Data-driven numerical analysis of Koopman operators for dynamical systems

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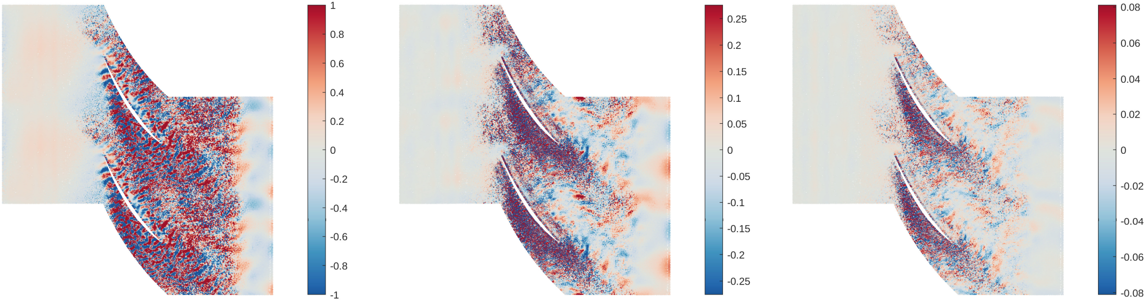
Based on: Matthew Colbrook and Alex Townsend, "*Rigorous data-driven computation of spectral properties of Koopman operators for dynamical systems*" (available on arXiv)



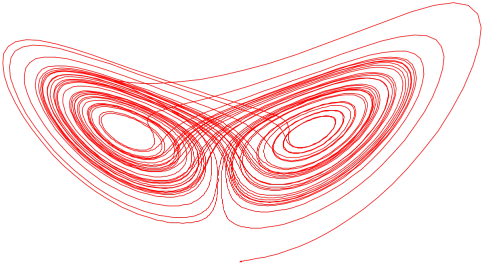
The setup: discrete-time dynamical system

Dynamical system: State $\boldsymbol{x} \in \Omega \subset \mathbb{R}^d$, $\quad F : \Omega \to \Omega, \quad \boldsymbol{x}_{n+1} = F(\boldsymbol{x}_n)$.

Given snapshot data: $\{\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)}\}_{m=1}^{M}$ with $\boldsymbol{y}^{(m)} = F(\boldsymbol{x}^{(m)})$.

Broad goal: Learn properties of the dynamical system.

Applications: Biochemistry, classical mechanics, climate, electronics, epidemiology, finance, fluids, molecular dynamics, neuroscience, robotics, ... (anything evolving in time).



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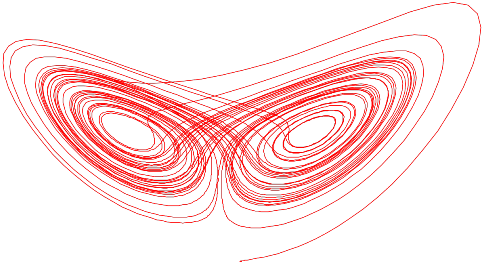
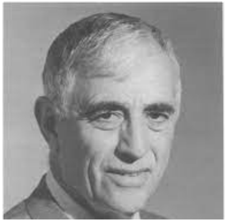


Immediate difficulties:

- F is **unknown**
- F is typically **nonlinear**
- system could be **chaotic**

Koopman operators



Vol. 17, 1931 *MATHEMATICS: B. O. KOOPMAN* 315

HAMILTONIAN SYSTEMS AND TRANSFORMATIONS IN HILBERT SPACE

By B. O. Koopman

Department of Mathematics, Columbia University

Communicated March 23, 1931

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Observable $g : \Omega \to \mathbb{C}$

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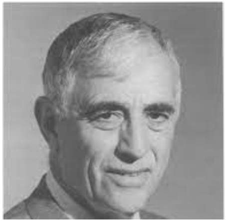

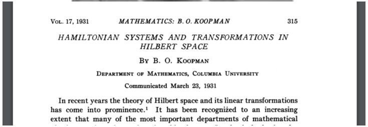

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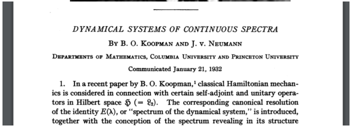

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GOAL: Learn spectral properties of $\mathcal{K}$. Spectrum, $\sigma(\mathcal{K}) = \{z \in \mathbb{C} : \mathcal{K} - z \text{ not invertible}\}$.

Why spectra?

Suppose $(\lambda, \varphi_\lambda)$ is an eigenfunction-eigenvalue pair of $\mathcal{K}$, then

$$\varphi_\lambda(\boldsymbol{x}_n) = [\mathcal{K}^n \varphi_\lambda](\boldsymbol{x}_0) = \lambda^n \varphi_\lambda(\boldsymbol{x}_0).$$

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Suppose system is measure-preserving (e.g., Hamiltonian, ergodic,...), $\forall g \in L^2(\Omega, \omega)$

$$g = \underbrace{\sum_{\text{e-vals } \lambda} c_\lambda \varphi_\lambda}_{\text{discrete spectral part}} + \underbrace{\int_{[-\pi,\pi]_{\mathrm{per}}} \phi_{\theta,g} \, d\theta}_{\text{continuous spectral part}}.$$

φ_λ are eigenfunctions of $\mathcal{K}$, $c_\lambda \in \mathbb{C}$, $\phi_{\theta,g}$ are "continuously parametrised" eigenfunctions.

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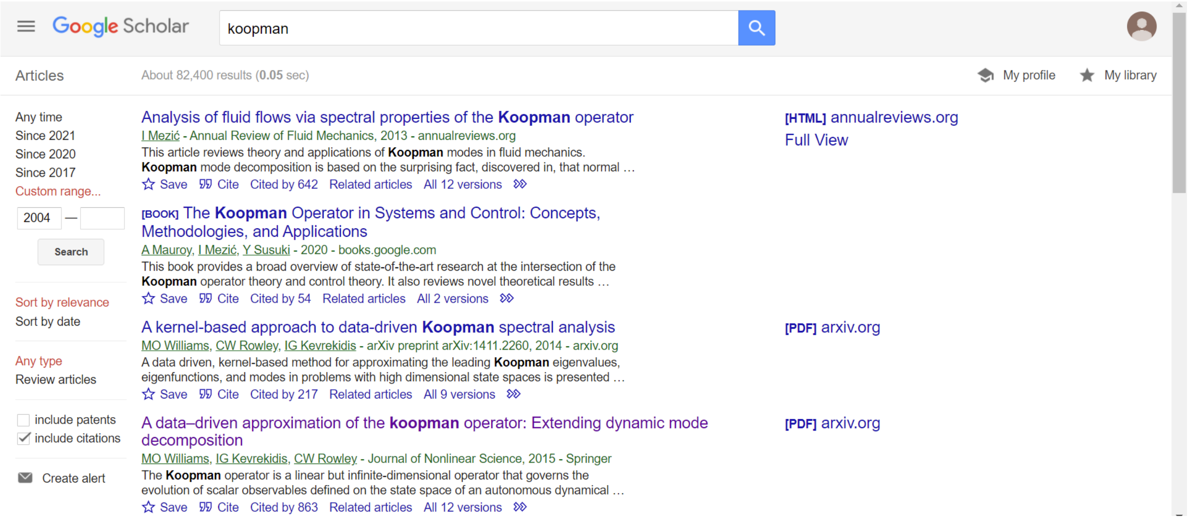
Koopman mode decomposition

$$g(\boldsymbol{x}_n) = [\mathcal{K}^n g](\boldsymbol{x}_0) = \sum_{\text{e-vals } \lambda} c_\lambda \lambda^n \varphi_\lambda(\boldsymbol{x}_0) + \int_{[-\pi,\pi]_{\mathrm{per}}} e^{in\theta} \phi_{\theta,g}(\boldsymbol{x}_0)\, d\theta.$$

· I. Mezić "*Spectral properties of dynamical systems, model reduction and decompositions*," Nonlin. Dyn., 2005.

