The Distributional Koopman Operator

SIAM DS25, Data Driven Modeling of Dynamical Systems via the Transfer Operator

Maria Oprea, May 12th 2025

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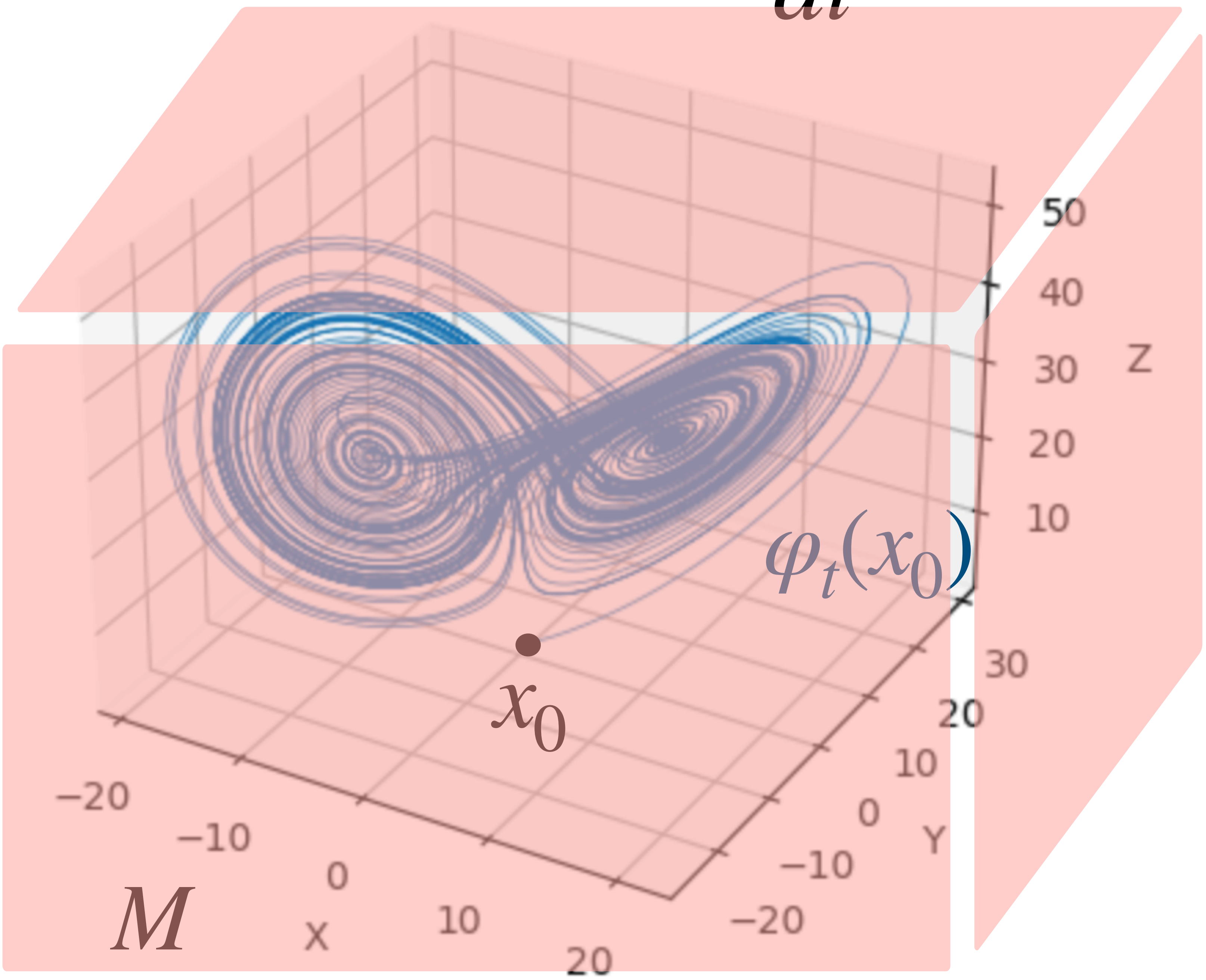
The Koopman operator K_t

Dynamics on M:

$$\varphi : \mathbb{R} \times M \to M, \frac{d}{dt}\varphi_t(x) = f(x)$$



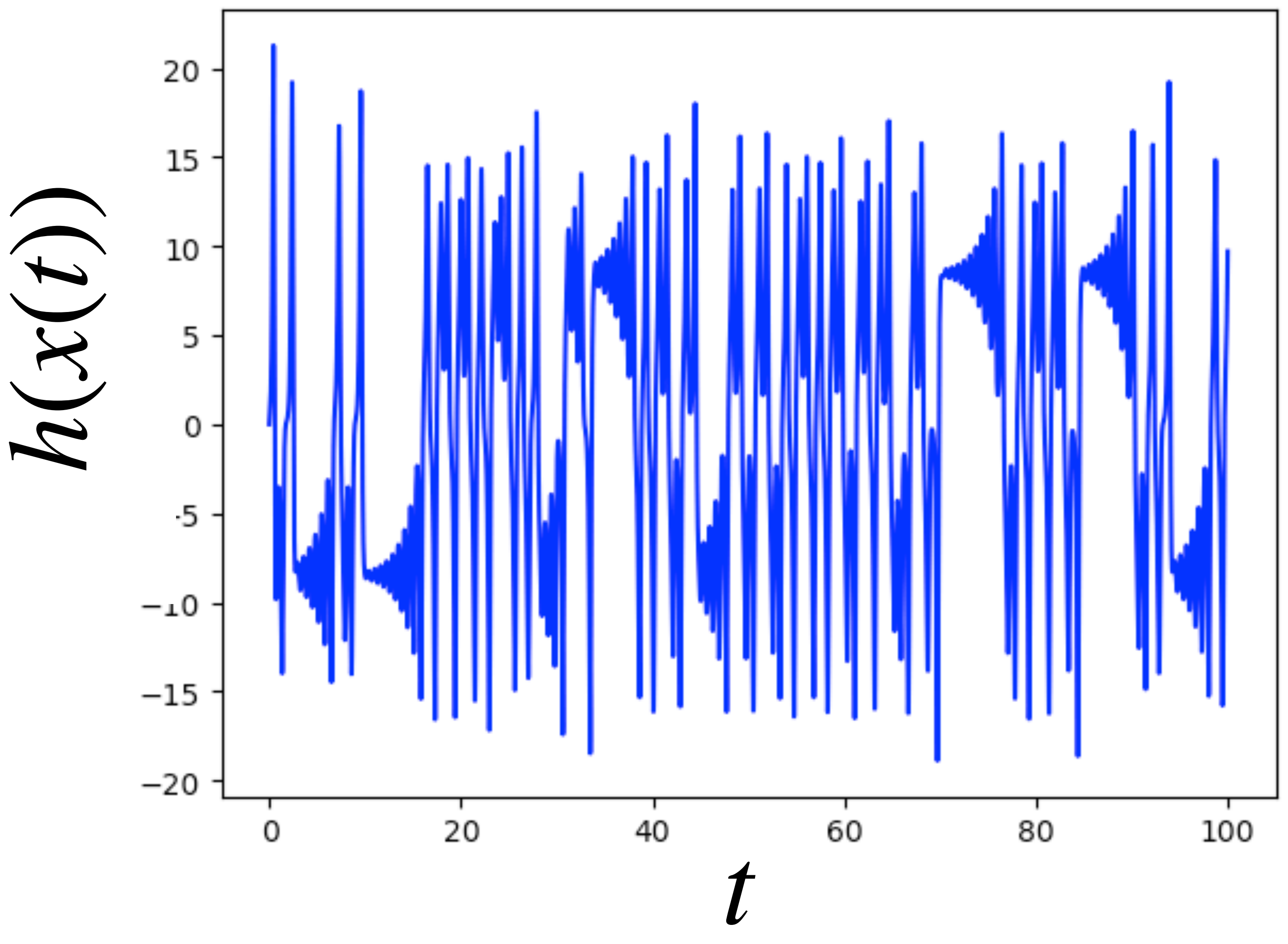
Measurement

$$\hat{h} : M \to \mathbb{R}$$

$$\hat{h} \in L^\infty(M)$$

Dynamics of observables:

$$K_t : L^\infty(M) \to L^\infty(M), K_t\hat{h} = \hat{h} \circ \varphi_t$$



Introducing randomness

$(\Omega, \mathscr{F}, p)$

$\theta_t : \Omega \to \Omega, \theta_t \# p = p$

Source of randomness

$\longrightarrow$

M

$\Phi_t(\omega, \cdot\,)$

State

Random dynamical systems: $\Phi : \mathbb{R} \times \Omega \times M \to M$ with cocycle propriety

$$\Phi_{t+s}(\omega, x) = \Phi_t(\theta_s \omega, x) \circ \Phi_s(\omega, x) \ \forall x, \omega$$

