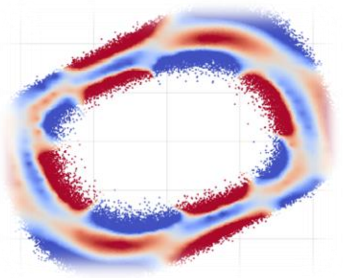
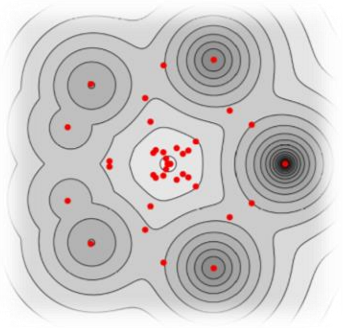
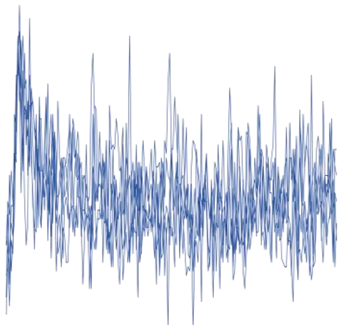
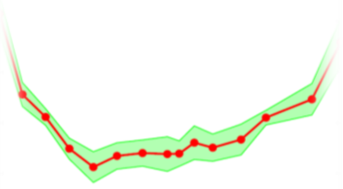








Going beyond expectations: Stochastic ResDMD

Matthew Colbrook
University of Cambridge

22/08/2023

Joint work with:

Qin Li

Ryan Raut

Alex Townsend

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

Stochastic Dynamical System

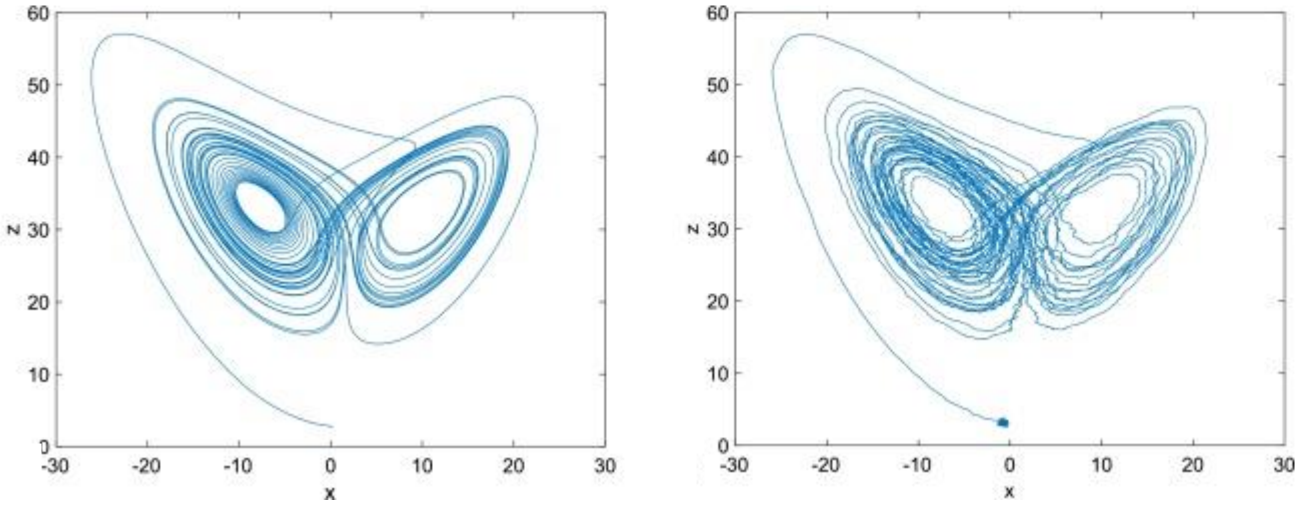
State $x \in \Omega \subseteq \mathbb{R}^d$, i.i.d. random variables $\tau_1, \tau_2, \ldots$

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 or uncertainty, or truly random process.



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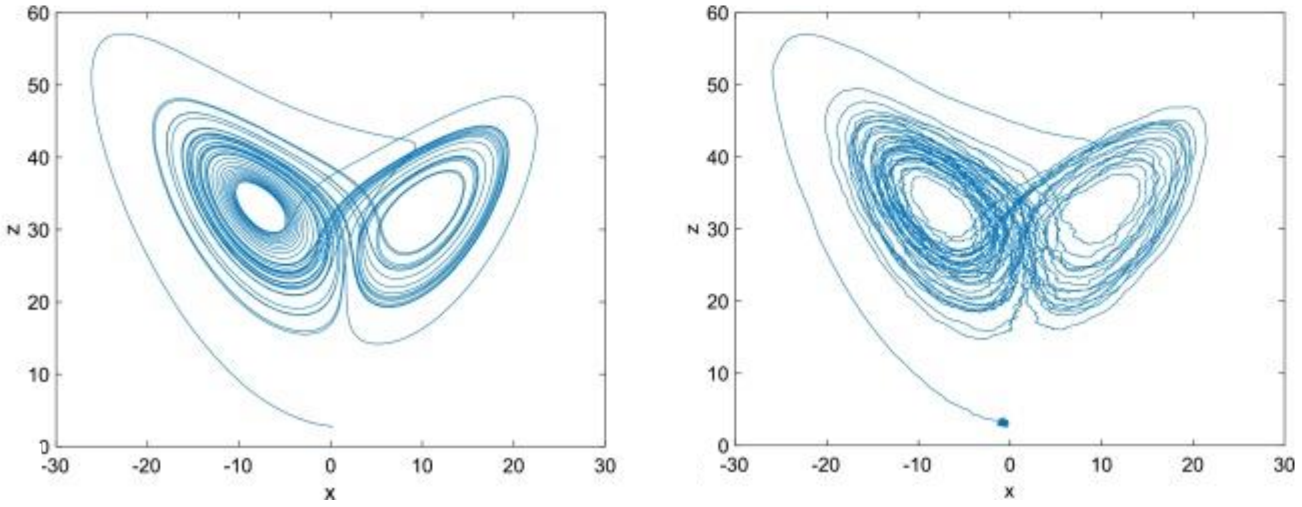
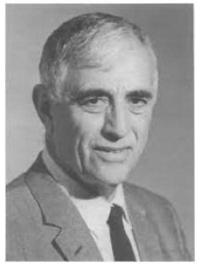