Lots of interest!



· I. Mezić, A. Banaszuk "*Comparison of systems with complex behavior*," Physica D, 2004.
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Challenges

Global understanding of nonlinear dynamics in state-space:

"*a mathematical grand challenge of the 21st century*"

· M. Budišić, R. Mohr, I. Mezić "*Applied Koopmanism*," Chaos, 2012.
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Solutions in this talk:

(S1) Compute smoothed approximations of spectral measures with explicit high-order convergence rates.

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(S2) Compute spectral properties of $\mathcal{K}$ directly, as opposed to restrictions of $\mathcal{K}$ to finite-dimensional subspaces.

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(S2) Compute spectral properties of $\mathcal{K}$ directly, as opposed to restrictions of $\mathcal{K}$ to finite-dimensional subspaces.

(S3) Compute residuals associated with the spectrum with error control, providing convergence without spectral pollution.

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(S4) Handle chaotic systems using single time steps.

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Part 1: Computing residuals and spectra.

General Koopman operators.

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

Extended dynamic mode decomposition (EDMD)

Subspace $\mathrm{span}\{\psi_j\}_{j=1}^{N_K} \subset L^2(\Omega,\omega)$, $\Psi(\boldsymbol{x}) = \begin{bmatrix}\psi_1(\boldsymbol{x}) & \cdots & \psi_{N_K}(\boldsymbol{x})\end{bmatrix} \in \mathbb{C}^{1\times N_K}$.

$$\text{For } \{\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)} = F(\boldsymbol{x}^{(m)})\}_{m=1}^{M}, \quad \Psi_X = \begin{pmatrix}\Psi(\boldsymbol{x}^{(1)})\\ \vdots \\ \Psi(\boldsymbol{x}^{(M)})\end{pmatrix} \in \mathbb{C}^{M\times N_K}, \quad \Psi_Y = \begin{pmatrix}\Psi(\boldsymbol{y}^{(1)})\\ \vdots \\ \Psi(\boldsymbol{y}^{(M)})\end{pmatrix} \in \mathbb{C}^{M\times N_K}.$$

· M. Williams, I. Kevrekidis, C. Rowley "*A data–driven approximation of the Koopman operator: Extending dynamic mode decomposition*," J. Nonlin. Sci., 2015.

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$$\text{Given} \quad g = \sum_{j=1}^{N_K} \psi_j \boldsymbol{g}_j, \quad \text{seek } K_{\mathrm{EDMD}} \in \mathbb{C}^{N_K\times N_K} \text{ with} \quad \mathcal{K}g \approx \sum_{j=1}^{N_K} \psi_j [K_{\mathrm{EDMD}}\boldsymbol{g}]_j.$$

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$$\min_{B\in\mathbb{C}^{N_K\times N_K}} \int_\Omega \max_{\|\boldsymbol{g}\|_{\ell^2}=1} \left|\mathcal{K}g - \sum_{j=1}^{N_K} \psi_j [B\boldsymbol{g}]_j\right|^2 d\omega(\boldsymbol{x}) \approx \sum_{m=1}^{M} w_m \left\|\Psi(\boldsymbol{y}^{(m)}) - \Psi(\boldsymbol{x}^{(m)})B\right\|_2^2.$$

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Solution: $K_{\mathrm{EDMD}} = (\Psi_X^* W \Psi_X)^\dagger (\Psi_X^* W \Psi_Y) \quad (W = \mathrm{diag}(w_1, ..., w_M))$

Large data limit: $\lim_{M\to\infty} [\Psi_X^* W \Psi_X]_{jk} = \langle \psi_k, \psi_j\rangle$ and $\lim_{M\to\infty} [\Psi_X^* W \Psi_Y]_{jk} = \langle \mathcal{K}\psi_k, \psi_j\rangle$

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Residual DMD (ResDMD): A new matrix

If $g=\sum_{j=1}^{N_K}\psi_j\boldsymbol{g}_j\in\mathrm{span}\{\psi_j\}_{j=1}^{N_K}$ and λ are a candidate eigenfunction-eigenvalue pair then

$$\begin{aligned}\|\mathcal{K}g-\lambda g\|^2_{L^2(\Omega,\omega)}&=\sum_{j,k=1}^{N_K}\boldsymbol{g}_k\overline{\boldsymbol{g}_j}\left[\langle\mathcal{K}\psi_k,\mathcal{K}\psi_j\rangle-\lambda\langle\psi_k,\mathcal{K}\psi_j\rangle-\overline{\lambda}\langle\mathcal{K}\psi_k,\psi_j\rangle+|\lambda|^2\langle\psi_k,\psi_j\rangle\right]\\&\approx\sum_{j,k=1}^{N_K}\boldsymbol{g}_k\overline{\boldsymbol{g}_j}\left[\Psi_Y^*W\Psi_Y-\lambda[\Psi_X^*W\Psi_Y]^*-\overline{\lambda}\Psi_X^*W\Psi_Y+|\lambda|^2\Psi_X^*W\Psi_X\right]_{jk}\\&=\boldsymbol{g}^*\left[\Psi_Y^*W\Psi_Y-\lambda[\Psi_X^*W\Psi_Y]^*-\overline{\lambda}\Psi_X^*W\Psi_Y+|\lambda|^2\Psi_X^*W\Psi_X\right]\boldsymbol{g}\end{aligned}$$

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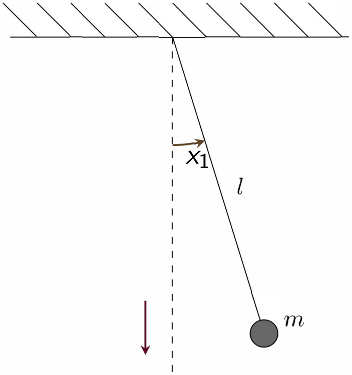
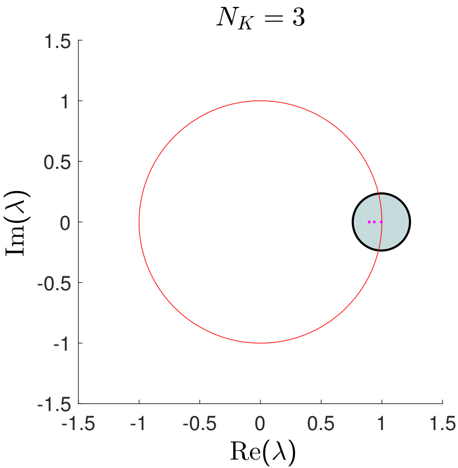
New matrix: $\Psi_Y^*W\Psi_Y$ with $\lim_{M\to\infty}[\Psi_Y^*W\Psi_Y]_{jk}=\langle\mathcal{K}\psi_k,\mathcal{K}\psi_j\rangle$

Example: nonlinear pendulum

$$\dot{x}_1 = x_2, \quad \dot{x}_2 = -\sin(x_1), \quad \text{with} \quad \Omega = [-\pi, \pi]_{\text{per}} \times \mathbb{R}.$$





Computed pseudospectra ($\epsilon = 0.25$). Eigenvalues of K_{EDMD} shown as dots (spectral pollution).