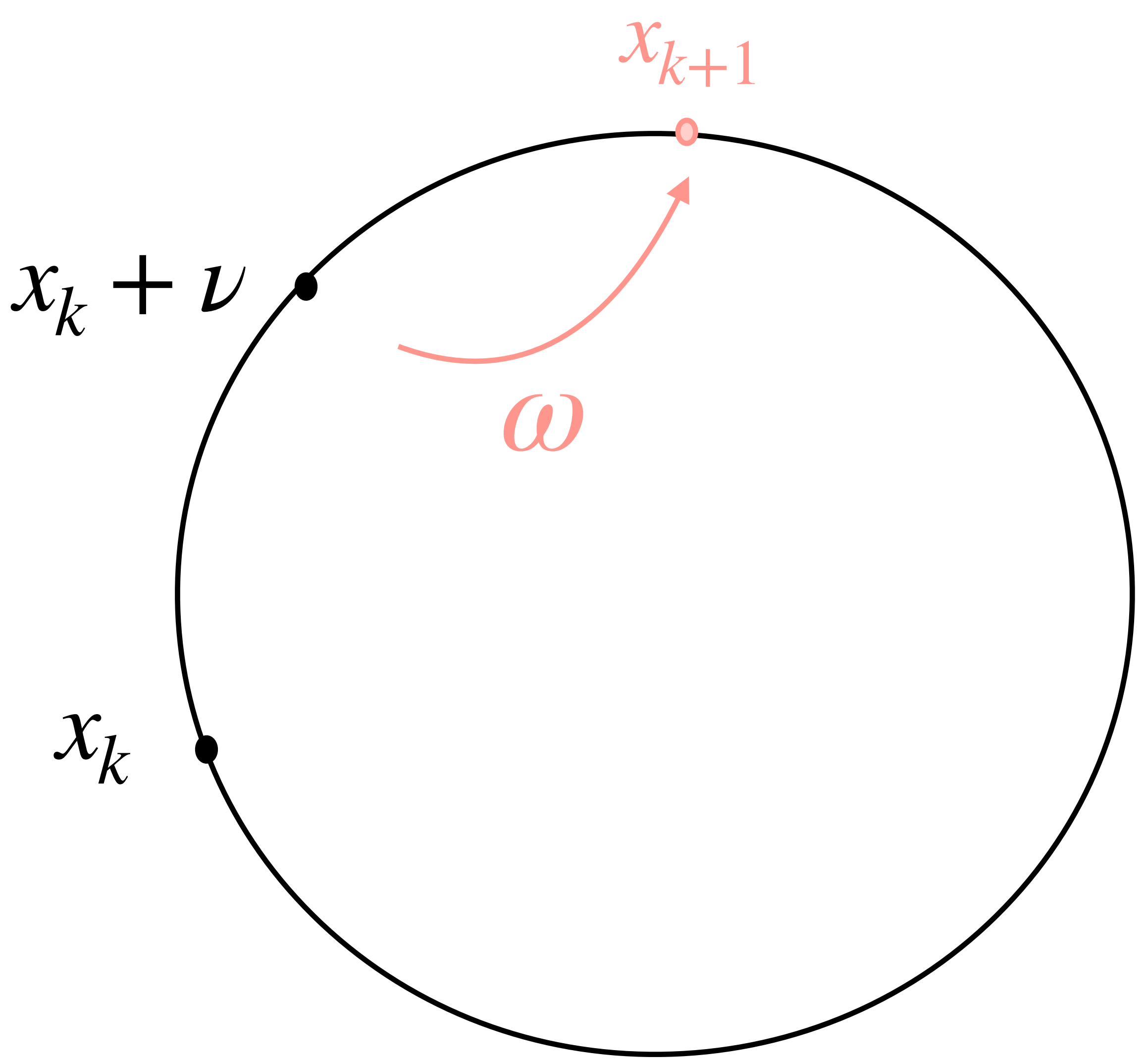
Example: Random rotations on a circle

$\omega = (\omega_0, \omega_1, \ldots)$

p = Bernoulli measure

$\theta(\omega_0, \omega_1, \ldots) = (\omega_1, \ldots)$

$\Phi_1(\omega, x) = x + \nu + \omega_0 \bmod 2\pi$



Introducing randomness

Random dynamical systems: $\Phi : \mathbb{R} \times \Omega \times M \to M$ with cocycle propriety

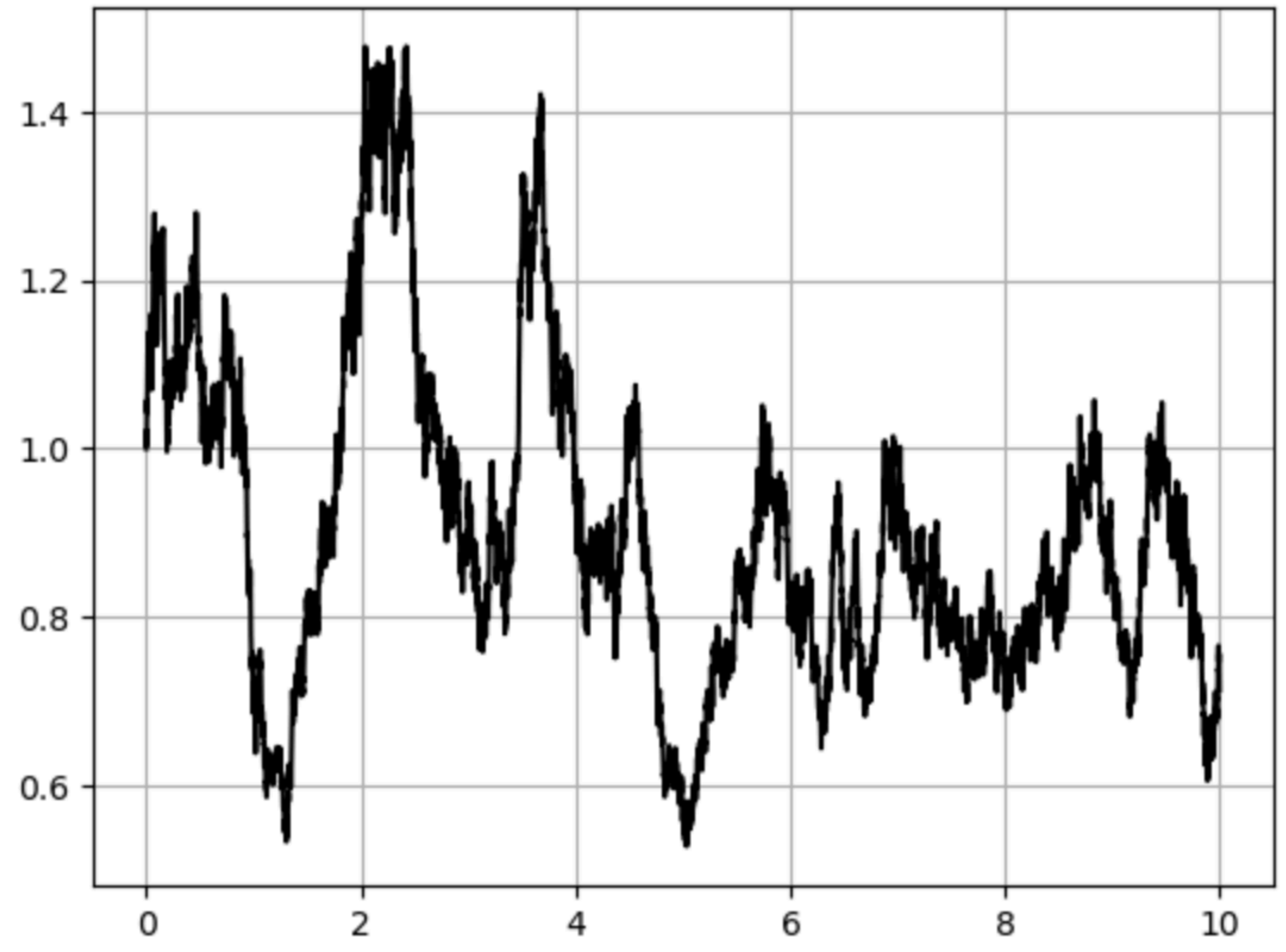
$$\Phi_{t+s}(\omega, x) = \Phi_t(\theta_s \omega, x) \circ \Phi_s(\omega, x) \ \forall x, \omega$$

Example: SDEs $dX_t = a(X_t)dt + b(X_t)d\omega_t$

$\Omega = \mathscr{C}[0,1]$ continuous functions

$\theta_t \omega(s) = \omega(t+s) - \omega(s)$ shift

Wiener measure with σ-algebra generated by cylinder sets[1]