Goal: Verified learning from data $\{x^{(m)}, y^{(m)} = F_{\tau_m}(x^{(m)})\}_{m=1}^{M}$.

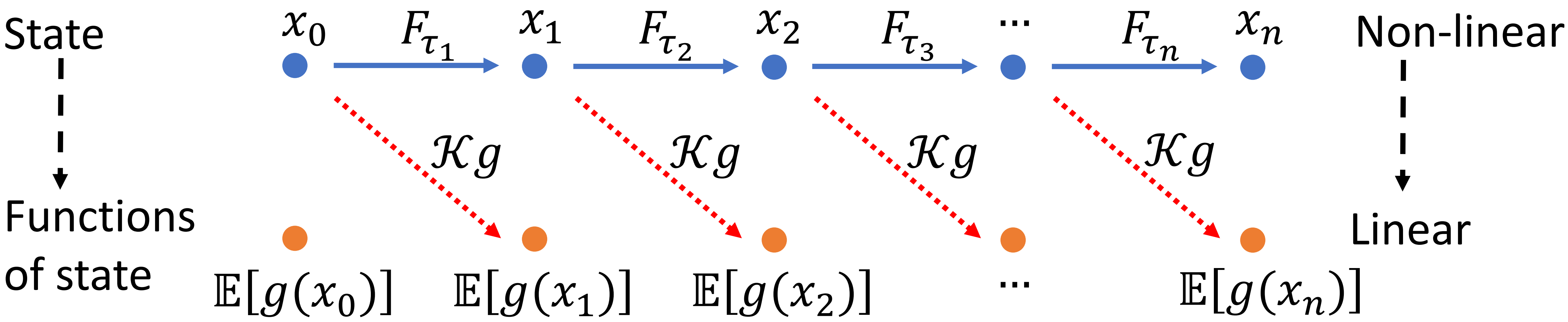
Koopman Operator

Koopman



von Neumann

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



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:

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

Turn into discrete-time system with step 0.3.

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

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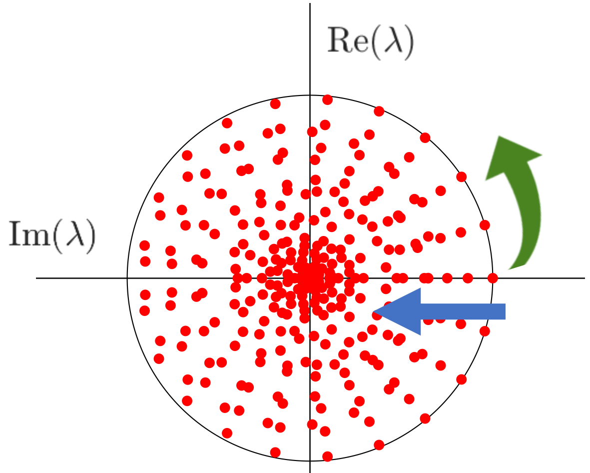

Eigenvalues λ

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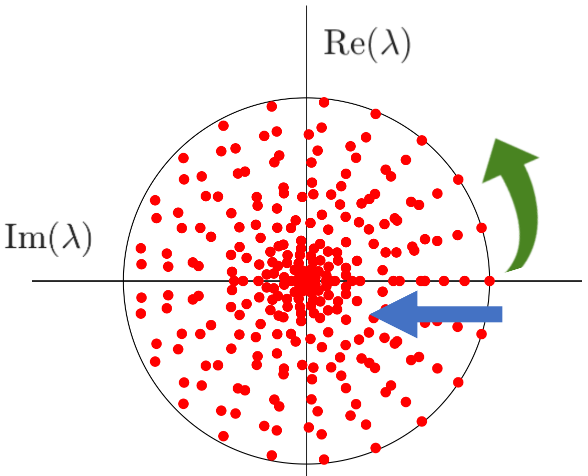