ResDMD: Avoiding spectral pollution

$$\mathrm{res}(\lambda, g)^2 = \frac{\boldsymbol{g}^* \left[\Psi_Y^* W \Psi_Y - \lambda[\Psi_X^* W \Psi_Y]^* - \overline{\lambda}\Psi_X^* W \Psi_Y + |\lambda|^2 \Psi_X^* W \Psi_X\right] \boldsymbol{g}}{\boldsymbol{g}^* \left[\Psi_X^* W \Psi_X\right] \boldsymbol{g}}.$$

Algorithm:

1. Compute K_{EDMD}, its eigenvalues and eigenvectors.
2. For each eigenpair (λ, g), compute $\mathrm{res}(\lambda, g)$.
3. Discard eigenpairs with $\mathrm{res}(\lambda, g) > \epsilon$, for accuracy tolerance $\epsilon > 0$.

Theorem (No spectral pollution, compute residuals from above.)

Let Λ_M denote the eigenvalue output of above algorithm. Then

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

BUT: typically does not capture all of spectrum!

ResDMD: Computing pseudospectra (and spectra)

$$\sigma_\epsilon(\mathcal{K}) := \cup_{\|\mathcal{B}\|\leq\epsilon}\sigma(\mathcal{K}+\mathcal{B}), \quad \lim_{\epsilon\downarrow 0}\sigma_\epsilon(\mathcal{K}) = \sigma(\mathcal{K})$$

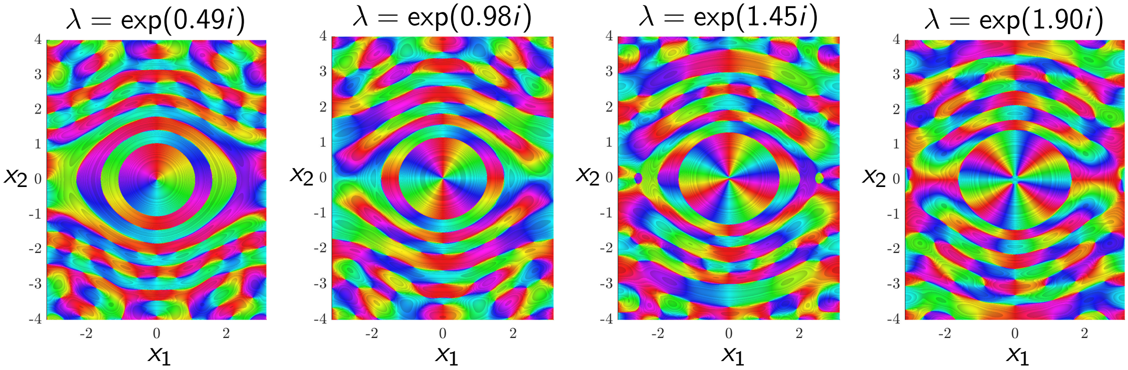
Algorithm:

1. Compute $\Psi_X^* W \Psi_X$, $\Psi_X^* W \Psi_Y$, and $\Psi_Y^* W \Psi_Y$.
2. For each z_j in a computational grid, compute $\tau_j = \min_{\boldsymbol{g}\in\mathbb{C}^{N_K}} \mathrm{res}(z_j, \sum_{k=1}^{N_K} \psi_k \boldsymbol{g}_k)$ and the corresponding singular vectors $\boldsymbol{g}_{(j)}$ (generalised SVD problem).
3. Output: $\{z_j : \tau_j < \epsilon\}$ (estimate of $\sigma_\epsilon(\mathcal{K})$) and ϵ-pseudo-eigenfunctions $\{\boldsymbol{g}_{(j)} : \tau_j < \epsilon\}$.

Theorem

No spectral pollution: $\{z_j : \tau_j < \epsilon\} \subset \sigma_\epsilon(\mathcal{K})$ *(as $M \to \infty$).*
Spectral inclusion: *Converges uniformly to $\sigma_\epsilon(\mathcal{K})$ on bounded subsets of $\mathbb{C}$ as $N_K \to \infty$.*

Example: pseudo-eigenfunctions of nonlinear pendulum



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

Part 2: Dealing with continuous spectra - computing spectral measures.

In this part, we assume that dynamics are measure-preserving.

This is equivalent to $\mathcal{K}$ being an isometry[a]:

$$\|\mathcal{K}g\|_{L^2(\Omega,\omega)} = \|g\|_{L^2(\Omega,\omega)}, \quad \forall g \in L^2(\Omega,\omega).$$

Spectrum lives inside the **unit disk**.

[a]For analysts: we actually consider unitary extensions of $\mathcal{K}$ with 'canonical' spectral measures.

Diagonalising infinite-dimensional operators

Finite-dimensional: $A \in \mathbb{C}^{n\times n}$ with $A^*A = AA^*$ has orthonormal basis of e-vectors $\{v_j\}_{j=1}^n$

$$v = \left(\sum_{j=1}^n v_j v_j^*\right) v, \quad v \in \mathbb{C}^n \qquad Av = \left(\sum_{j=1}^n \lambda_j v_j v_j^*\right) v, \quad v \in \mathbb{C}^n.$$

Infinite-dimensional: Operator $\mathcal{L} : \mathcal{D}(\mathcal{L}) \to \mathcal{H}$, ($\mathcal{H}$ = Hilbert space). Typically, no longer a basis of e-vectors. Spectral Theorem: Projection-valued spectral measure $\mathcal{E}$

$$g = \left(\int_{\sigma(\mathcal{L})} d\mathcal{E}(\lambda)\right) g, \quad g \in \mathcal{H} \qquad \mathcal{L}g = \left(\int_{\sigma(\mathcal{L})} \lambda\, d\mathcal{E}(\lambda)\right) g, \quad g \in \mathcal{D}(\mathcal{L}).$$

Scalar-valued spectral measures: $\nu_g(U) = \langle \underbrace{\mathcal{E}(U)}_{\text{projection}} g, g\rangle.$