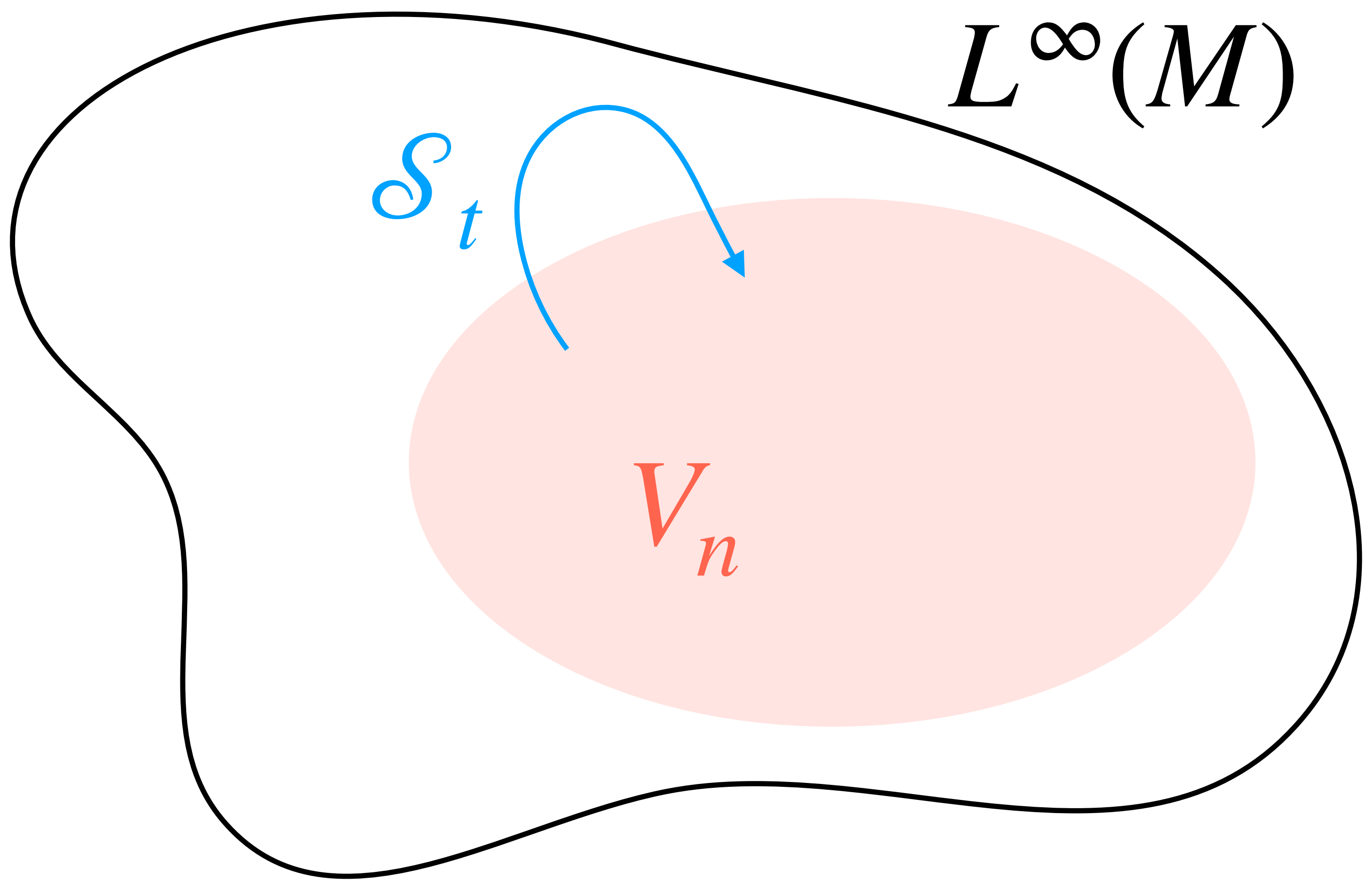


[1] P. Billingsley, Convergence of Probability Measures, A Wiley-Interscience Publication, 1999

The Stochastic Koopman operator (SKO)

Average value of the observable at time t:

$$\mathcal{S}_t : L^\infty(M) \to L^\infty(M), \mathcal{S}_t\hat{h}(x) = \mathbb{E}_{\omega\sim p}[\hat{h}(\Phi_t(\omega, x))]$$



Importance of SKO:

let $V_n = Span\{\hat{h}_1, \ldots, \hat{h}_n\}$ such that $\mathcal{S}_t V_n \subset V_n$

$$\text{Then } \mathcal{S}_t\hat{h}(x) = \sum_{i=1}^{n} \alpha_i \mathcal{S}_t\hat{h}_i(x) = \sum_{i=1}^{n} (\alpha S_m)_i \hat{h}_i(x)$$

matrix approximation

Eigenvalues and eigenvectors:

$$\mathcal{S}_t\hat{h}_i = \lambda_i\hat{h}_i \implies S_m \text{ diagonal}$$

1. M. Wanner and I. Mezic, Robust approximation of the stochastic Koopman operator, SIAM Journal on Applied Dynamical Systems, 21 (2022), pp. 1930–1951.
2. Črnjarić-Žic, Nelida, Senka Maćešić, and Igor Mezić. "Koopman operator spectrum for random dynamical systems." *Journal of Nonlinear Science* 30 (2020): 2007-2056.
3. Minghao Han, Jacob Euler-Rolle, Robert K. Katzschmann, DESKO: Stability-Assured Robust Control of Nonlinear Systems with a Deep Stochastic Koopman Operator

Dynamic Mode Decomposition[1]

$\hat{h}_i(x_{j+1})$

Choose V_n, what is the best approximation of $\mathcal{S}_t|_{V_n}$? $\quad argmin_{S_m} \sum_{i,j} |\mathcal{S}_t \hat{h}_i(x_j) - (S_m)_{ik} \hat{h}_k(x_j)|_2$

Given trajectory data: $\{x_j\}_{j=1}^m, m \geq n$

Compute :$(\Psi_m)_{ij} = \hat{h}_i(x_{j-1})$ and $(\Phi_m)_{ij} = \hat{h}_i(x_j)$

Return $S_m = \Phi_m \Psi_m^\dagger$

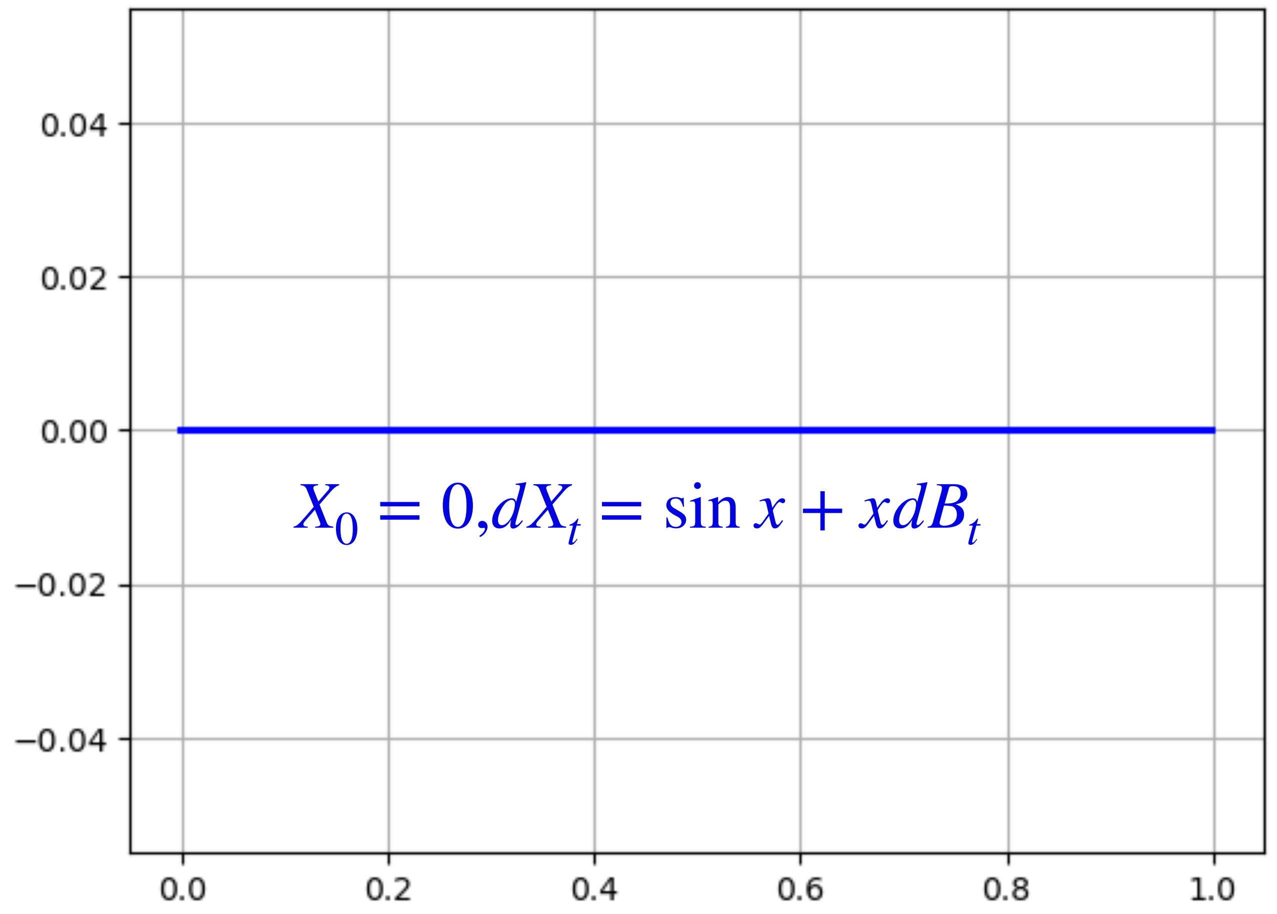
When $m \to \infty, S_m \to argmin \sum_{i=1}^{n} \|\mathcal{S}_t \hat{h}_i - (S_m)_{ik} \hat{h}_k\|^2_{L^2(M,\mu)} := S_\infty$

if $\{x_j\}_{j=1}^m$ ergodic, can interchange space and time averages

Matrix $S_m \in \mathbb{R}^{n \times n}$ vs finite rank operator $\mathcal{S}_m^n : V_n \to V_n$

