y_2})/2,$$

$$K_2 = (\Psi_{Y_1}^* W \Psi_{Y_1} + \Psi_{Y_2}^* W \Psi_{Y_2})/2, \qquad K_3 = (\Psi_{Y_1}^* W \Psi_{Y_2} + \Psi_{Y_2}^* W \Psi_{Y_1})/2.$$

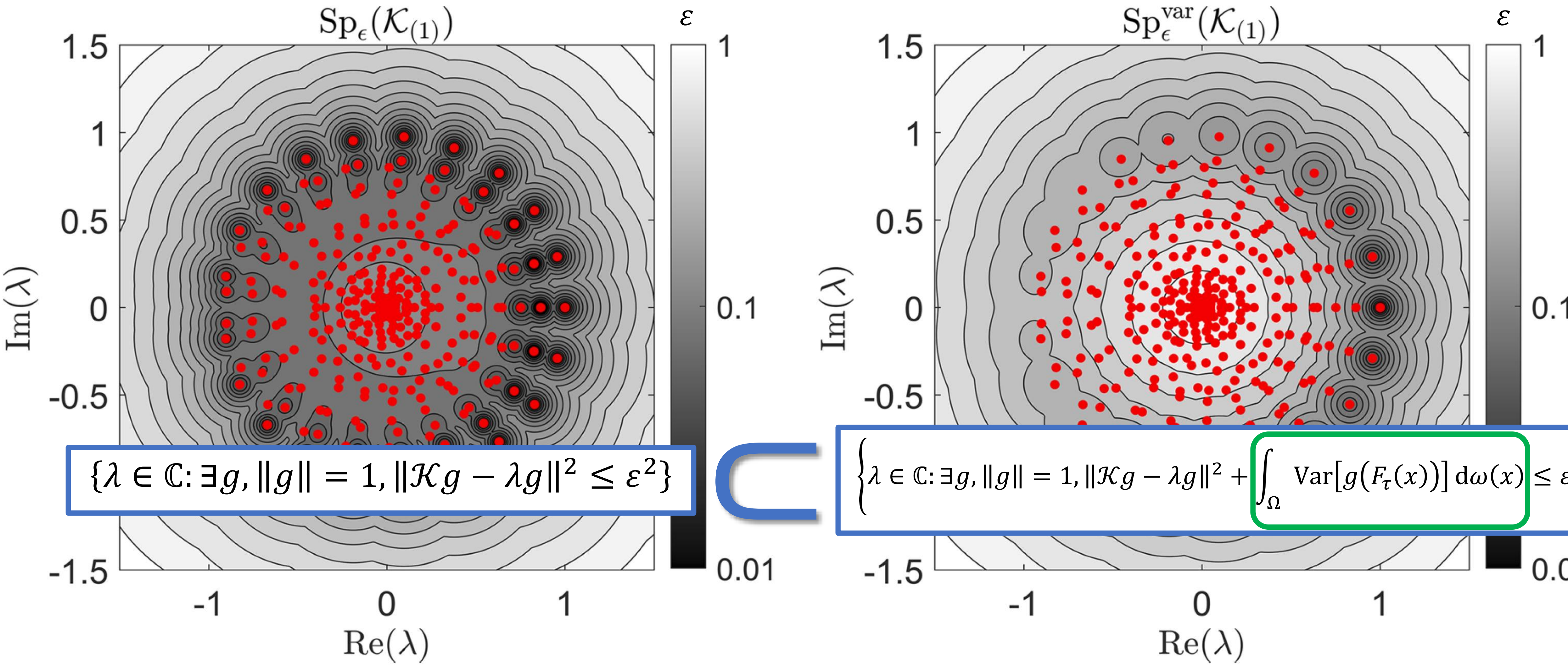
Residual for $\mathcal{K}$: $\|\mathcal{K}g - \lambda g\|^2 = \lim_{M\to\infty} \mathbf{g}^* \left[K_3 - \lambda K_1^* - \bar{\lambda} K_1 + |\lambda|^2 G\right] \mathbf{g}$

- Bound no projection errors.
- Spectral properties of $\mathcal{K} = \mathcal{K}_{(1)}$ without spurious eigenvalues.
- Verified dictionary, error bounds for trajectories.