Example: $\mathcal{L} = -\frac{d^2}{dx^2}$ and Fourier transform

$$\mathcal{L} = -\frac{d^2}{dx^2} \quad \xleftrightarrow[\text{spectral theorem}]{} \quad \text{projection-valued measure } \mathcal{E}$$

$$x \in [-\pi, \pi]_{\mathrm{per}}$$

$$\sigma(\mathcal{L}) = \{n^2 : n \in \mathbb{Z}_0\}$$

discrete spectrum

$$\hat{g}_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(x) e^{-ikx}\, dx$$

$$[\mathcal{E}([a,b])g](x) = \sum_{a \le k^2 \le b} \hat{g}_k e^{ikx}$$

$$\nu_g([a,b]) = \sum_{a \le k^2 \le b} |\hat{g}_k|^2$$

$$-\infty < x < \infty$$

$$\sigma(\mathcal{L}) = [0, +\infty)$$

continuous spectrum

$$\hat{g}(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} g(x) e^{-ikx}\, dx$$

$$[\mathcal{E}([a,b])g](x) = \int_{a \le k^2 \le b} \hat{g}(k) e^{ikx}\, dk$$

$$\nu_g([a,b]) = \int_{a \le k^2 \le b} |\hat{g}(k)|^2\, dk$$

Koopman mode decomposition

ν_g are spectral measures on $[-\pi,\pi]_{\mathrm{per}}$

Lebesgue's decomposition theorem:

$$d\nu_g(\lambda) = \underbrace{\sum_{\text{e-vals } \lambda_j} \langle \mathcal{P}_{\lambda_j} g, g\rangle \, \delta(\lambda-\lambda_j) d\lambda}_{\text{discrete part}} \qquad + \underbrace{{\color{red}\rho_g(\lambda)}\, d\lambda + d\nu_g^{(\mathrm{sc})}(\lambda)}_{\text{continuous part}}$$

$$g = \sum_{\text{e-vals } \lambda_j} c_{\lambda_j} \underbrace{\varphi_{\lambda_j}}_{\text{e-functions}} \qquad + \underbrace{\int_{[-\pi,\pi]_{\mathrm{per}}} \phi_{\theta,g}\, d\theta}_{\text{ctsly param e-functions}}.$$

$$g(\boldsymbol{x}_n) = [\mathcal{K}^n f](\boldsymbol{x}_0) = \sum_{\text{e-vals } \lambda_j} c_{\lambda_j} \lambda_j^n \varphi_{\lambda_j}(\boldsymbol{x}_0) \qquad + \int_{[-\pi,\pi]_{\mathrm{per}}} e^{in\theta} \phi_{\theta,f}(\boldsymbol{x}_0)\, d\theta.$$

Computing ν_g provides diagonalisation of non-linear dynamical system!

Plemelj-type formula

$$\underbrace{K_\epsilon(\theta) = \frac{1}{2\pi} \cdot \frac{(1+\epsilon)^2 - 1}{1 + (1+\epsilon)^2 - 2(1+\epsilon)\cos(\theta)}}_{\text{Poisson kernel for unit disc}}, \quad \underbrace{\mathtt{C}_{\nu_g}(z) := \frac{1}{2\pi} \int_{[-\pi,\pi]_{\mathrm{per}}} \frac{e^{i\theta}\, d\nu_g(\theta)}{e^{i\theta} - z}}_{\text{generalised Cauchy transform}}$$

Plemelj-type formula

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$$\begin{aligned}
\nu_g^\epsilon(\theta_0) &= \underbrace{\int_{[-\pi,\pi]_{\mathrm{per}}} K_\epsilon(\theta_0 - \theta)\, d\nu_g(\theta)}_{\text{smoothed measure}} \\
&= \mathtt{C}_{\nu_g}\left(e^{i\theta_0}(1+\epsilon)^{-1}\right) - \mathtt{C}_{\nu_g}\left(e^{i\theta_0}(1+\epsilon)\right) \\
&= \underbrace{\frac{-1}{2\pi}\left[\langle(\mathcal{K} - e^{i\theta_0}(1+\epsilon))^{-1}g, \mathcal{K}^* g\rangle + e^{-i\theta_0}\langle g, (\mathcal{K} - e^{i\theta_0}(1+\epsilon))^{-1} g\rangle\right]}_{\text{approximate using matrices } \Psi_X^* W \Psi_X, \Psi_X^* W \Psi_Y, \Psi_Y^* W \Psi_Y}
\end{aligned}$$

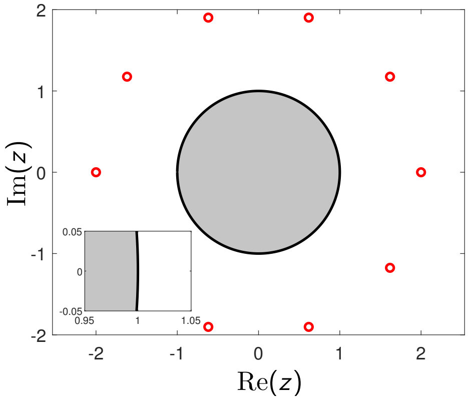
Compute smoothed approximations using ResDMD discretisations of size N_K.

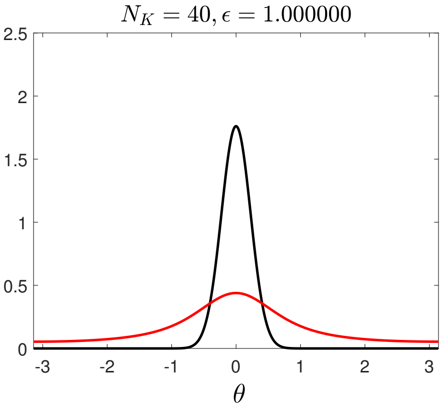
Example on $\ell^2(\mathbb{N})$ with known spectral measure

$$\mathcal{K} = \begin{bmatrix} \overline{\alpha_0} & \overline{\alpha_1}\rho_0 & \rho_1\rho_0 & & & \\ \rho_0 & -\overline{\alpha_1}\alpha_0 & -\rho_1\alpha_0 & 0 & & \\ 0 & \overline{\alpha_2}\rho_1 & -\overline{\alpha_2}\alpha_1 & \overline{\alpha_3}\rho_2 & \rho_3\rho_2 & \\ & \rho_2\rho_1 & -\rho_2\alpha_1 & -\overline{\alpha_3}\alpha_2 & -\rho_3\alpha_2 & \ddots \\ & & 0 & \overline{\alpha_4}\rho_3 & -\overline{\alpha_4}\alpha_3 & \ddots \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \alpha_j = (-1)^j 0.95^{(j+1)/2}, \rho_j = \sqrt{1-|\alpha_j|^2}.$$

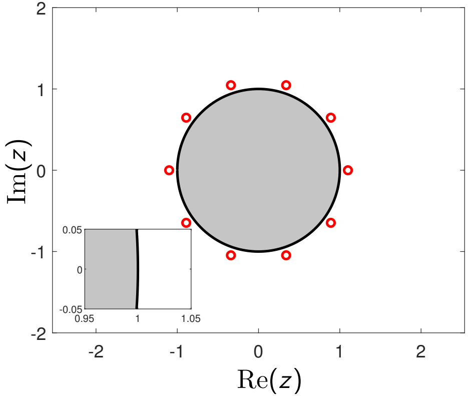
Generalised shift, typical building block of many dynamical systems (e.g., Bernoulli shifts).