[1]M. O. Williams, I. G. Kevrekidis, and C. W. Rowley, A data–driven approximation of the Koopman operator: Extending dynamic mode decomposition, Journal of Nonlinear Science, 25 (2015), pp. 1307–1346

Shortcomings of SKO



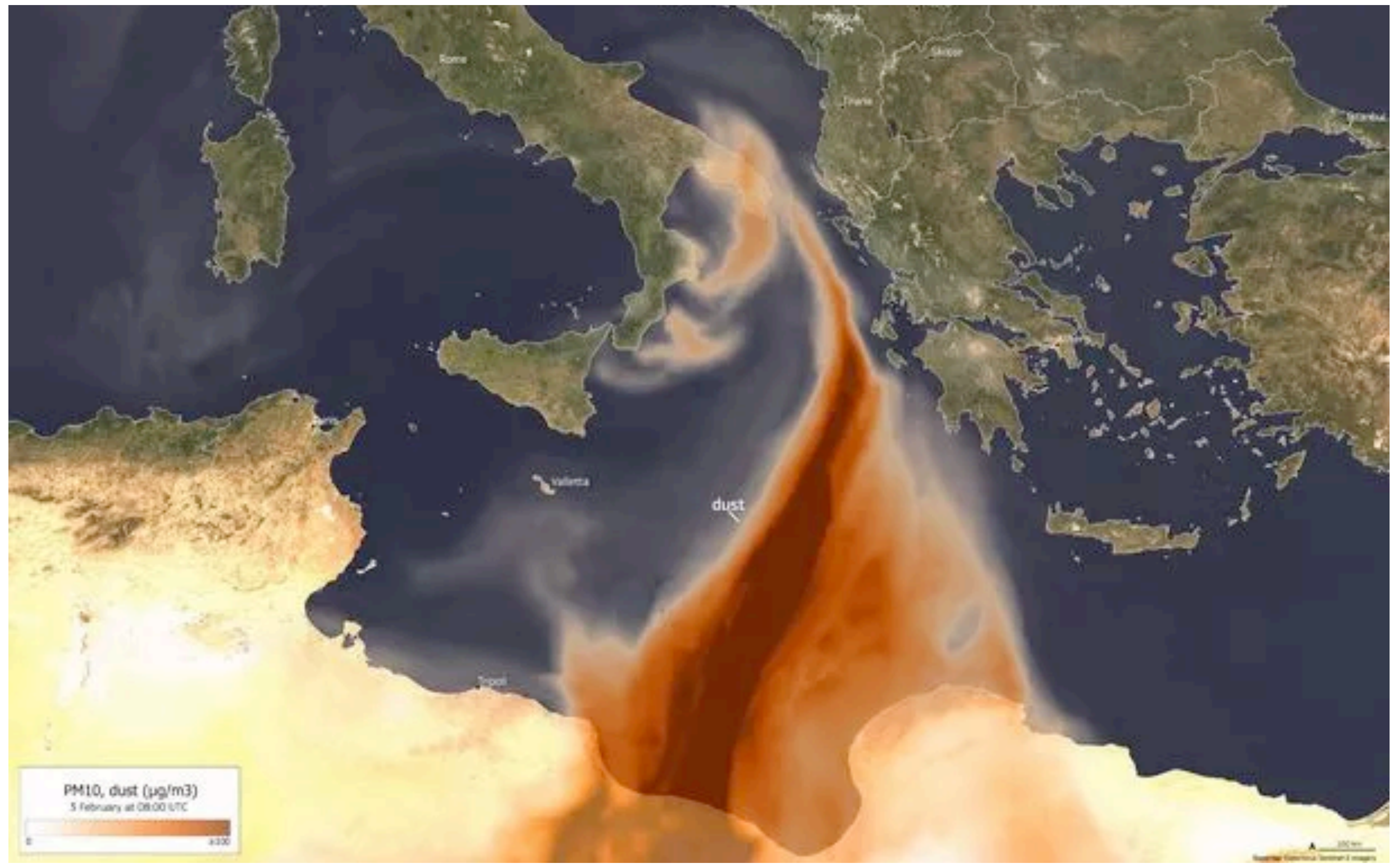
No higher order moment information

Dynamics might not be ergodic $\implies \nexists \mu$

Trajectory not representative

DMD cannot be applied when only aggregate data available

Unnatural $L^2(M, \mu)$ framework



Dust plume data off the coast of Libia

Credit: https://www.bristolpost.co.uk/news/uk-world-news/map-shows-blood-rain-dust-9920288

Lagrangian vs. Eulerian perspective

$x \in M$

$\hat{h} \in L^\infty(M)$

RDS: $\Phi : \mathbb{R} \times \Omega \times M \to M$

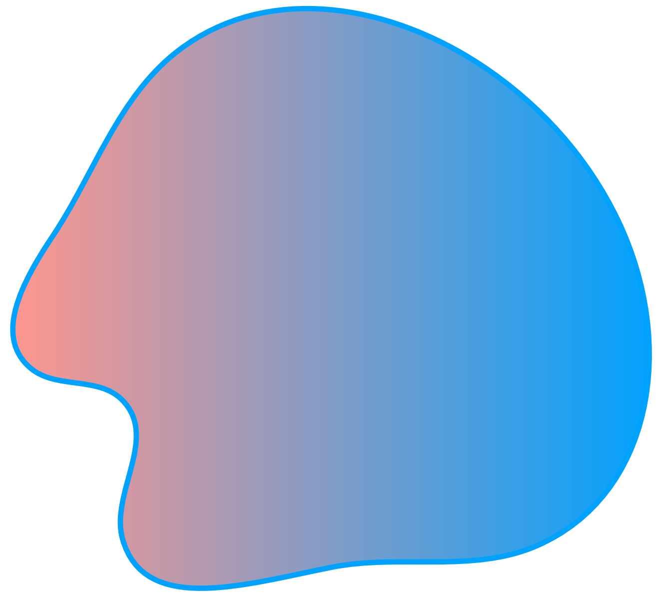
$\pi \in \mathscr{P}(M)$

$h : \mathscr{P}(M) \to \mathbb{R}$ continuous and bounded

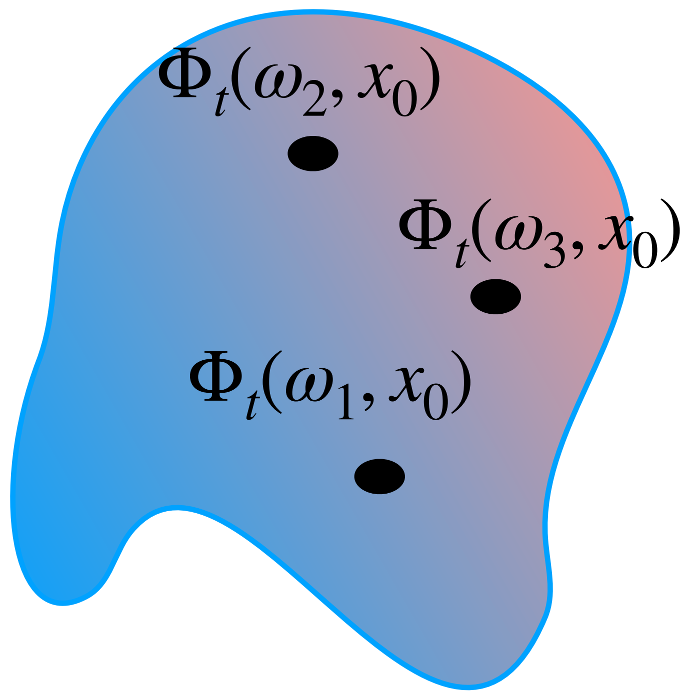
Transfer operator $T_t : \mathscr{P}(M) \to \mathscr{P}(M)$