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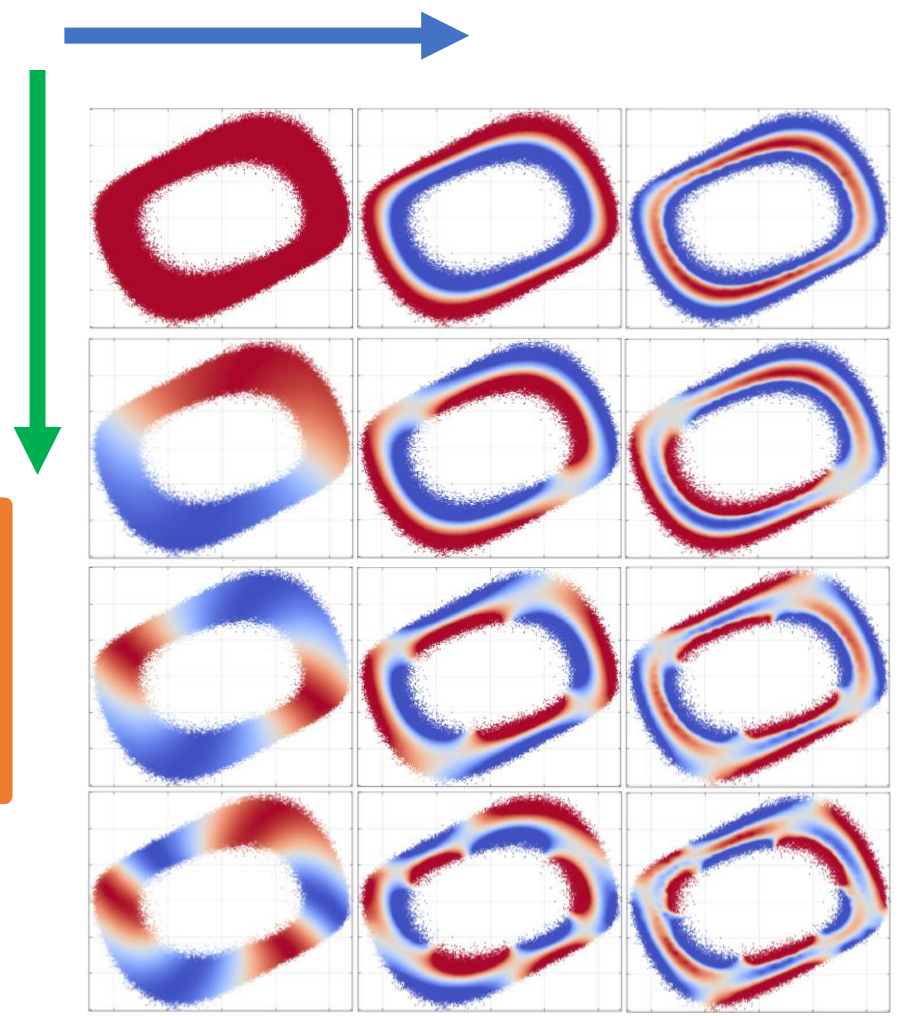
Eigenfunctions g_λ



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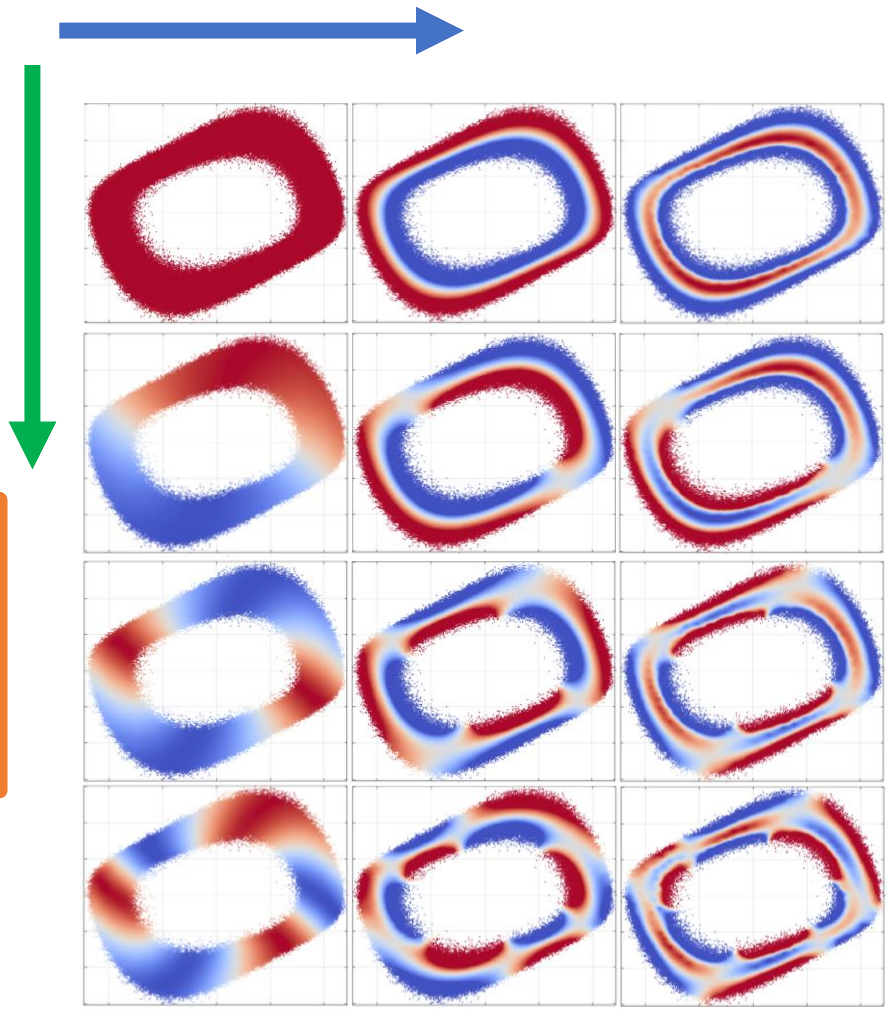
Eigenfunctions g_λ