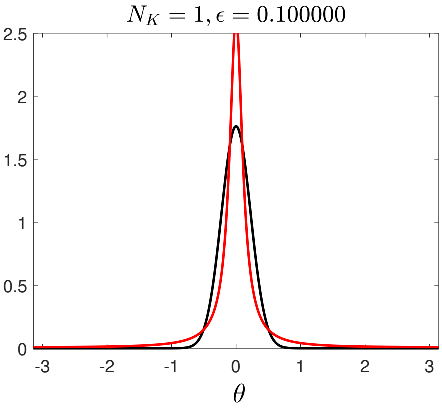
Fix N_K, vary ϵ



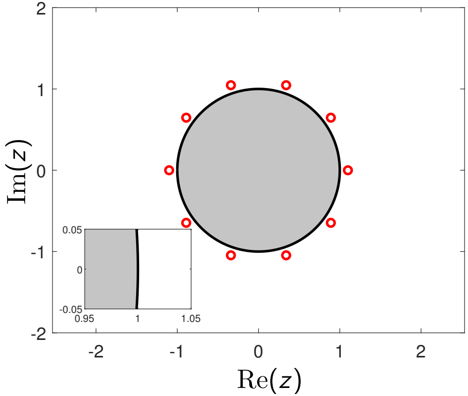


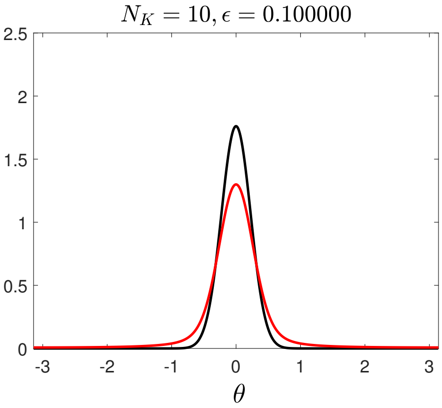
Fix ϵ, vary N_K





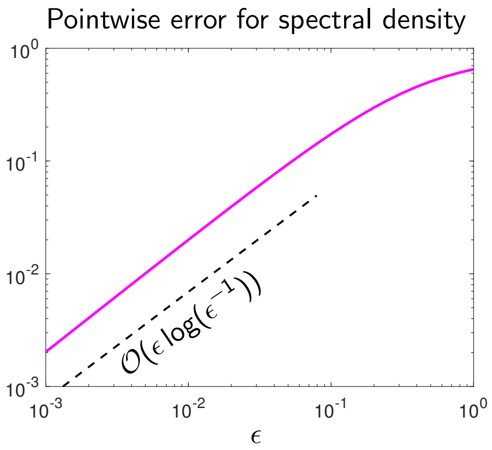
Adaptive $N_K(\epsilon)$ (or $\epsilon(N_K)$): New matrix $\Psi_Y^* W \Psi_Y$ key!

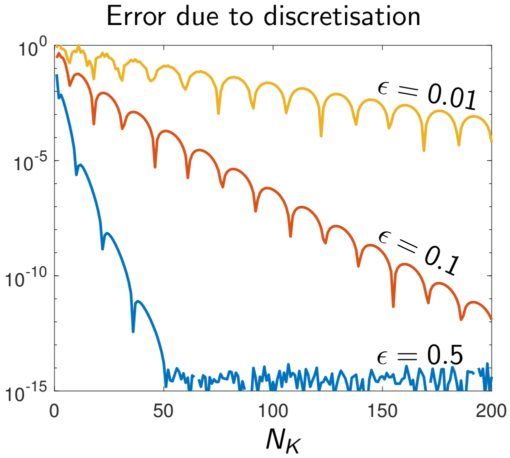




Slow convergence!

Problem: As $\epsilon \downarrow 0$, error is $\mathcal{O}(\epsilon \log(\epsilon^{-1}))$ and $N_K(\epsilon) \to \infty$.





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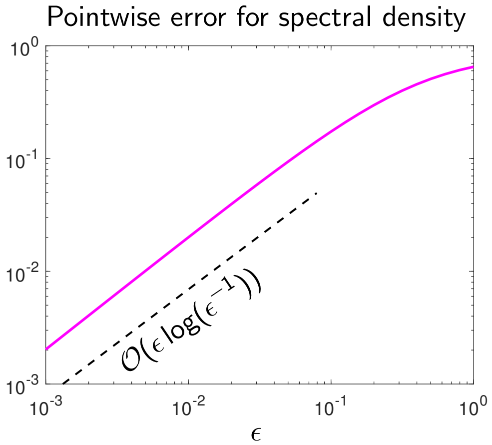
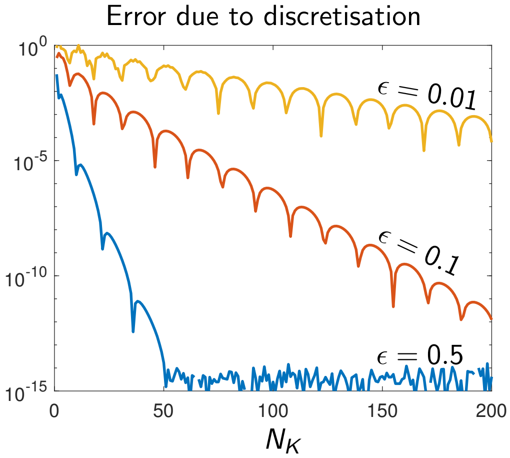




Critical in data-driven computations where we want N_K to be as small as possible.

Question: Can we improve the convergence rate in ϵ?

High-order kernels

Idea: Replace the Poisson kernel by

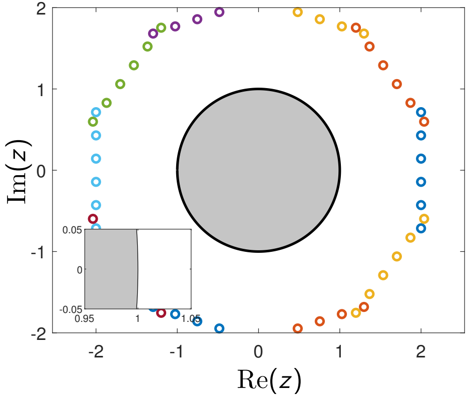
$$K_\epsilon(\theta) = \frac{e^{-i\theta}}{2\pi} \sum_{j=1}^{m} \left[\frac{c_j}{e^{-i\theta} - (1+\epsilon \overline{z_j})^{-1}} - \frac{d_j}{e^{-i\theta} - (1+\epsilon z_j)} \right]$$

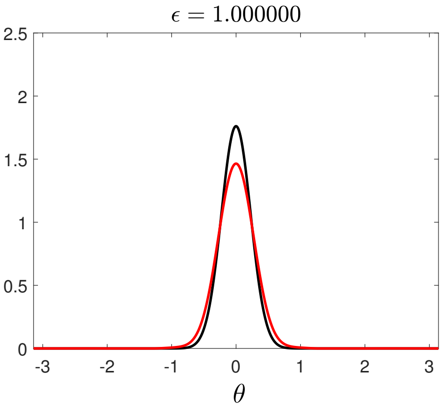
Simple way to select suitable z_j, c_j and d_j to achieve high-order kernel.

$$\nu_g^\epsilon(\theta_0) = \int_{[-\pi,\pi]_{\mathrm{per}}} K_\epsilon(\theta_0 - \theta)\, d\nu_g(\theta) = \sum_{j=1}^{m} \left[c_j \mathtt{C}_{\nu_g} \left(e^{i\theta_0}(1+\epsilon \overline{z_j})^{-1} \right) - d_j \mathtt{C}_{\nu_g} \left(e^{i\theta_0}(1+\epsilon z_j) \right) \right]$$