π_0

$\frac{1}{m}\sum_j \delta_{x_j}$



$\xrightarrow{T_t}$



$\pi_t = T_t(\pi_0)$

$\frac{1}{m}\sum_j \delta_{x_{j+1}}$

The definition of DKO

$$\mathscr{D}_t h(\pi) = h \circ T_t(\pi)$$

Linearity ✓

Semi-group propriety $\mathscr{D}_{t+s} = \mathscr{D}_t \circ \mathscr{D}_s$ ✓

Invariant subspace $H_1 = \{h : \mathscr{P}(M) \to \mathbb{R}$ linear and bounded $\}$

Generalizes SKO when restricted to H_1

- Evaluation at delta: $\mathscr{D}_t h(\delta_x) = \mathscr{S}_t \hat{h}(x)$
- Integrate the $x-$uncertainty: $\mathscr{D}_t h(\pi) = \mathbb{E}_{X\sim\pi}\big[[\mathscr{S}_t \hat{h}](X)\big]$
- Same eigenvalues: $\mathscr{S}_t \hat{h} = \lambda \hat{h} \implies \mathscr{D}_t h = \lambda h$

Observables on $\mathscr{P}(M)$

Linear: $h(\pi) = \int \hat{h}(x)d\pi(x), \hat{h} \in L^\infty(M)$

Centered moments: $h(\pi) = \mathbb{E}_{X\sim\pi}\left[\left(\hat{h}(X) - \mathbb{E}_{X\sim\pi}[\hat{h}(X)]\right)^n\right]$

Inner product: $\Lambda : (\Theta, \mathbb{P}) \to \mathscr{P}(M)$ ⟶ Random measure

$$\Lambda\#\mathbb{P} := P \in \mathscr{P}(\mathscr{P}(M))$$

$$\langle h_1, h_2 \rangle := \int h_1 \circ \Lambda(\theta) h_2 \circ \Lambda(\theta) d\mathbb{P} = \int h_1(\pi)h_2(\pi)dP$$

Hilbert space: $(V_n, \langle \cdot , \cdot \rangle)$, where $V_n = Span\{h_1, \ldots, h_n\}$ ⟶ Finite dimensional

DMD Algorithm

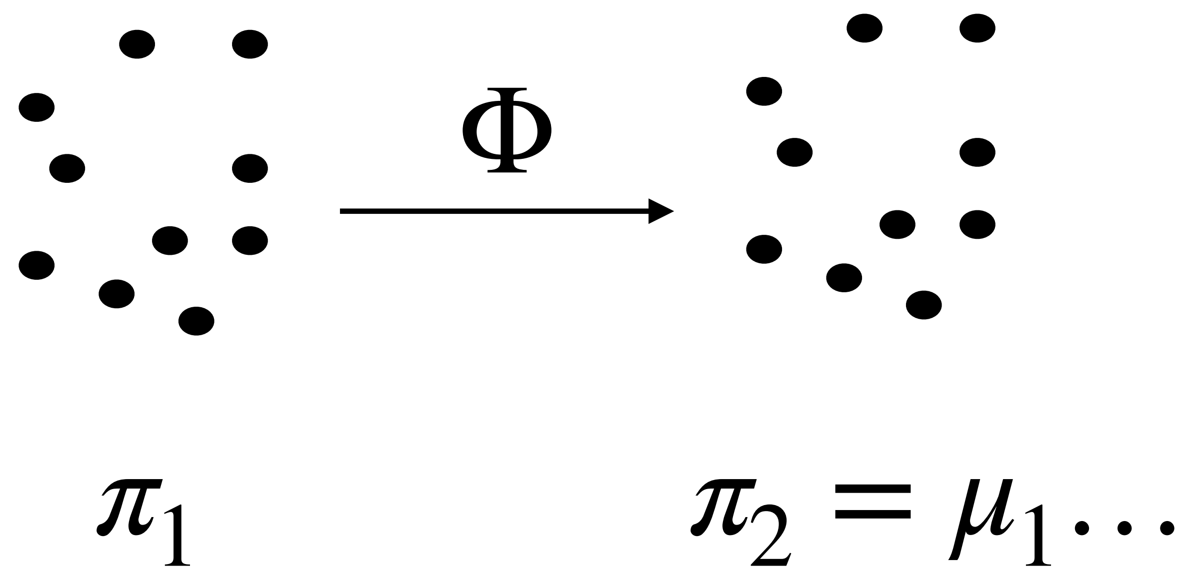
Choose V_n, what is the best approximation of $\mathscr{D}_t|_{V_n}$? $argmin_{D_m} \sum_{i,j} |\mathscr{D}_t h_i(\pi_j) - (D_m)_{ik} h_k(\pi_j)|_2^2$

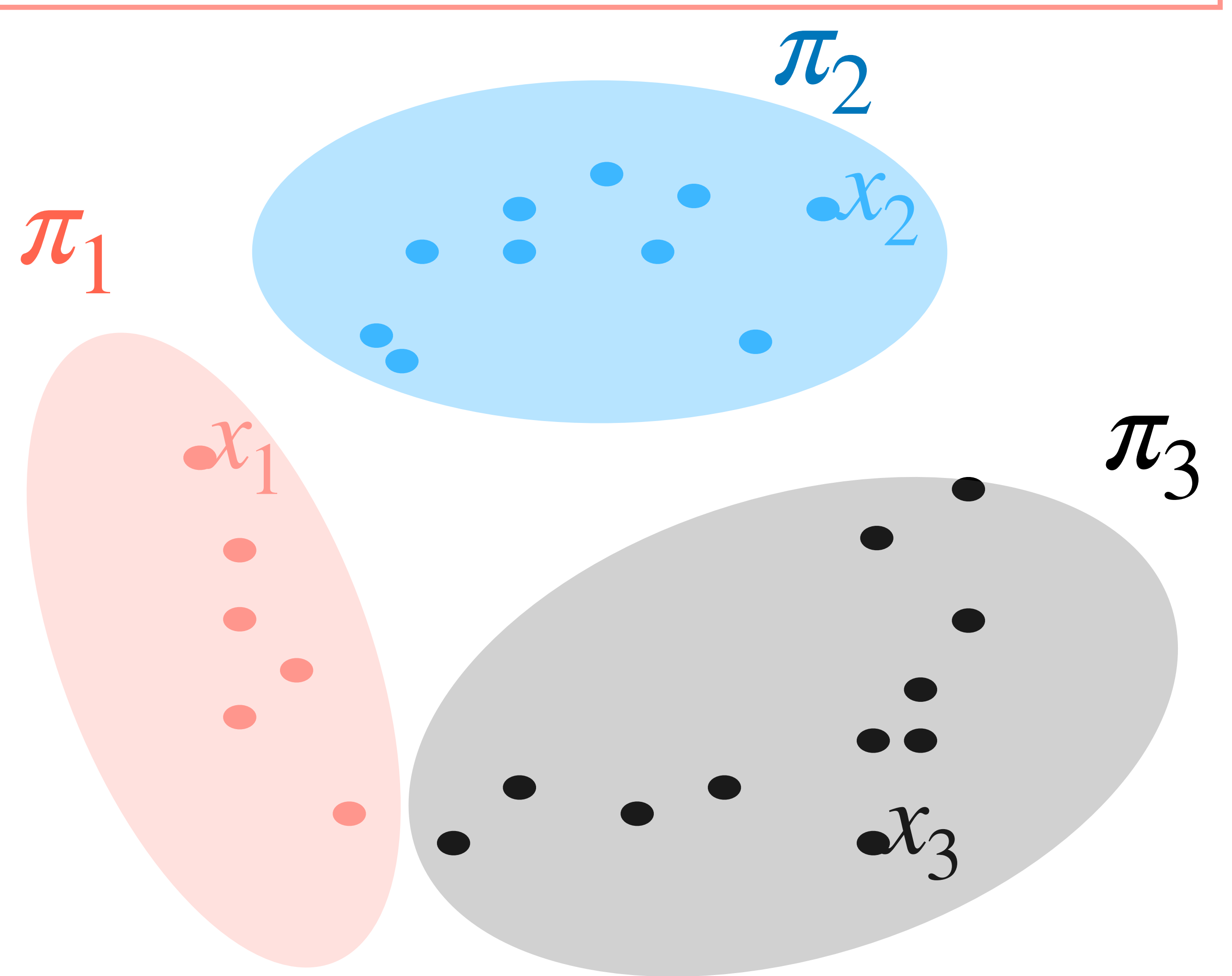
Given distributional data: $\{\pi_j\}_{j=1}^m, \{\mu_j = T_t \pi_j\}_{j=1}^m$

Compute :$(\Psi_m)_{ij} = h(\pi_j)$ and $(\Phi_m)_{ij} = h_i(\mu_j)$

Return $D_m = \Phi_m \Psi_m^\dagger$

Ways to obtain densities





Convergence guarantees

Define a Hilbert Schmidt norm for $Z_n = \{\mathscr{E} : V_n \to H, \mathscr{E} \text{ linear}\}$:

$$\|\mathscr{E}\|_{HS} = \|G^{-1}E\|_F, \text{ where } G_{ik} = \langle h_i, h_k \rangle, E_{ik} = \langle \mathscr{E}h_i, \mathscr{E}h_k \rangle$$