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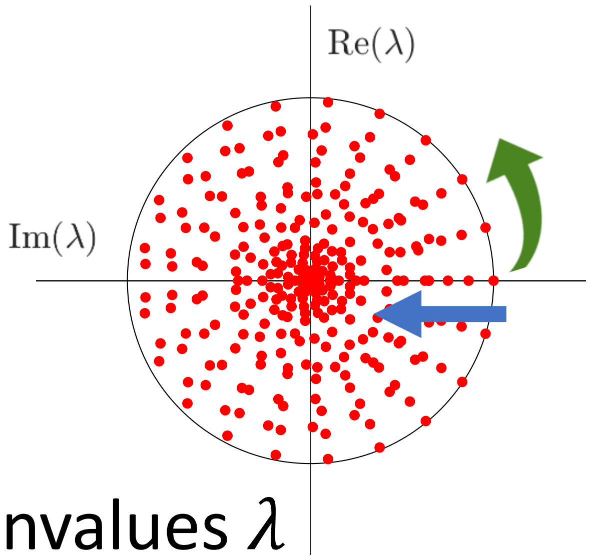

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$$\mathbb{E}\left[g_\lambda\left(F_{\tau_n} \circ \cdots \circ F_{\tau_1}(x)\right)\right] = [\mathcal{K}^n g_\lambda](x) = \lambda^n g_\lambda(x)$$

Is this enough?

Time for an example!

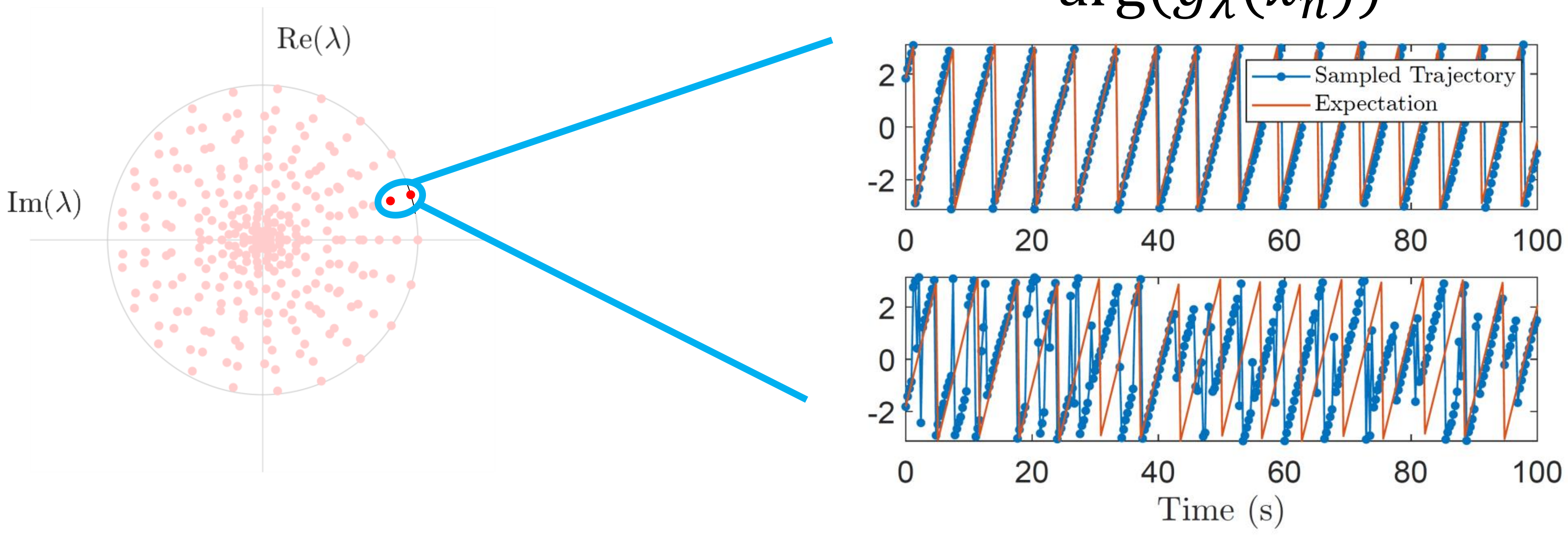
Stochastic Van der Pol oscillator:

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

Turn into discrete-time system with step 0.3.

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

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



$\approx 0.956 + 0.290i$

$\approx 0.825 + 0.250i$

Time for an example!

Stochastic Van der Pol oscillator:

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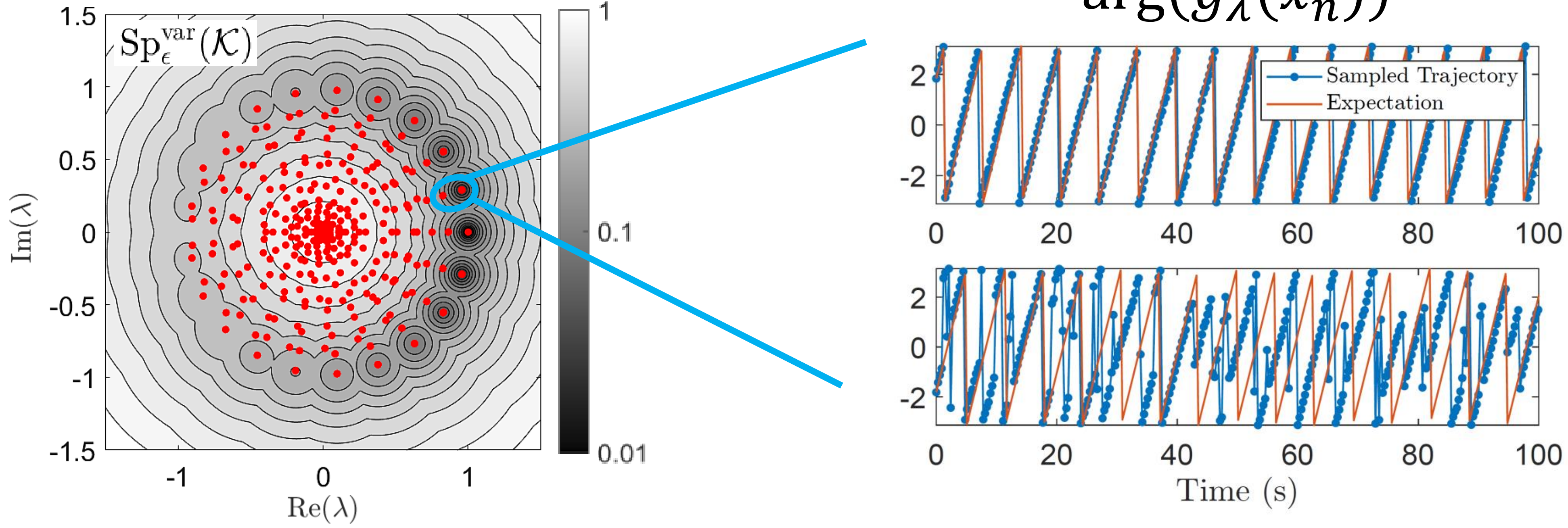