Variance: $\int_\Omega \mathrm{Var}\left[g\left(F_\tau(x)\right)\right] \mathrm{d}\omega(x) = \lim_{M\to\infty} \mathbf{g}^* [K_2 - K_3] \mathbf{g}$

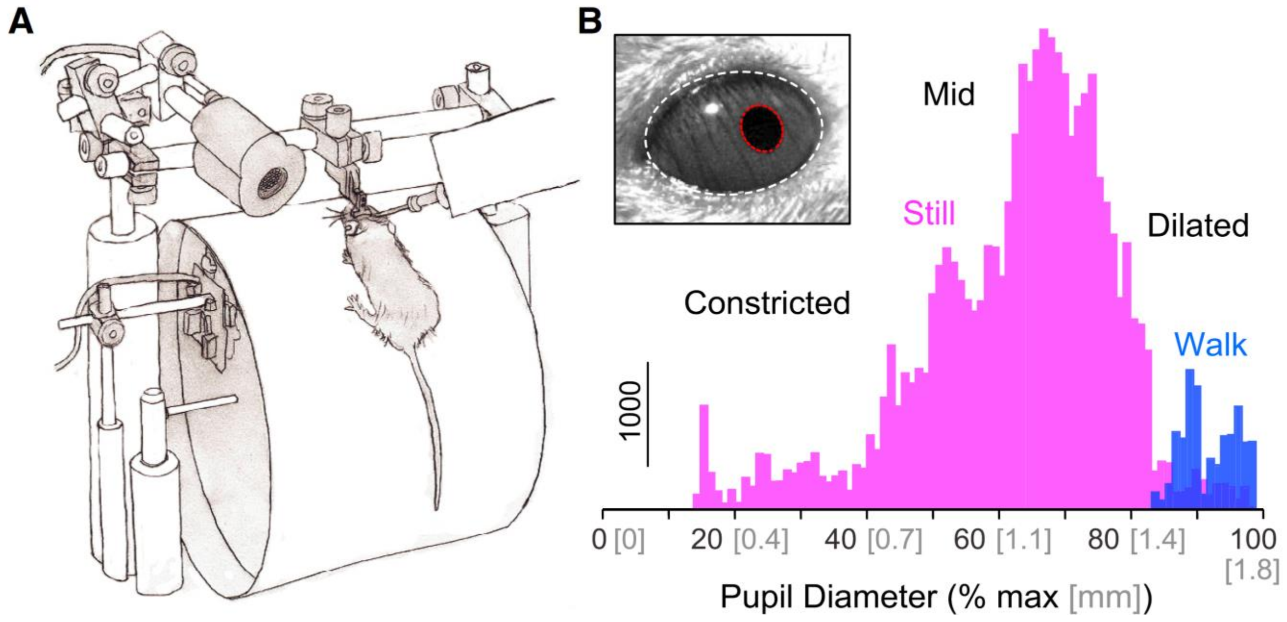
Spot the difference!

$$\mathrm{d}X_1 = X_2\mathrm{d}t, \qquad \mathrm{d}X_2 = [0.5(1 - X_1^2)X_2 - X_1]\mathrm{d}t + 0.2\mathrm{d}B_t, \qquad \Delta t = 0.3$$



$$\{\lambda \in \mathbb{C}: \exists g, \|g\| = 1, \|\mathcal{K}g - \lambda g\|^2 \leq \varepsilon^2\} \subset \left\{\lambda \in \mathbb{C}: \exists g, \|g\| = 1, \|\mathcal{K}g - \lambda g\|^2 + \int_\Omega \mathrm{Var}[g(F_\tau(x))]\, \mathrm{d}\omega(x) \leq \varepsilon^2\right\}$$