∞ -data

Minimize the HS norm of the residual operator: $\mathscr{D}_t^n = arg \min_{\mathscr{C}:V_n \to V_n} \|\mathscr{D}_t - \mathscr{C}\|_{HS}$

First order optimality: $D_\infty = YG^{-1}$, where $Y_{ik} = \langle h_i \circ T_t, h_k \rangle = \int h_i(T_t(\pi))h_k(\pi)dP$

m -data

$$D_m = \Phi_m \Psi_m^\dagger = \frac{1}{m}\Phi_m \Psi_m^\top \left(\frac{1}{m}\Psi_m \Psi_m^\top \right)^{-1}$$

$$\frac{1}{m}\sum_j h_i(T_t(\pi_j))h_k(\pi_j) \qquad \frac{1}{m}\sum_j h_i(\pi_j)h_k(\pi_j)$$

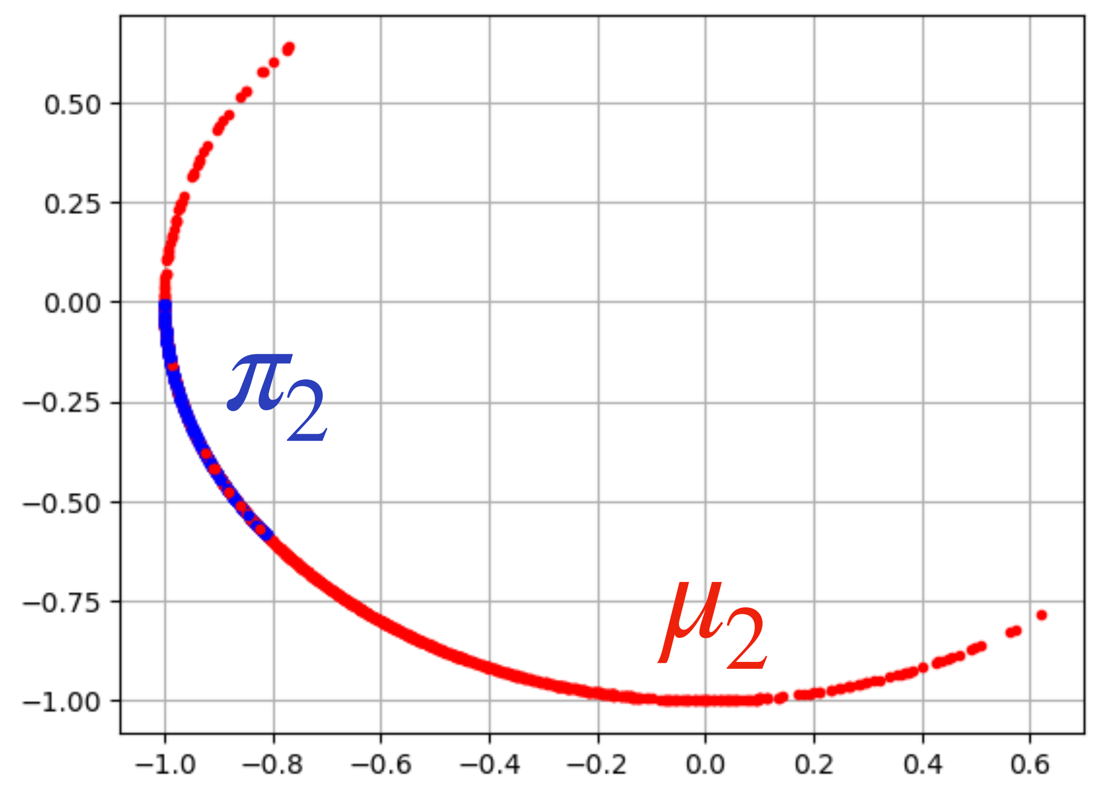
Convergence guarantees

Theorem (O., Townsend, Yang, 2025) Let $h_1, \ldots, h_n$ be linearly independent and assume the condition number of $G_{ik} = \langle h_i, h_k \rangle$ is bounded. If for any fixed m, $\pi_1, \ldots, \pi_m \sim P$ I.i.d then D_m converges to **the best matrix approximation** D_∞ of the DKO on $V_n = Span\{h_i\}_{i=1}^n$

$$\|D_m - D_\infty\|_F \to 0 \iff \|\mathcal{D}_t^n - \mathcal{D}_m^n\|_{HS} \to 0$$