$\approx 0.956 + 0.290i$

$\approx 0.825 + 0.250i$

Dynamic Mode Decomposition (DMD)

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

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

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

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

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

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

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

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

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

- 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

The missing matrix: Residual DMD

Only if system deterministic!

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

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

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

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.
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Decomposing the residual

$$\lim_{M\to\infty} \mathbf{g}^*\left[K_2 - \lambda K_1{}^* - \bar{\lambda} K_1 + |\lambda|^2 G\right]\mathbf{g}$$
$$= \mathbb{E}[\|g \circ F_\tau - \lambda g\|^2]$$
$$= \|\mathcal{K}g - \lambda g\|^2 + \int_\Omega \mathrm{Var}[g(F_\tau(x))]\, \mathrm{d}\omega(x)$$

Squared residual   Integrated variance

Decomposing the residual

$$\lim_{M\to\infty} \mathbf{g}^*\left[K_2 - \lambda {K_1}^* - \bar{\lambda} K_1 + |\lambda|^2 G\right]\mathbf{g}$$
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Squared residual — Integrated variance

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

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

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Measure of statistical coherency.

Sampler of the results we prove

Representation of higher moments via batched Koopman operators:

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

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

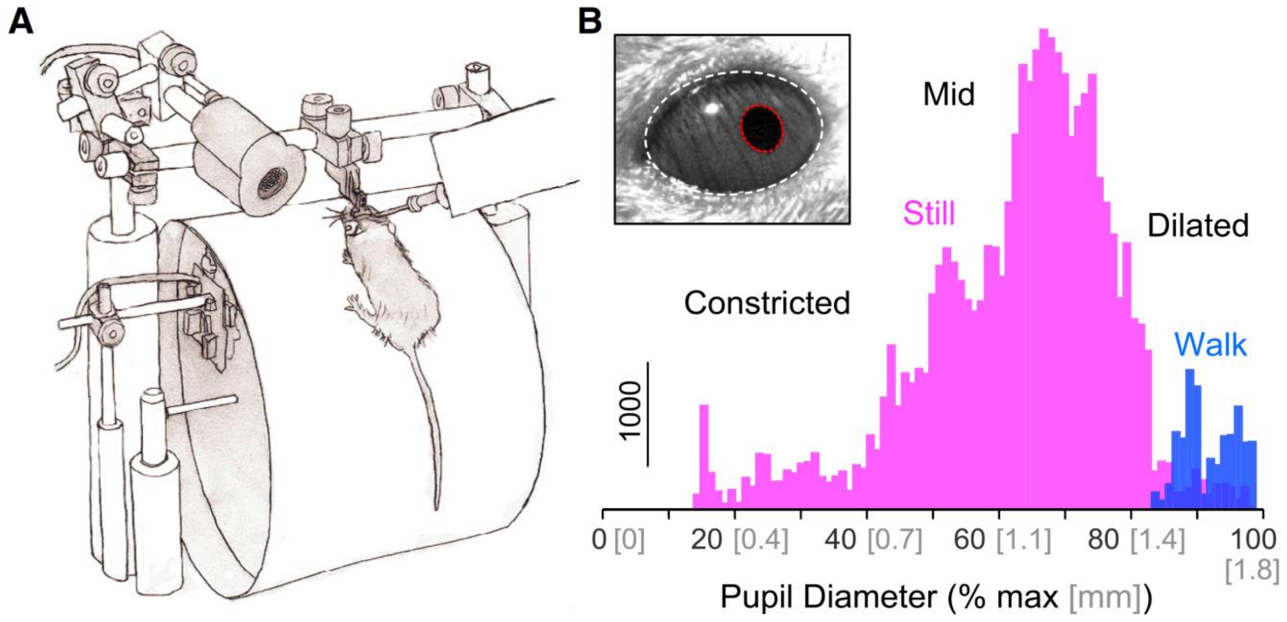
Computation of spectrum of $\mathcal{K}$ without issues such as spurious eigenvalues.

