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EDMD FOR THE KOOPMAN OPERATOR AND GENERATOR

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The Generator (Continued)

Basic EDMD

Semigroup

The Chapman-Kolmogorov equation implies that the Koopman operators form a semigroup:

Definition

A familiy of bounded linear operators $\mathcal{T}^\tau,\ \tau \geq 0$ on a Banach space X is called a **strongly continuous semigroup** if:
(i) $\mathcal{T}^0 = \mathrm{Id}$.
(ii) $\mathcal{T}^{\tau_1+\tau_2} = \mathcal{T}^{\tau_1}\mathcal{T}^{\tau_2}$ for all $0 \leq \tau_1 \leq \tau_2$.
(iii) $\lim_{\tau\to 0} \mathcal{T}^\tau x = x$ for all $x \in X$.

The Generator

In accordance with semigroup theory, we define:

Definition

The generator $\mathcal{L}$ of the semigroup of Koopman operators $\mathcal{K}^\tau$ on $L^2_\mu(\mathbb{X})$ acts on a function f by

$$\mathcal{L}f := \lim_{\tau \to 0} \frac{1}{\tau}(\mathcal{K}^\tau - \mathrm{Id})f,$$

whenever this limit exists. The domain of of the generator is the set of all f where the above limit exists, is denoted $\mathcal{D}(\mathcal{L})$.

Generator and Time Evolution

We also know from semigroup theory that:

Theorem

The generator $\mathcal{L}$ is defined on a dense subspace $\mathcal{D}(\mathcal{L})$. Consider the function $v(\tau, x) = \mathcal{K}^\tau f(x)$ for $f \in \mathcal{D}(\mathcal{L})$. Then we have the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}\tau} v(\tau, x) = \mathcal{L} v(\tau, x).$$

This is the analogue of $\dot{y} = Ly$ from last night's talk. The dynamics of the expectation value of a function in $\mathcal{D}(\mathcal{L})$ are linear.

The Generator of an SDE

Proposition

Let $f \in C_0^\infty(\mathbb{R}^d)$ and X_t solve an SDE with drift b and diffusion σ. Then $f \in \mathcal{D}(\mathcal{L})$ and the action of the generator is given by

$$\mathcal{L}f(x) = b(x) \cdot \nabla f(x) + \frac{1}{2} a(x) : \nabla^2 f(x).$$

Proof

Proof.

$$
\begin{aligned}
\mathcal{L}f(x) &= \lim_{\tau\to 0}\frac{1}{\tau}\mathbb{E}^x(f(X_\tau)-f(X_0)) \\
&= \lim_{\tau\to 0}\frac{1}{\tau}\mathbb{E}^x\left[\int_0^\tau \nabla f^T(X_s)b(X_s)+\frac{1}{2}a(X_s):\nabla^2 f(X_s)\,\mathrm{d}s\right] \\
&\quad + \mathbb{E}^x\left[\int_0^\tau \nabla f^T(X_s)\sigma(X_s)\,\mathrm{d}B_s\right] \\
&= \lim_{\tau\to 0}\frac{1}{\tau}\mathbb{E}^x\left[\int_0^\tau \nabla f^T(X_s)b(X_s)+\frac{1}{2}a(X_s):\nabla^2 f(X_s)\,\mathrm{d}s\right] \\
&= \nabla f^T(x)b(x)+\frac{1}{2}a(x):\nabla^2 f(x).
\end{aligned}
$$

Generators and PDEs

Corollary

Let $f \in C_0^\infty(\mathbb{R}^d)$ and consider the function $v(\tau, x) = \mathcal{K}^\tau f(x)$, with X_τ solution of an SDE. Then v solves the PDE

$$\frac{\partial}{\partial \tau} v(\tau, x) = \mathcal{L} v(\tau, x) = b(x) \cdot \nabla_x v(\tau, x) + \frac{1}{2} a(x) : \nabla_x^2 v(\tau, x).$$

Summary

- Markovian stochastic dynamics are defined by a transition kernel.
- Time evolution of expectation values of observable functions is carried out by the semigroup of Koopman operators.
- The time evolution of these expectations in linear (in function space).
- For an SDE, this time evolution corresponds to a PDE. In particular, the "system matrix" is an unbounded differential operator.