Application

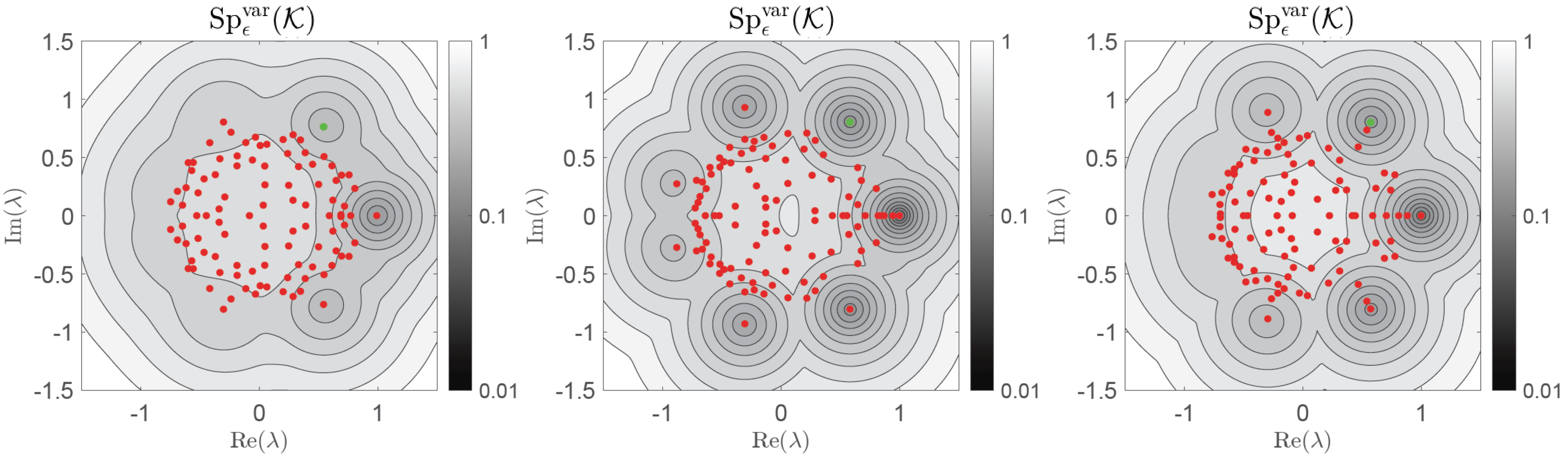


- Large populations of neurons.
- Mice shown drifting grating.
- 15 stochastic Koopman operators according to arousal level (pupil diameter).
- $N = 100$ basis functions.

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.