$\mathtt{C}_{\nu_g}(z)$ **computed using ResDMD.**

High-order kernels

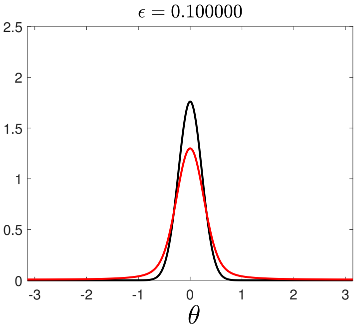




High-order kernels

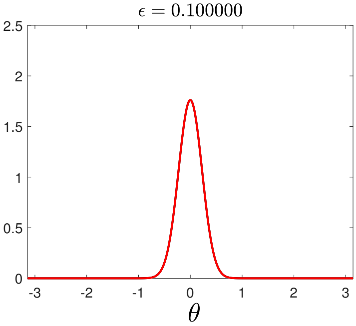
$$m = 1$$

$$\mathtt{C}_{\nu_g}\left(e^{i\theta_0}(1+\epsilon)^{-1}\right) - \mathtt{C}_{\nu_g}\left(e^{i\theta_0}(1+\epsilon)\right)$$



$$m = 6$$

$$\sum_{j=1}^{m}\left[c_j \mathtt{C}_{\nu_g}\left(e^{i\theta_0}(1+\epsilon\overline{z_j})^{-1}\right) - d_j \mathtt{C}_{\nu_g}\left(e^{i\theta_0}(1+\epsilon z_j)\right)\right]$$



Convergence

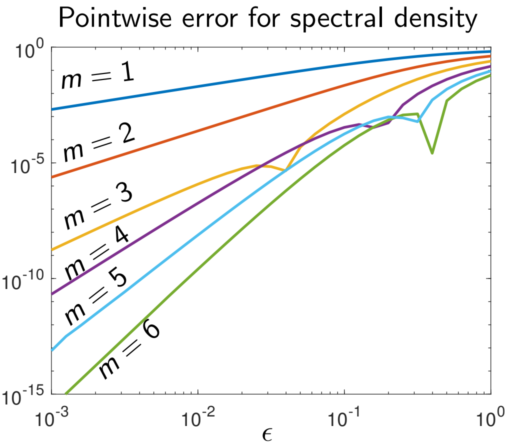
$\mathcal{O}(\epsilon^m \log(\epsilon^{-1}))$ convergence for:

- Pointwise recovery of the density ρ_g
- L^p recovery of ρ_g
- Weak convergence

$$\lim_{\epsilon \downarrow 0} \int_{[-\pi,\pi]_{\mathrm{per}}} \phi(\theta)\nu_g^\epsilon(\theta)\, d\theta = \int_{[-\pi,\pi]_{\mathrm{per}}} \phi(\theta)\, d\nu_g(\theta),$$

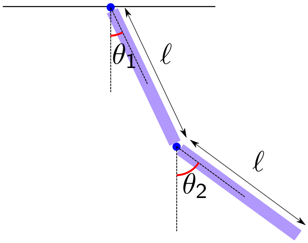
for periodic continuous ϕ.

Also recover discrete part of measure.
(i.e., eigenvalues of $\mathcal{K}$)



Evaluate at P values of θ: Parallelisable $\mathcal{O}(N_K^3 + PN_K)$ computation.

Example: double pendulum (chaotic)



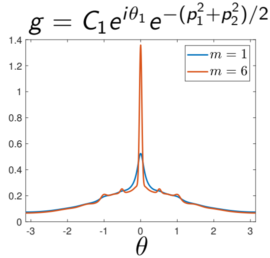
$$\dot{\theta}_1 = \frac{2p_1 - 3p_2\cos(\theta_1 - \theta_2)}{16 - 9\cos^2(\theta_1 - \theta_2)},$$

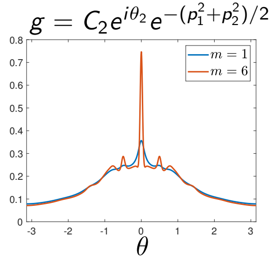
$$\dot{\theta}_2 = \frac{8p_2 - 3p_1\cos(\theta_1 - \theta_2)}{16 - 9\cos^2(\theta_1 - \theta_2)},$$

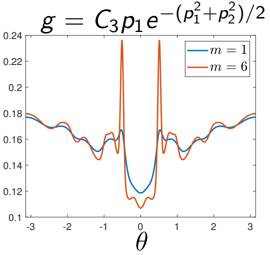
$$\dot{p}_1 = -3(\dot{\theta}_1\dot{\theta}_2\sin(\theta_1 - \theta_2) + \sin(\theta_1)),$$

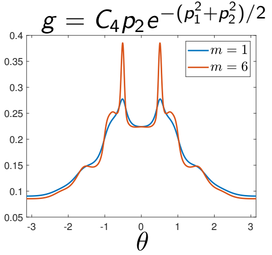
$$\dot{p}_2 = -3(-\dot{\theta}_1\dot{\theta}_2\sin(\theta_1 - \theta_2) + \frac{1}{3}\sin(\theta_2)),$$

where $p_1 = 8\dot{\theta}_1 + 3\dot{\theta}_2\cos(\theta_1 - \theta_2)$,
$p_2 = 2\dot{\theta}_2 + 3\dot{\theta}_1\cos(\theta_1 - \theta_2)$



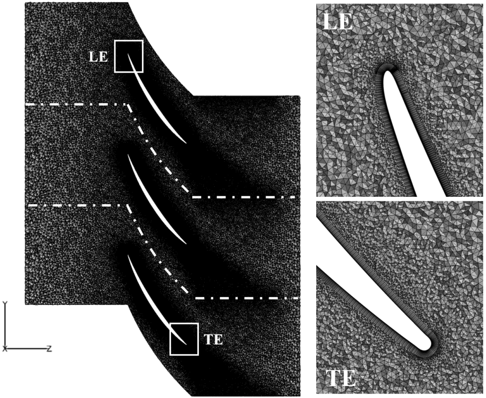






Part 3: High-dimensional dynamical systems and learned dictionaries.

Curse of dimensionality



Scalar field

$\Omega \subset \mathbb{R}^d$, d = number of grid/mesh points

E.g., polynomial dictionary up to tot. deg. 5.

Small grid: $d = 5 \times 5 \Rightarrow N_K \approx 50,000$.

Example later: $d \approx 300,000 \Rightarrow N_K \approx 2 \times 10^{25}$
$\gg$ **number of stars in known universe!!!!**

Conclusion: Infeasible to use hand-crafted dictionary when $d \gtrapprox 25$.

Kernelized EDMD

- Kernelized EDMD: $\mathcal{O}(d)$ cost using “kernel trick”.
- Forms $\widetilde{K}_{\mathrm{EDMD}} \in \mathbb{C}^{M \times M}$ with subset of eigenvalues of $K_{\mathrm{EDMD}} \in \mathbb{C}^{N_K \times N_K}$.
- Implicitly learns dictionary: eigenfunctions of $\widetilde{K}_{\mathrm{EDMD}} \in \mathbb{C}^{M \times M}$.

· M. Williams, C. Rowley, and I. Kevrekidis “*A kernel-based method for data-driven Koopman spectral analysis*,” J. Comput. Dyn., 2015.