References

Oksendal, *Stochastic Differential Equations* (2013)

Pazy, *Semigroups of linear operators and applications to partial differential equations* (2012)

Bakry, Gentil, Ledoux, *Analysis and Geometry of Markov Diffusion Operators* (2014)

The Generator (Continued)

Basic EDMD

Galerkin Projection of the Koopman Operator: EDMD

Consider the Koopman operator $\mathcal{K}^\tau$ on the Hilbert space L^2_μ. Choose an N-dimensional subspace $\mathbb{W}$ with basis $\{\psi_i\}_{i=1}^N$ (the functions g from last night). Find a matrix K, such that, for any function $\psi_v \in \mathbb{W}$ with coefficient vector v, we have that $\psi_{Kv} - \mathcal{K}^\tau \psi_v$ is as small as possible. By standard best-approximation in Hilbert space, the optimal matrix representation is

$$K^\tau = G^{-1}A, \qquad A_{ij} = \left\langle \psi_i, \mathcal{K}^\tau \psi_j \right\rangle_\mu, \qquad G_{ij} = \left\langle \psi_i, \psi_j \right\rangle_\mu .$$

Data-Based Approximation

If the process X_t is ergodic, i.e. time averages converge to spatial averages, we can approximate the Galerkin projection based on simulation data:

Proposition

Let μ be the unique invariant measure of the process X_t. Moreover, let $\{x_k\}_{k=1}^{\infty}$ be an infinitely long realization of the process, started from the initial distribution μ and sampled at time step τ. Then, with probability one

$$G_{ij} = \langle \psi_i, \psi_j \rangle_\mu = \lim_{m \to \infty} \frac{1}{m} \sum_{k=1}^{m} \psi_i(x_k)\psi_j(x_k)$$

$$A_{ij} = \langle \psi_i, \mathcal{K}^t \psi_j \rangle_\mu = \lim_{m \to \infty} \frac{1}{m-1} \sum_{k=1}^{m-1} \psi_j(x_k)\psi_j(x_{k+1}).$$

Williams et al, *J. Nonlinear Sci.* (2015), Klus, Nüske, et al, *J. Nonlinear Sci.* (2018)

Comments

- With matrices $\Psi_X = [\psi_i(x_k)]$, $\Psi_Y = [\psi_i(x_{k+1})] \in \mathbb{R}^{N\times(m-1)}$, we basically obtain EDMD:

$$K \approx (\Psi_X \Psi_X^T)^{-1} \Psi_X \Psi_Y^T = (\Psi_X^T)^\dagger \Psi_Y^T.$$

- The lag time τ can also equal an integer multiple of the elementary time step between data points. In this case, all pairs with time spacing τ in between can be used ("sliding window").
- Similar results can be obtained for non-stationary systems, upon replacing a single long trajectory by many short ones.

Example: Markov State Model

For $k = 1, \ldots, N$, let S_k be a subset of $\mathbb{X}$ such that $S_k \cap S_l = \emptyset$ if $k \neq l$, and $\mathbb{X} = \bigcup_{k=1}^{N} S_k$. Let $\mathbb{W} = \{\mathbf{1}_{S_k}\}_{k=1}^{N}$ be the subspace spanned by the indicator functions of those sets.

Proposition

Let $S_k,\ k = 1, \ldots, N$ and $\mathbb{W}$ as described above. Then the resulting matrix approximation $T = G^{-1}A$ is a stochastic transition matrix of conditional transition probabilities between the discrete sets S_k. If the dynamics are reversible w.r.t. to the invariant measure μ, then T is also a reversible transition matrix.

Dellnitz and Junge, *SIAM J. Numer. Anal.* (1999), Schütte et al, *J. Comp. Phys.* (1999), Prinz et al, *J. Chem. Phys.* (2011)