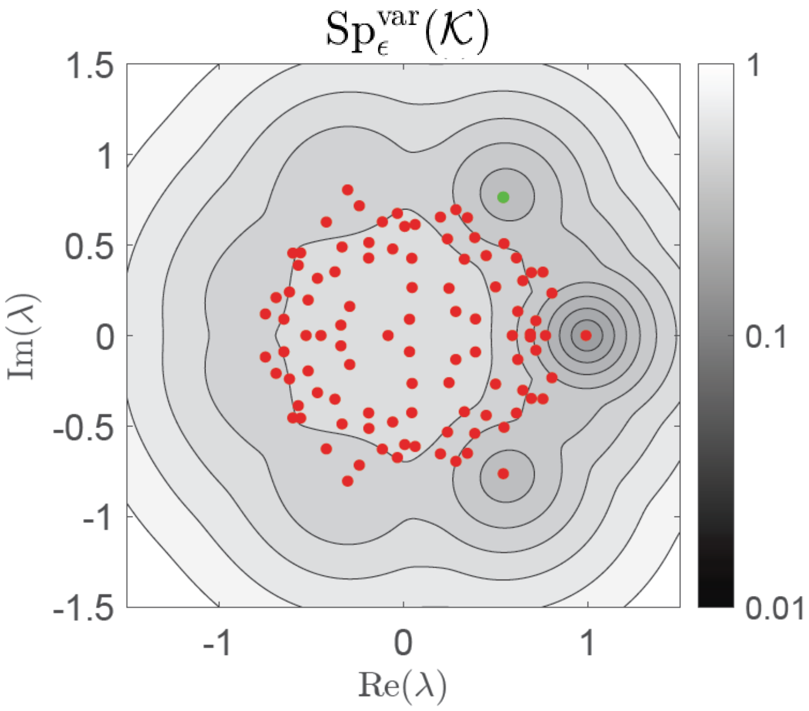
Variance pseudospectra of mouse # 11

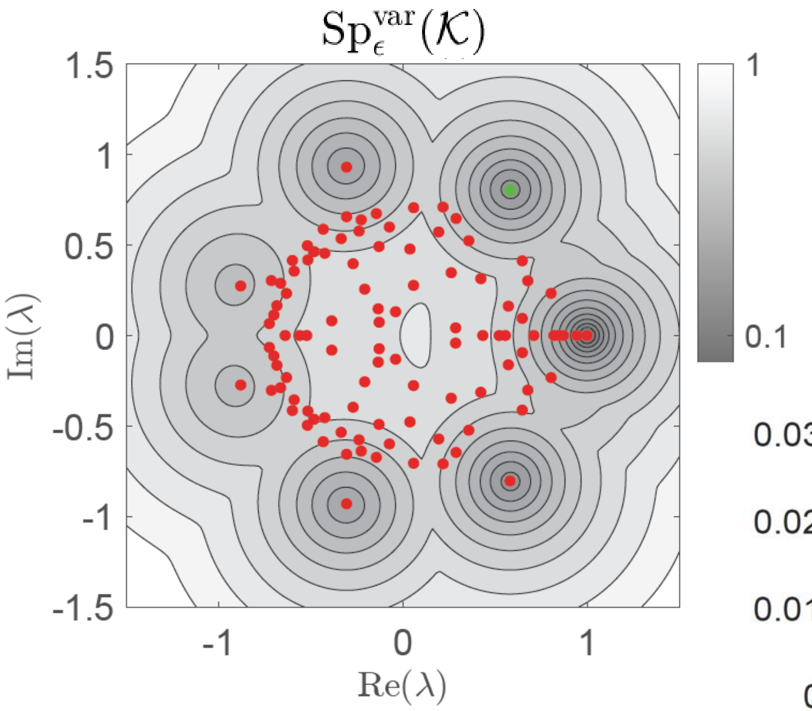


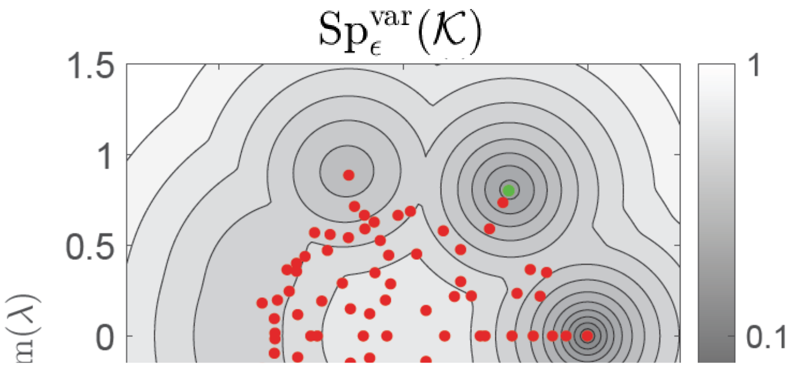
pupil diameter 8% pupil diameter 28% pupil diameter 43%

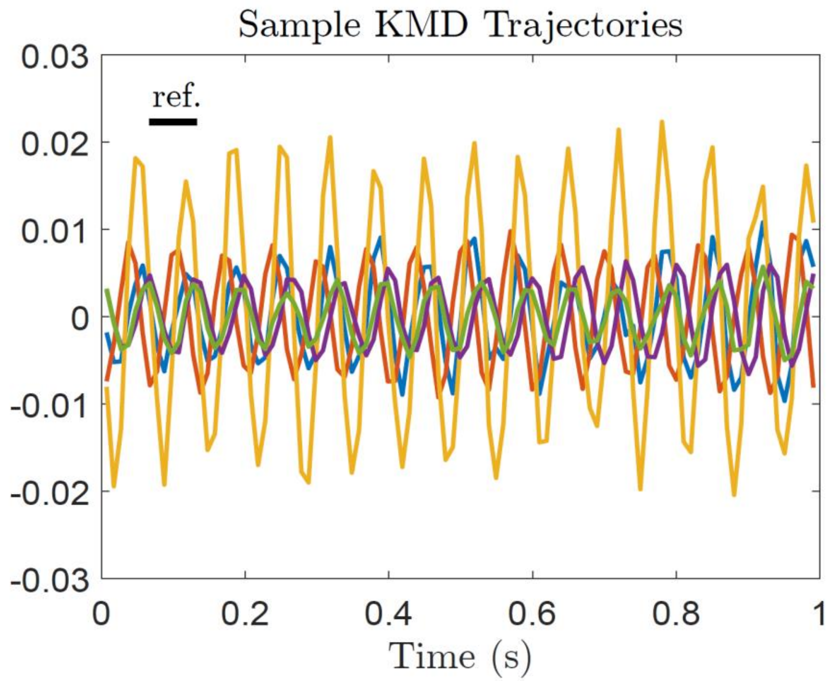
$$\|\mathcal{K}g - \lambda g\|^2 + \int_\Omega \mathrm{Var}[g(F_\tau(x))] \, \mathrm{d}\omega(x)$$