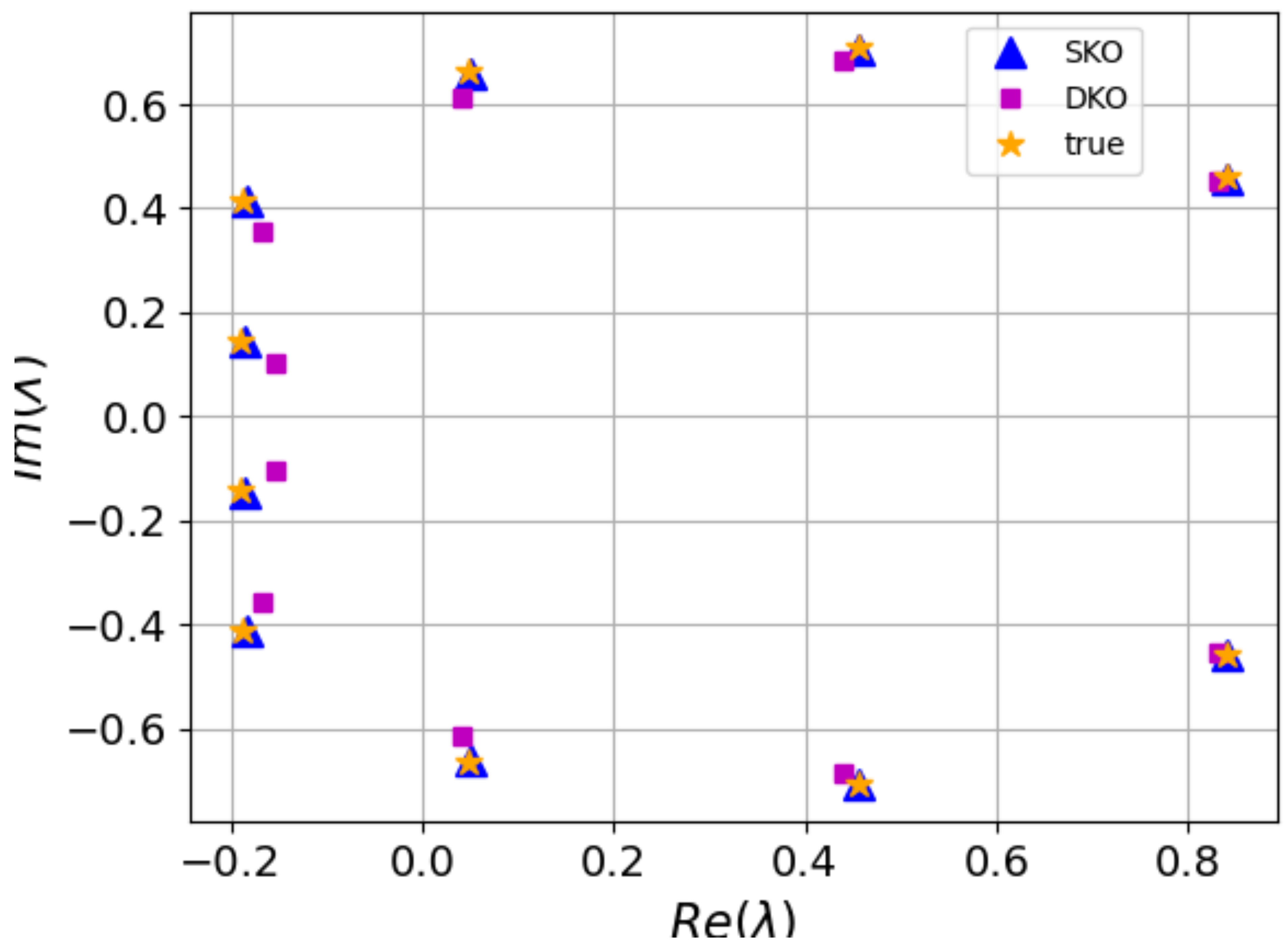
Numerical results

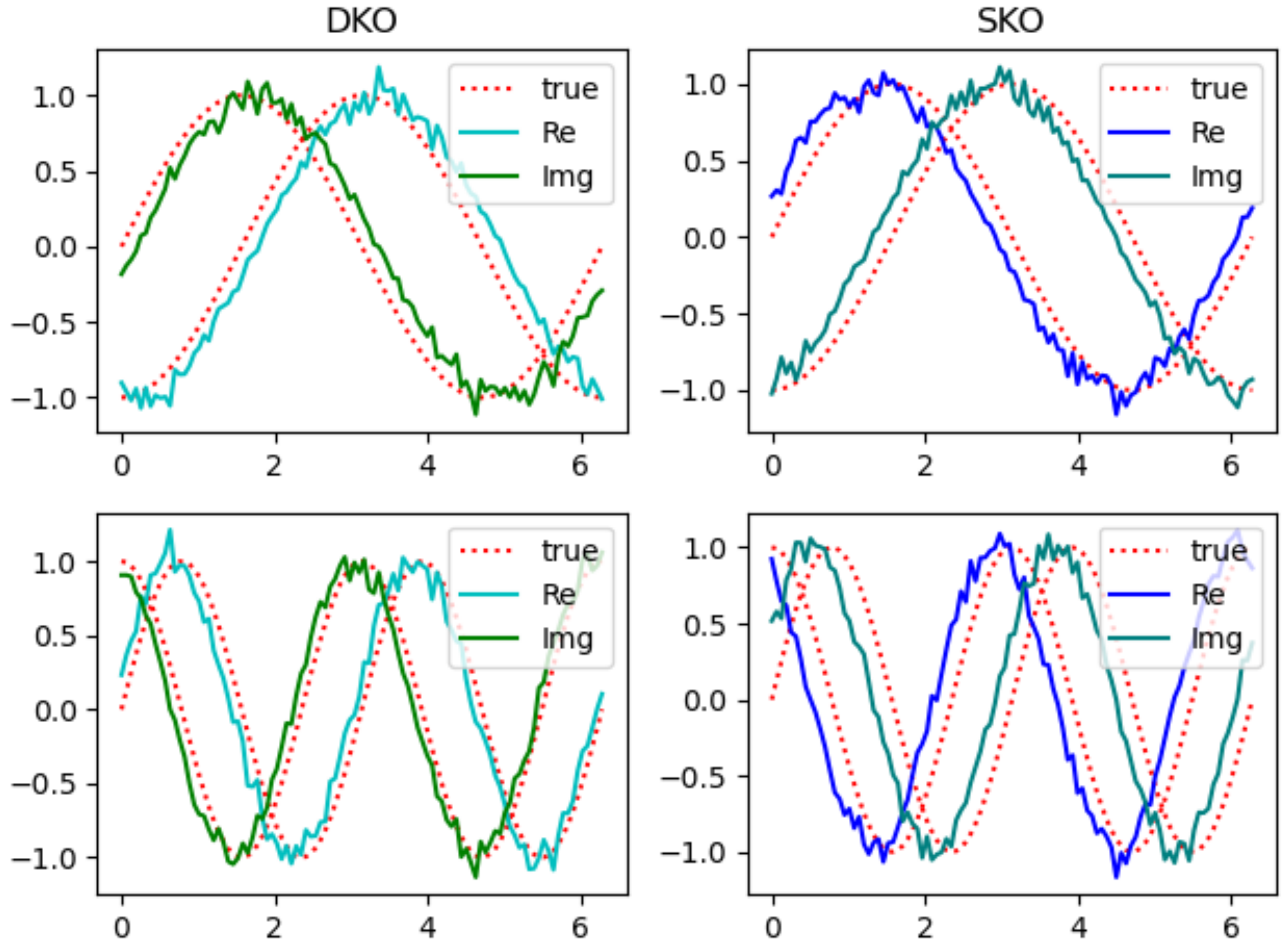
Random rotations on a circle $\theta_{t+1} = \theta_t + \nu + \omega_t,\ \nu = 0.5$



Observables $\hat{h}_i = 1_{\left[i\frac{2\pi}{N},(i+1)\frac{2\pi}{N}\right]}$

Measures $\pi_i = Unif\left[j\frac{2\pi}{N},(j+1)\frac{2\pi}{N}\right]$





Numerical results

Variance for an SDE

$$dX_t = -\sin X_t dt + e^{-0.5(x-1)^2} d\omega_t$$

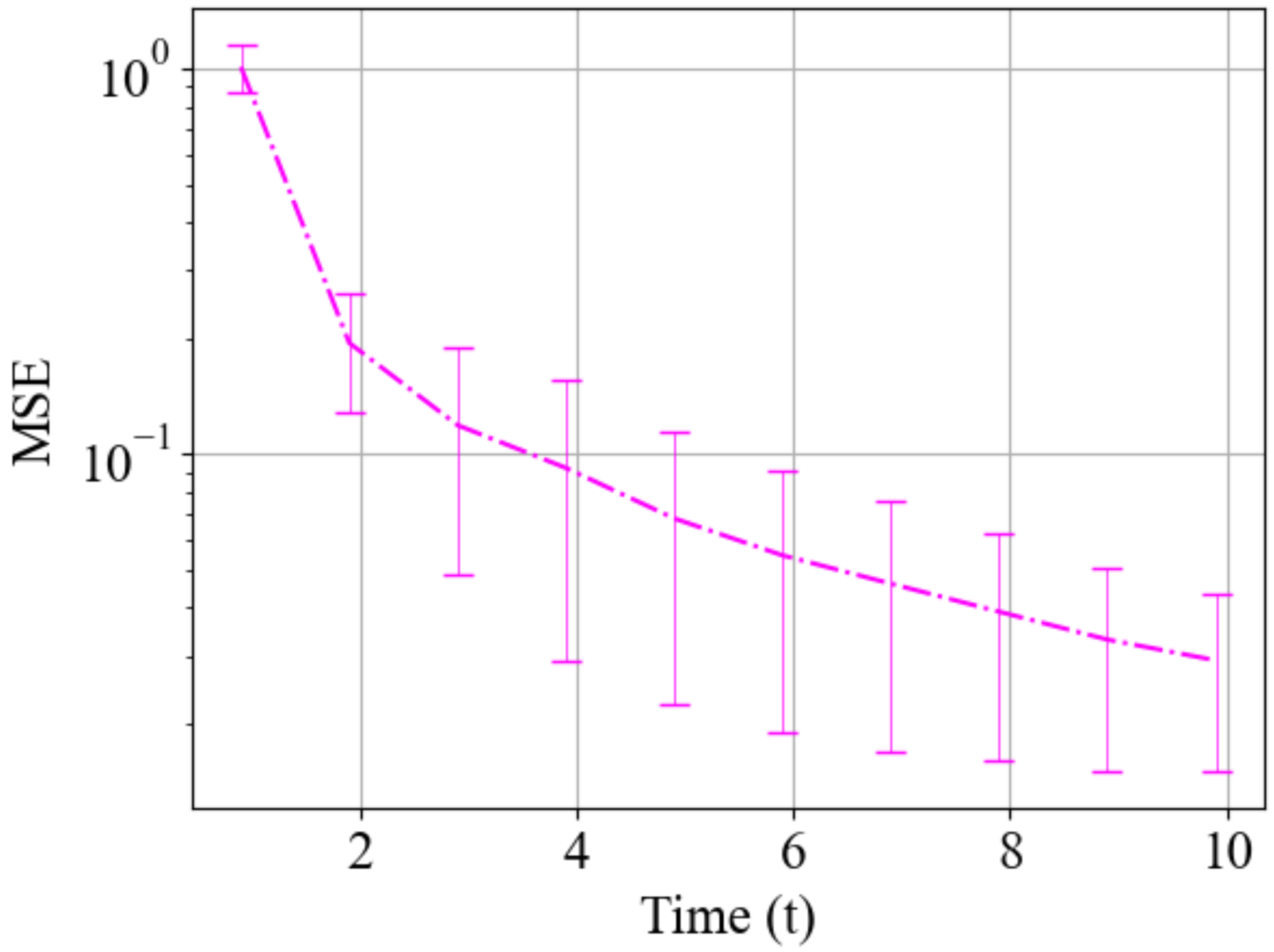
Start with radial basis functions with $n = 9$