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

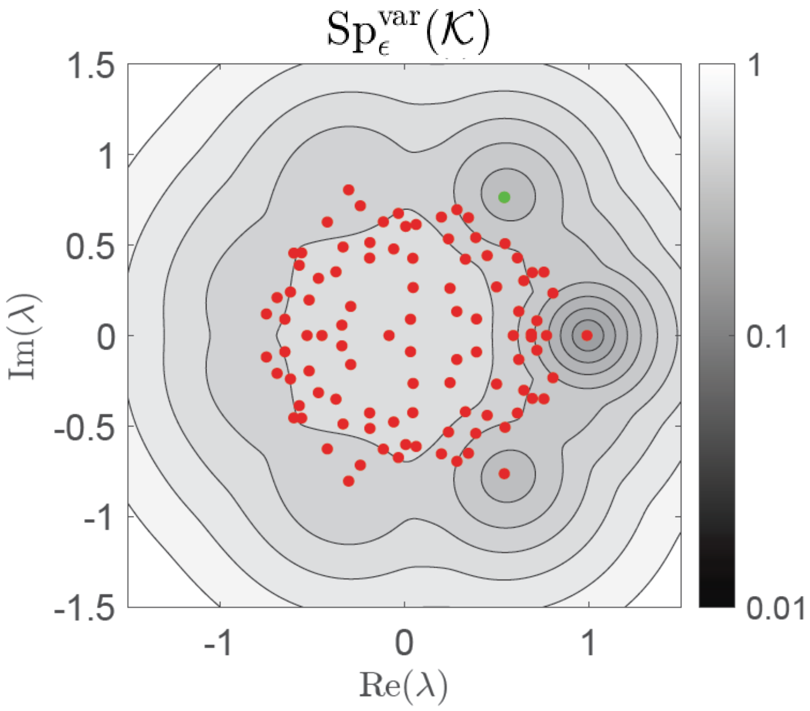


- Monitoring of large populations of neurons.
- Mice shown a drifting grating.
- Separate stochastic Koopman operators according to 15 different arousal levels (indexed by pupil diameter).

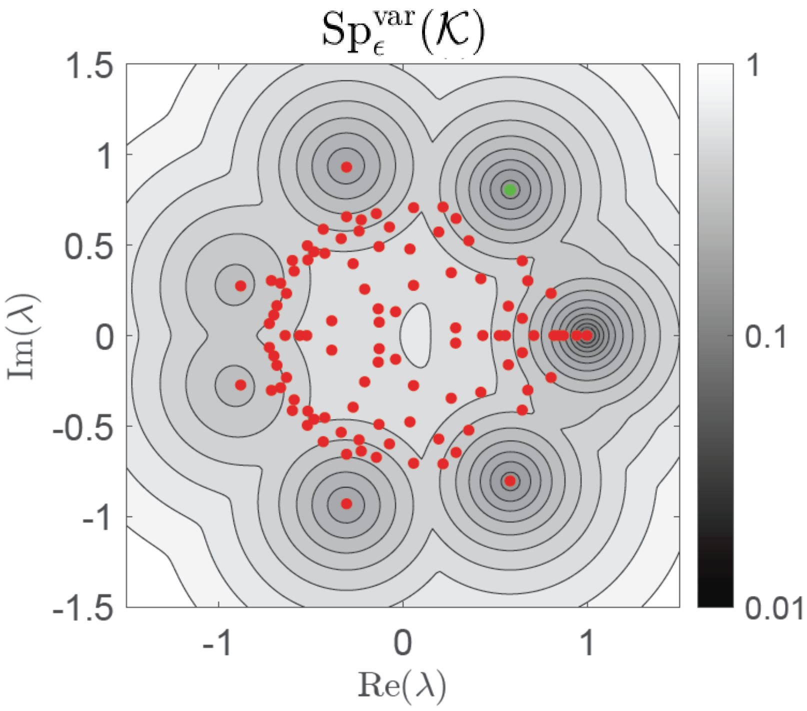
Standard DMD does not provide verification…

- 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.