Variance pseudospectra of mouse # 11







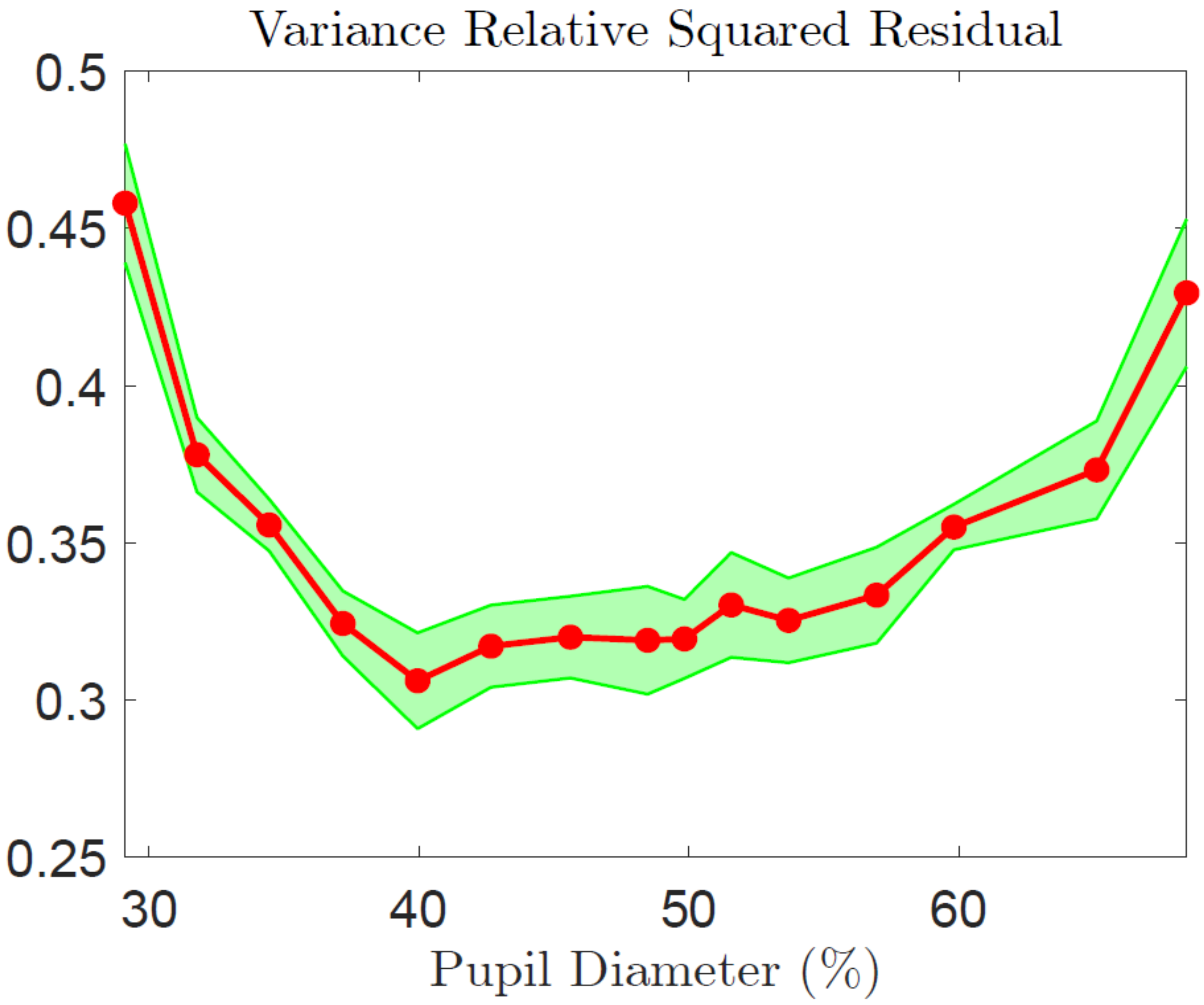


pupil diameter 8%

pupil diameter 28%

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

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.*

Conclusion: Crucial to move "beyond expectations" in Koopman setting

- Variance-ε-pseudospectrum measures statistical coherency.

Definition: For $\varepsilon > 0$, the variance-ε-pseudospectrum is

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

- Batched Koopman operators separate variance and residual.

Definition: For $g \in L^2(\Omega^r)$, $\left[\mathcal{K}_{(r)} g\right](x_1, \dots, x_r) = \mathbb{E}\left[g\left(F_\tau(x_1), \dots, F_\tau(x_r)\right)\right]$.

➢ **Verified data-driven** methods for Koopman operators of **stochastic systems**.

➢ Methods are **cheap**, **easy-to-use**, come with **convergence guarantees**.

References

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