$$\hat{h}_i = e^{-\epsilon(x-c_i)^2}$$

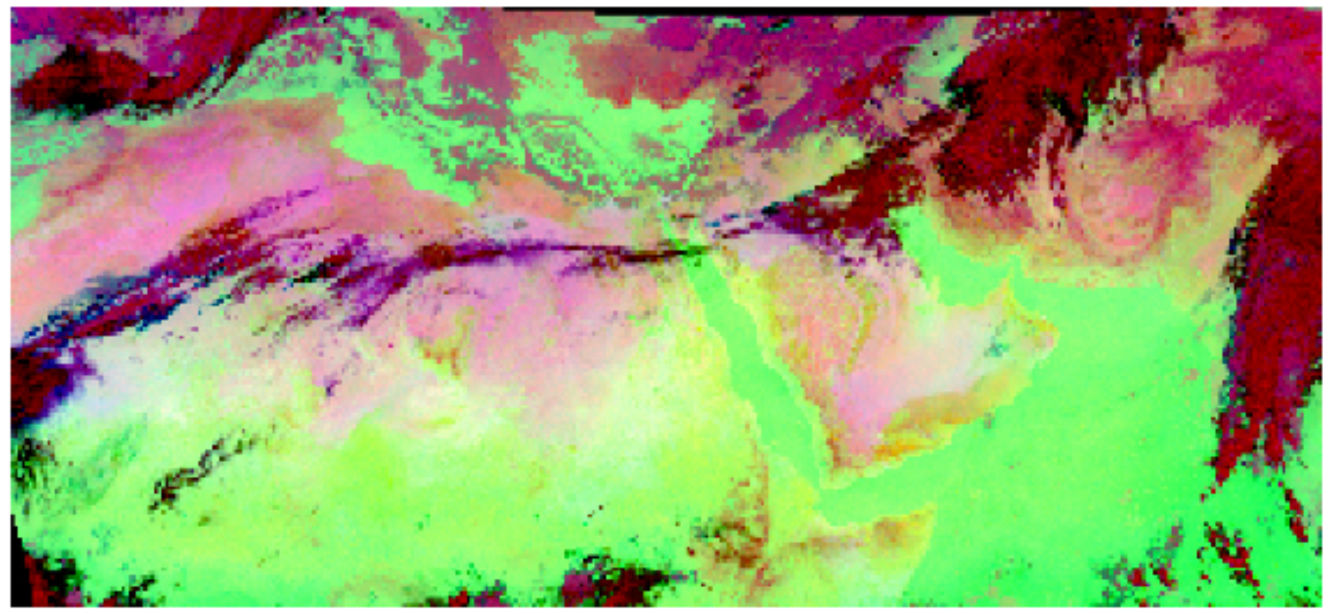
Observables $\mathbb{E}_\pi[\hat{h}_i \hat{h}_k], \mathbb{E}_\pi[\hat{h}_i]\mathbb{E}_\pi[\hat{h}_k]$

Measures $\{\pi_j\}_{j=1}^{20}, \pi_0 = \mathcal{N}(0,1)$

Observe for time T = 2 and predict for time T = 10



Numerical results



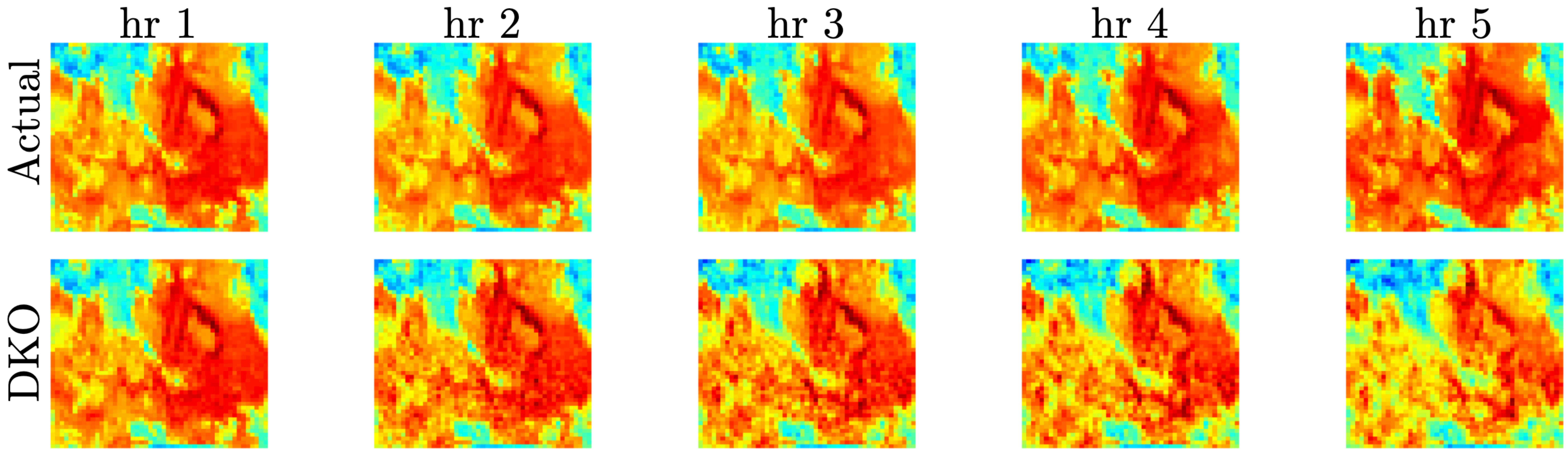
Dust plume DUSTScan2022 data

Dataset = hourly dust observations from SEVIRI on Meteosat-8

Data = pictures of dust density as a function of deviation from magenta

Observables = average over patches of PDI index over 50x50 pixels

Use 28 days worth of data and predict the following 5 hours



Thank you for your attention!

M.O., Alex Townsend, Yunan Yang, The Distributional Koopman Operator for Random Dynamical Systems, arXiv preprint, 2025

Transfer operator

Satisfies the Fokker Plank equation

$$\partial T_t(\pi) = -\nabla \cdot \Big(f(x)\pi_t - \nabla \cdot (g(x)\pi_t\Big)$$

Definition

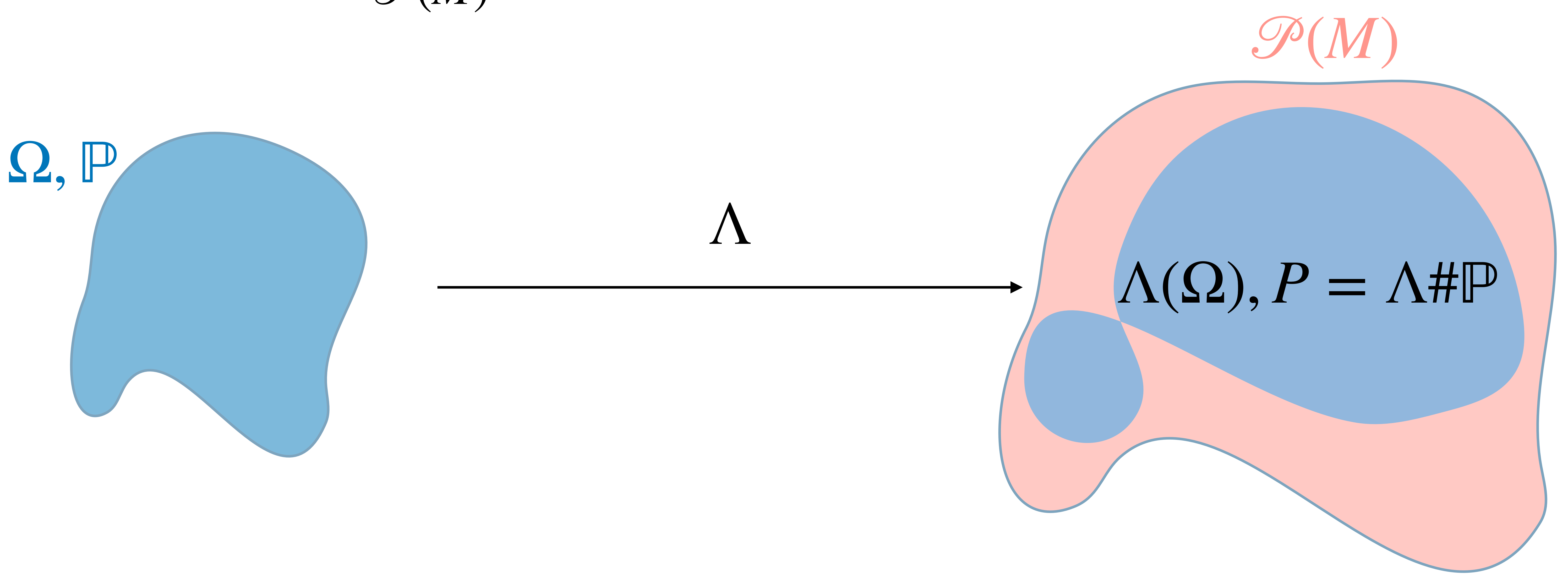
$$\int_M \hat{h}(x)\, d\Big(T_t\pi\Big)(x) = \int_\Omega \int_M \hat{h}(x)\, d\Bigg(\Phi_t(\omega, \cdot\,)\#\pi\Bigg)(x)\, dp(\omega),$$

Adjoint of SKO

$$\langle \mathcal{S}_t \hat{h}, \pi \rangle = \langle \hat{h}, T_t\pi \rangle$$

An inner product structure on H

Holy grail: $\langle h_1, h_2 \rangle = \int_{\mathscr{P}(M)} h_1(\pi) h_2(\pi) dP$ ⟵ Does not exist



Enough to define on a dense subset of $\mathscr{P}(M)$ and extend by continuity

|{ space of all empirical measures} | = |[0,1]|

Sample empirical measures $\pi_j \sim \Lambda \# \mathbb{P}$ and let $\langle h_1, h_2 \rangle = \frac{1}{m} \sum_{j=1}^{m} h_1(\pi_j) h_2(\pi_j)$ ✓

Details for the numerical examples

Random rotations on a circle $\omega \sim Unif[-0.5, 0.5]$

used 20 measures, each with 1000 samples