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Still face the challenges:

(C1) Continuous spectra.
(C2) Lack of finite-dimensional invariant subspaces.
(C3) Spectral pollution.
(C4) Chaotic behaviour.

· M. Williams, C. Rowley, and I. Kevrekidis "*A kernel-based method for data-driven Koopman spectral analysis*," J. Comput. Dyn., 2015.

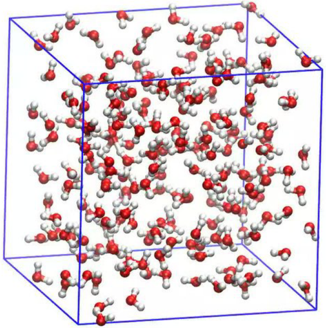
A solution: two sets of snapshot data

Two data sets: $\{\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)}\}_{m=1}^{M'}$ and $\{\hat{\boldsymbol{x}}^{(m)}, \hat{\boldsymbol{y}}^{(m)}\}_{m=1}^{M''}$.

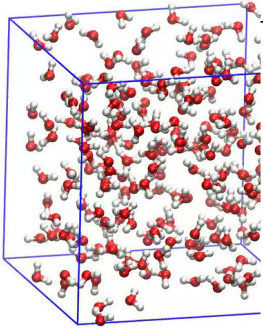
1. Apply kernel EDMD to $\{\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)}\}_{m=1}^{M'}$.
2. Compute the dominant N_K'' eigenvectors of $\widetilde{K}_{\mathrm{EDMD}}$ (learned dictionary $\{\psi_j\}_{j=1}^{N_K''}$).
3. Apply above **ResDMD** algorithms with $\{\hat{\boldsymbol{x}}^{(m)}, \hat{\boldsymbol{y}}^{(m)}\}_{m=1}^{M''}$ and the dictionary $\{\psi_j\}_{j=1}^{N_K''}$.

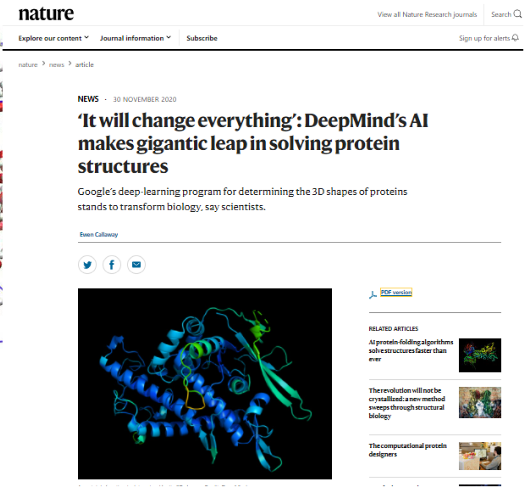
Key advantages of ResDMD: Convergence theory and a posterior verification of dictionary.

Overcomes the above challenges...



Molecular dynamics





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Ewen Callaway

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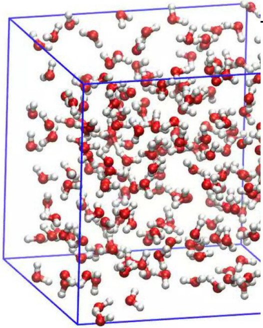

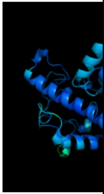

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'It will chang
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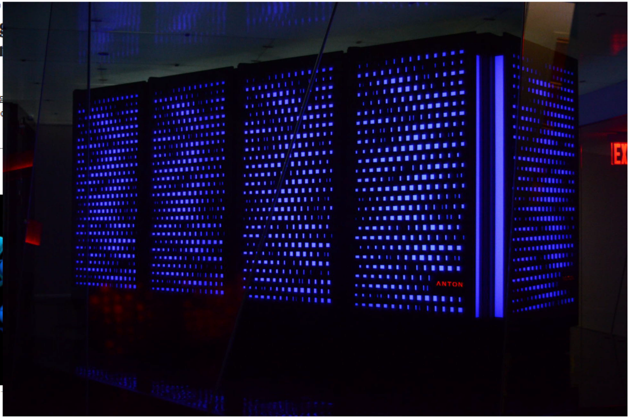
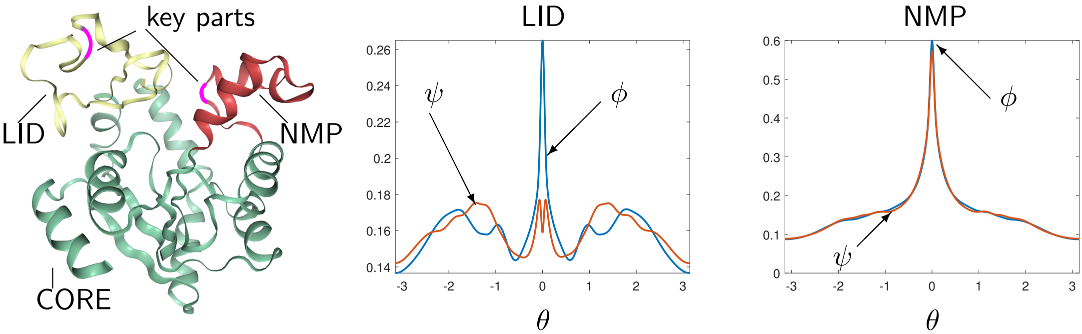
Google's deep-learning
stands to transform bi

Ewen Callaway



www.mdanalysis.org/MDAnalysisData/adk_equilibrium.html

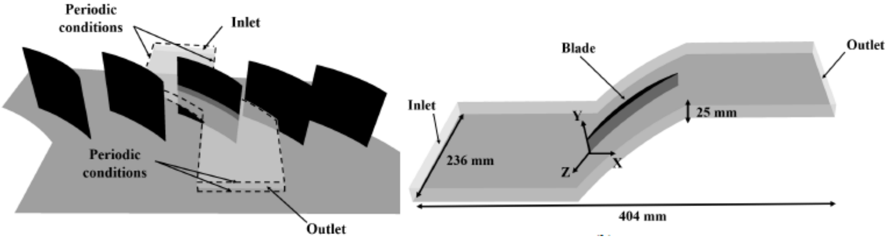
Spectral measures in molecular dynamics, $d = 20{,}046$



Left: ADK with three domains: CORE (green), LID (yellow) and NMP (red).
Middle and right: Spectral measures with respect to the dihedral angles of the selected parts.

