



The distributional Koopman operator

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Abstract:

The expected evolution of an observable in a random dynamical system is captured by the Stochastic Koopman (SKO) operator. It's computation uses the dynamic mode decomposition (DMD) algorithm that relies on the availability of tracking information. In this work, we introduce the Distributional Koopman Operator (DKO), a novel framework which incorporates higher moment information, and avoids the need for particle tracking in its computation. The core idea is to extend the Koopman operator to act on observables of probability distributions, leveraging the transfer operator to propagate these distributions forward in time. We analyse the proprieties of this new operator, and show how one can recover information about higher order moments from this formulation. Lastly, we design an algorithm to compute the DKO from data.

RANDOM DYNAMICAL SYSTEMS

HILBERT SCHMIDT STRUCTURE OF OBSERVABLES

Other observables:

Variance $h(\pi) = \text{Var}_{X \sim \pi}(\hat{h}(X))$
Evaluation of densities $h(\pi) = \pi(x_0)$

Inner product:

$\Lambda : (\Theta, \mathbb{P}) \rightarrow \mathcal{P}(M)$ random measure with dense image
 $\Rightarrow$ Measure on $\mathcal{P}(M)$: $\Lambda \# \mathbb{P}$

$\langle h_1, h_2 \rangle = \int_{\Theta} h_1 \circ \Lambda(\theta) h_2 \circ \Lambda(\theta) d\mathbb{P}(\theta)$

Hilbert Schmidt norm:

Finite dimensional space $V_n = \text{Span}\{h_1, \dots, h_n\}$
For an operator $\mathcal{E} : V_n \rightarrow H$ define $\|\mathcal{E}\|_{HS} = \|G^{-1}E\|_F$, where
 $G_{ik} = \langle h_i, h_k \rangle$ and $E_{ik} = \langle \mathcal{E}h_i, \mathcal{E}h_k \rangle$

DISTRIBUTIONAL DMD

Best approximation to $\mathcal{D}_t|_{V_n}$ is $\text{argmin}_{\mathcal{D}_n} \|\mathcal{D}_t - \mathcal{D}^n\|_{HS} \rightarrow$ matrix D^n

Assume finite data: $\{\pi_j\}_{j=1}^m$ and $\{\mu_j = T_t \pi_j\}_{j=1}^m$

Distributional DMD Algorithm:

- Compute $(\Phi_m)_{ij} = h_i(\pi_j)$ and $(\Psi_m)_{ij} = h_i(\mu_j)$
- $D_m^n = \Psi_m \Phi_m^\dagger$

Convergence guarantee
In the limit as $m \rightarrow \infty$, if G has bounded condition number and $\pi_j \sim \Lambda \# \mathbb{P}$

$\|D_m^n - D^n\|_F \rightarrow 0$

NUMERICAL EXPERIMENTS

Random rotations on the circle: $x_{t+1} = x_t + \frac{\pi}{3} + \omega \mod 2\pi$

H_1 observables

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

Measures

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

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

Observables: $h(\pi) \in \mathbb{E}[\hat{h}_i \hat{h}_k], \mathbb{E}[\hat{h}_i] \mathbb{E}[\hat{h}_k]$

$\hat{h}_i$ are radial basis functions

Measures $\pi_j \Delta t, \pi_0 = \mathcal{N}(0,1), \Delta t = 0.1$

Observe $T = 2$, predict $T = 10$

DustSCAN22 dataset: Satellite data of dust of the coast of Libia

observe first 28 days
predict next 5h
observables = average
over 50x50 patches

Actual

hr 1

hr 2

hr 3

hr 4

hr 5

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Check out our paper on arXiv: https://arxiv.org/abs/2504.11643

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Source of randomness

State

Example: SDE's

$\Omega = \mathcal{C}[0,1]$,

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

STOCHASTIC KOOPMAN OPERATOR

Average value of an observable at time t

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

Linear $\Rightarrow$ Matrix representation on invariant subspace $V_n = \text{Span}\{\hat{h}_1, \dots, \hat{h}_n\}$

Since $\mathcal{S}_t V_n \not\subset V_n$ find the best approximation by minimizing residual

$\text{argmin}_{S^n \in \mathbb{R}^{n \times n}} \|\mathcal{S}_t \hat{h}_i - (S^n)_{ik} \hat{h}_k\|_{L^2(\mu)}$

Assume finite data $\{x_j\}_{j=1}^m$ trajectory that fills invariant measure μ

DMD Algorithm:

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

- $S_m^n = \Psi_m \Phi_m^\dagger$

TRANSFER OPERATOR

Evolution of a density π under the random dynamical system

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

Can be computed using empirical data.

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

$\Phi_t(\omega_1, x_0)$

$\pi_t = T_t(\pi_0)$

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

DISTRIBUTIONAL KOOPMAN OPERATOR

Lagrangian $\rightarrow$ Eulerian

Particles $x \in M$

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

Distributions $\pi \in \mathcal{P}(M)$

Functionals $h : \mathcal{P}(M) \rightarrow \mathbb{R}$ continuous & bounded

RDS $\Phi_t : \Omega \times M \rightarrow M$

Transfer $T_t : \mathcal{P}(M) \rightarrow \mathcal{P}(M)$

Definition

$\mathcal{D}_t : H \rightarrow H, \mathcal{D}_t h(\pi) = h \circ T_t(\pi)$

$H =$ space of all observables,

$\Rightarrow \mathcal{D}_t$ linear & semigroup propriety

As a generalization of SKO

$H_1 = \left\{ h(\pi) = \int \hat{h}(x) d\pi(x) \right\}$ linear observables

Evaluation at $\delta_x : \mathcal{D}_t h(\delta_x) = \mathcal{S}_t \hat{h}(x)$

Integrate the uncertainty: $\mathcal{D}_t h(\pi) = \mathbb{E}_{X \sim \pi}[\mathcal{S}_t \hat{h}(X)]$

$(\lambda, \hat{h})$ eigenpair of $\mathcal{S}_t \Rightarrow (\lambda, h)$ eigenpair of $\mathcal{D}_t$