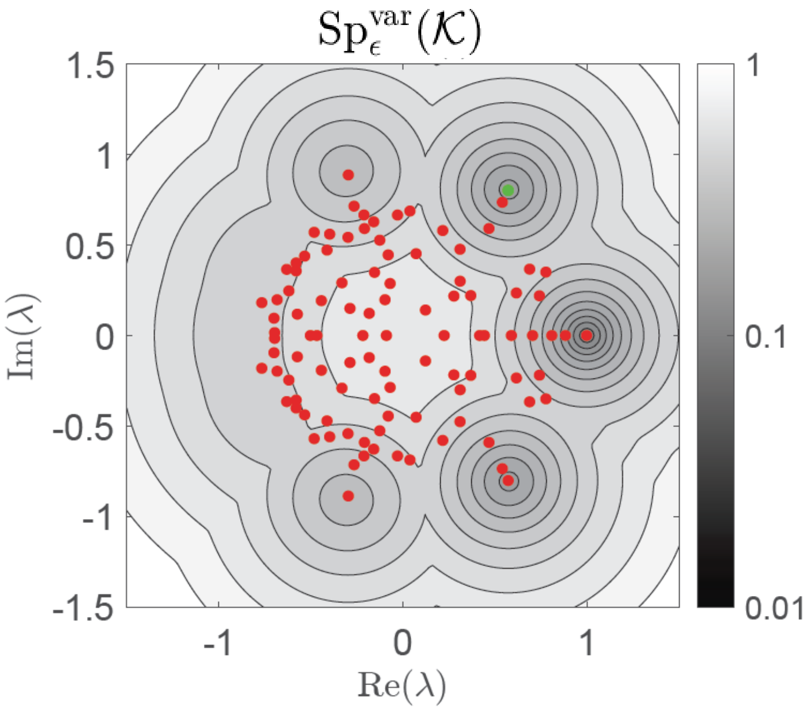
Variance pseudospectra of mouse # 11



pupil diameter 8%



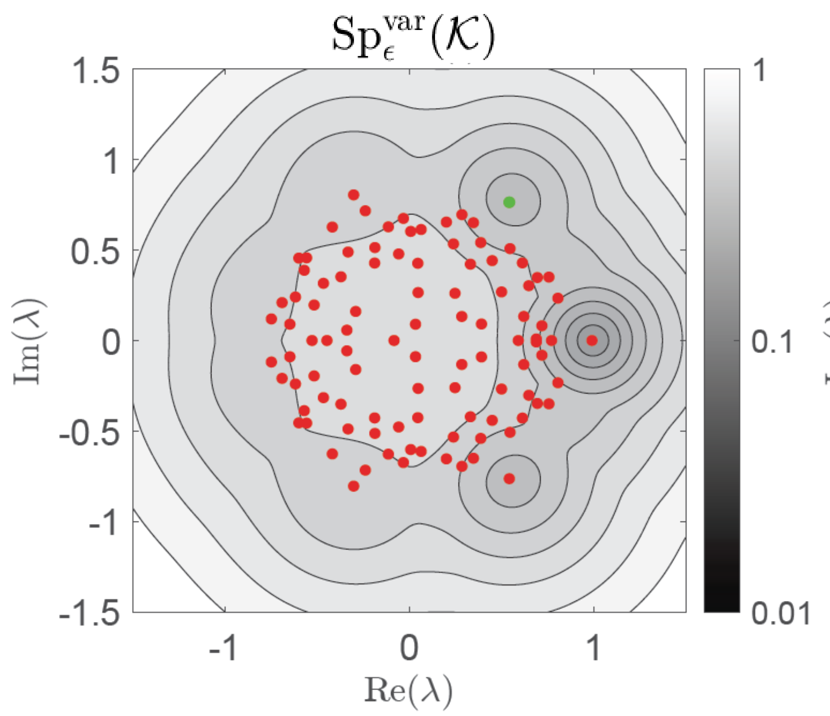
pupil diameter 28%



pupil diameter 43%

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

Variance pseudospectra of mouse # 11



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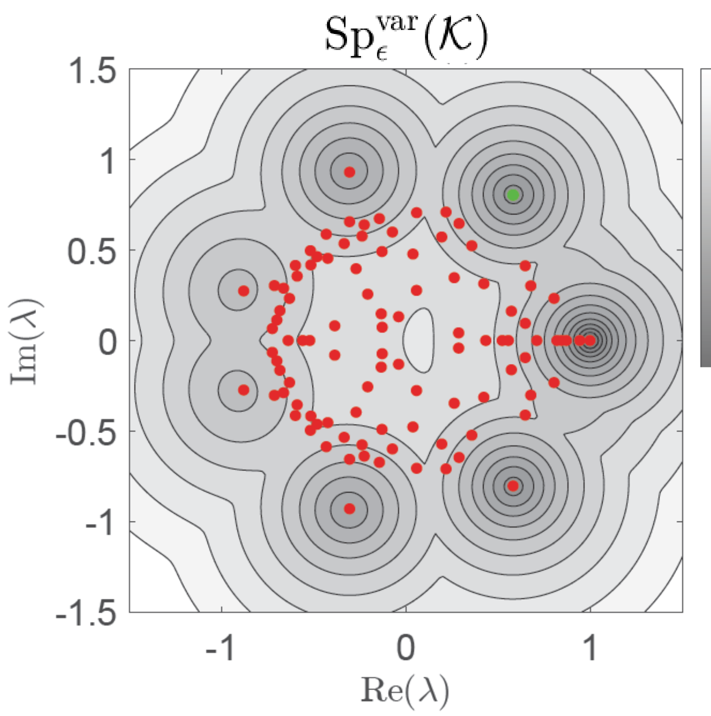