Turbulent flow past a cascade of aerofoils, $d = 295{,}122$

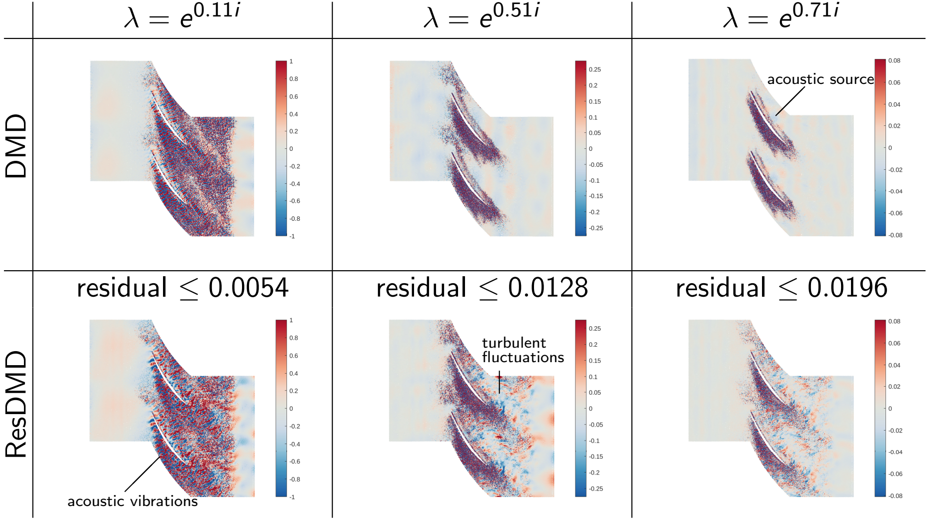
(Reynolds number 3.88×10^5.)



Motivation: Reduce noise sources (e.g., turbines, wings etc.).

· R. Koch, M. Sanjosé, and S. Moreau "*Large-Eddy Simulation of a Linear Compressor Cascade with Tip Gap: Aerodynamic and Acoustic Analysis*," AIAA Aviation, 2021.

Turbulent flow past a cascade of aerofoils, $d = 295{,}122$



Top row: Modes computed by DMD. **Bottom row:** Modes computed by ResDMD with residuals. Each column corresponds to different physical frequencies of noise pollution.

Concluding remarks

Summary: Rigorous and practical algorithms that overcome the challenges of (C1) Continuous spectra, (C2) Lack of finite-dimensional invariant subspaces, (C3) Spectral pollution, and (C4) Chaotic behaviour.

Part 1: Computed spectra, pseudospectra and residuals of general Koopman operators.

Idea: New matrix for residual $\Rightarrow$ ResDMD.

Part 2: Computed spectral measures of measure-preserving systems with high-order convergence. Density of continuous spectrum, discrete spectrum and weak convergence.

Idea: Convolution with rational kernels through the resolvent and ResDMD.

Part 3: Dealt with high-dimensional dynamical systems.

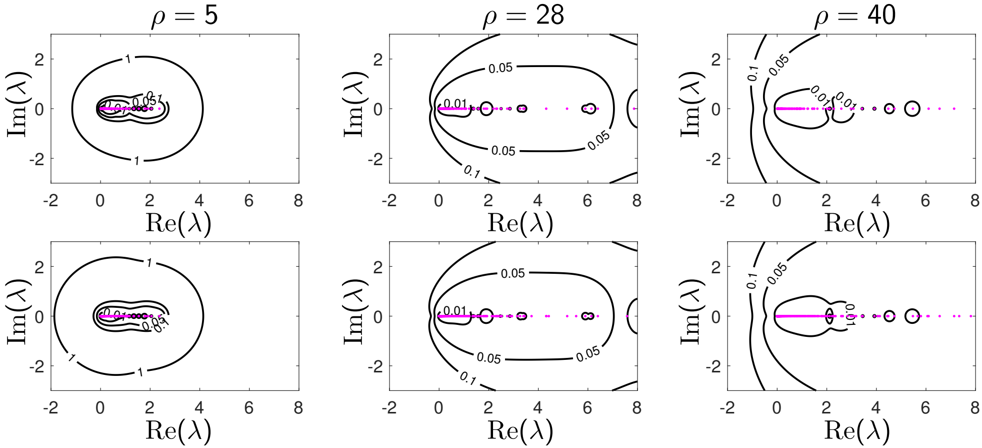
Idea: Kernel trick to learn dictionary, then apply ResDMD.

Details and code: http://www.damtp.cam.ac.uk/user/mjc249/home.html

If you have additional comments, questions, problems for collaboration, please get in touch!

Example: Lorenz and extended Lorenz systems

$$\dot{X} = 10\,(Y - X)\,, \quad \dot{Y} = X\,(\rho - Z) - Y, \quad \dot{Z} = XY - 8Z/3.$$



Top row: Lorenz system. **Bottom row:** Extended 11-dimensional Lorenz system.

· S. Moon et al. "*Periodicity and chaos of high-order Lorenz systems*," Inter. J. Bifur. Chaos, 2017.

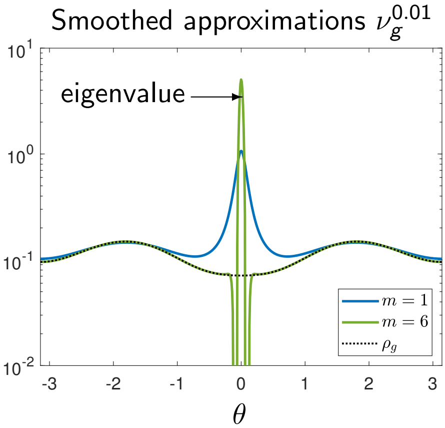
Example: Lorenz and extended Lorenz systems

$\rho = 5$				$\rho = 28$				$\rho = 40$			
$d = 3$		$d = 11$		$d = 3$		$d = 11$		$d = 3$		$d = 11$	
λ_j	r_j	λ_j	r_j	λ_j	r_j	λ_j	r_j	λ_j	r_j	λ_j	r_j
1.0108	4.9E-7	1.0108	8.6E-5	1.0423	5.1E-6	1.0346	2.6E-4	1.0689	4.6E-4	1.0046	6.2E-04
1.0217	3.8E-4	1.1550	1.1E-6	1.0712	7.9E-4	1.0423	1.9E-5	1.2214	2.9E-6	1.0868	1.1E-04
1.1550	5.1E-8	1.3339	1.0E-5	1.0862	6.3E-4	1.0472	4.8E-4	1.4191	9.9E-4	1.2214	1.3E-05
1.1675	7.6E-5	1.3380	5.2E-4	1.3839	7.5E-5	1.0594	7.7E-5	1.4823	4.9E-4	1.2419	8.3E-07
1.3340	1.3E-6	1.5410	4.0E-4	1.5810	4.4E-7	1.0598	2.0E-6	1.4916	4.8E-4	1.2452	6.7E-04
1.3385	6.9E-4			1.8065	7.4E-8	1.0685	9.8E-4	1.6216	5.2E-5	1.2526	1.2E-04
1.5410	3.1E-4			1.8829	5.8E-4	1.0707	9.4E-4	1.8527	1.7E-7	1.3498	1.7E-04
				2.8561	7.2E-5	1.0862	8.2E-4	2.1170	7.5E-8	1.3541	9.6E-04
				3.2633	2.9E-7	1.1964	2.4E-4	2.5857	3.7E-4	1.4251	1.5E-04
				5.8954	3.1E-4	1.3675	1.3E-6	3.9223	6.2E-5	1.4788	6.9E-04

Eigenvalues computed using Algorithm 1 with $\epsilon = 0.001$ along with the computed residuals r_j.

Example: tent map, $F(x) = 2\min\{x, 1-x\}$, $\Omega = [0,1]$

$$g(\theta) = C|\theta - 1/3| + C\sin(20\theta) + \begin{cases} C, & \theta > 0.78, \\ 0, & \theta \leq 0.78. \end{cases}$$



Added benefit: Avoid oversmoothing, and have better localisation of singular parts.