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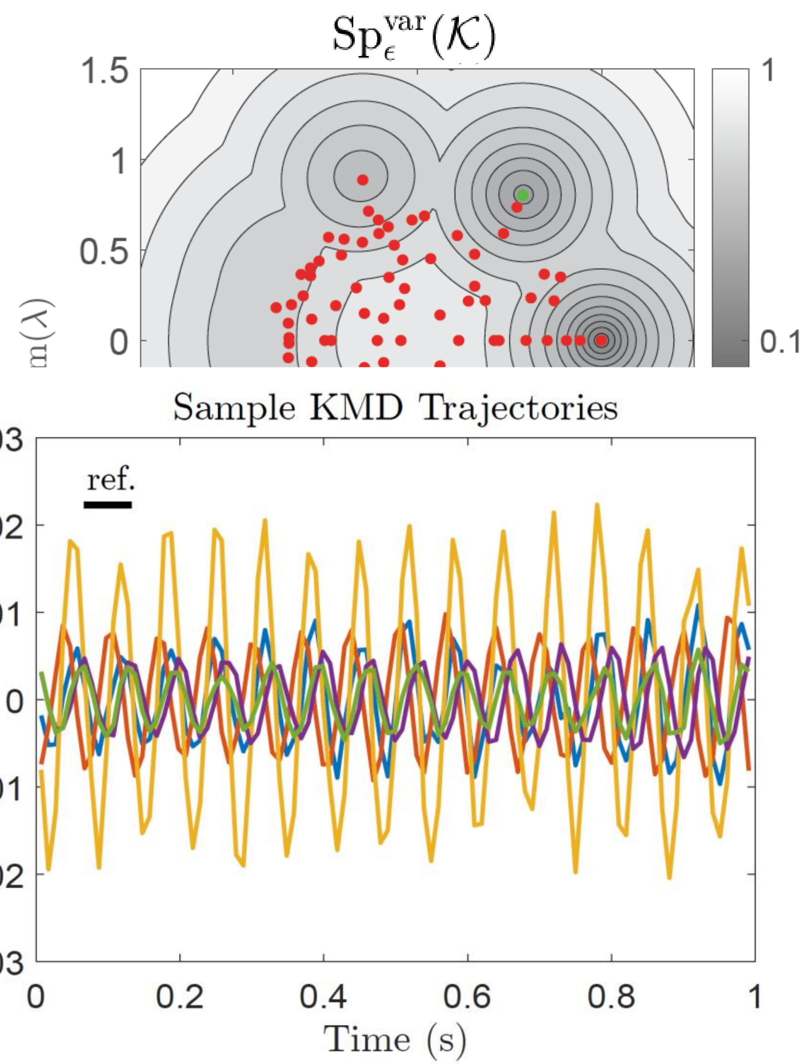
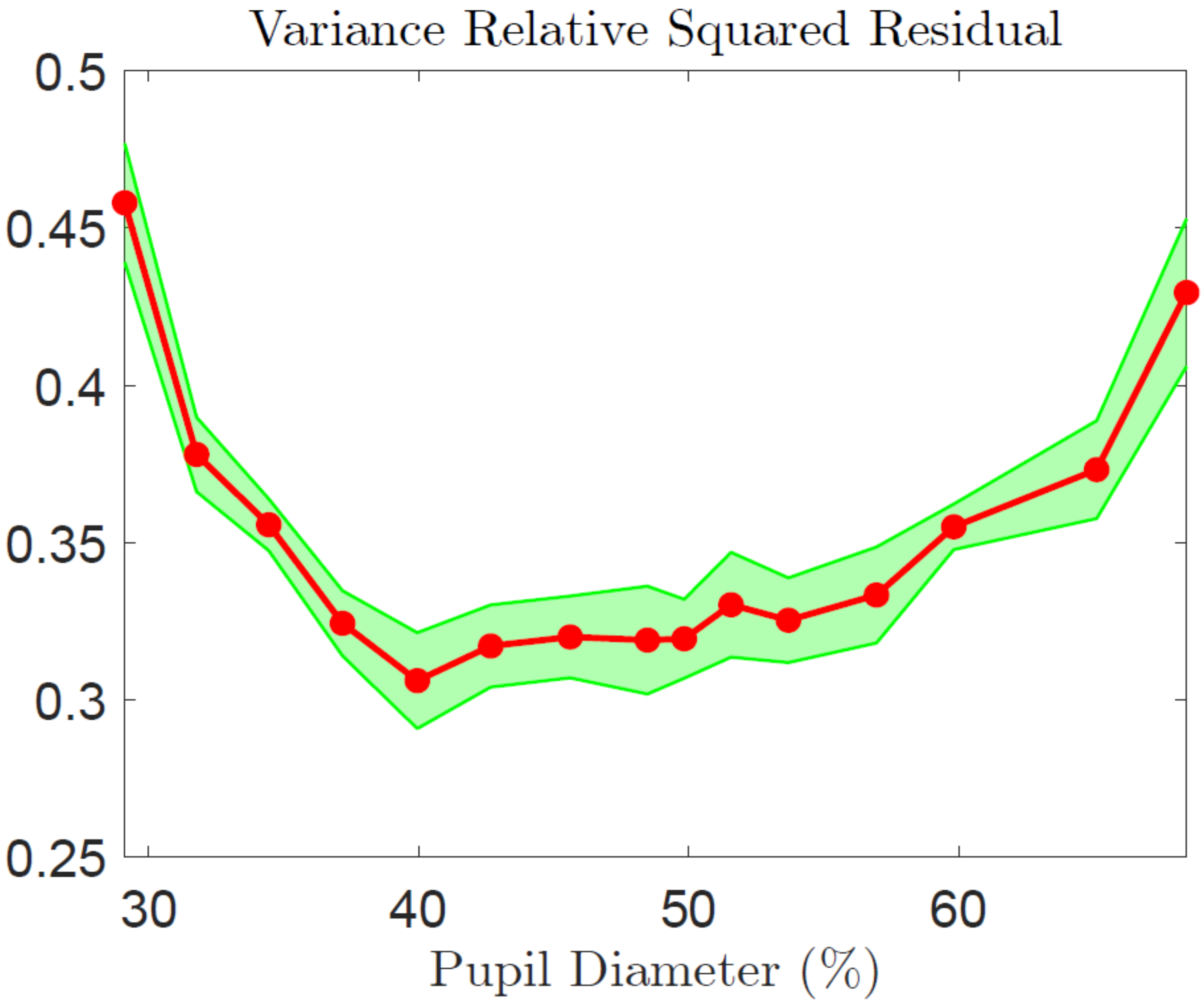


$$\|\mathcal{K}g - \lambda g\|^2 + \int_\Omega \mathrm{Var}[g(F_\tau(x))]\,\mathrm{d}\omega(x)$$

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

- **Verified data-driven** methods for Koopman operators of **stochastic systems**.
- Methods are **cheap**, **easy-to-use**, come with **convergence guarantees**.
- It is crucial **to move beyond expectations** when **studying projection errors** (dealing with infinite dimensions).

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

Please get in touch if you have suggestions, comments, or collaborative ideas!

References

[1] 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).

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

[3] 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.

[4] 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).

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

[6] 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.

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