Ergodicity of Markov processes: theory and computation (4)

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Overview

Last three times:

1. Find a small set $C$
2. Use Lyapunov function to estimate $\eta_C$
3. Create an atom $\alpha$. Estimate $\eta_\alpha$
4. Use renewal theory to estimate the coupling time $\tau_C$

Today: Data-driven computing for ergodicity and invariant probability measures.

Why data-driven? Traditional methods do not work in high dimension!
Outline: Data-driven computation

I. Invariant probability measure
   - Combine traditional PDE solver with simulation data.
   - Data-driven solver for invariant probability measure.

II. Geometric/power-law ergodicity
   - How fast does SDE converge to $\pi$?
   - Estimate coupling time from data.
Noise perturbations

ODE system

\[
\frac{dX}{dt} = f(X)
\]

stochastic differential equation (SDE)

\[
dX_t = f(X_t)dt + \epsilon \sigma(x)dW_t.
\]
Noise perturbations

1. Theory for discrete-time Markov process still works
2. Transition kernel becomes time-dependent

\[ P^t(x, A) = \mathbb{P}[\Phi_t \in A | \Phi_0 = x] \]

3. Infinitesimal generator

\[ \mathcal{L} u = \lim_{t \to 0} \frac{P^t u - u}{t} = \sum_{i=1}^{n} f_i u_{x_i} + \frac{1}{2} \epsilon^2 \sum_{i,j=1}^{n} a_{ij} u_{x_i x_j} \]

where \( A = \{ a_{ij} \}_{i,j=1}^{d} = \sigma \sigma^T \)
Fokker-Planck equation and its steady-state

**Invariant probability measure**
- Let \( P^t(x, \cdot) \) be the transition kernel of the SDE
- A probability measure \( \mu \) is said to be invariant if
  \[
  \mu(A) = \int \mu(dx) P^t(x, A) \quad \text{for any measurable } A.
  \]

**Steady-state Fokker-Planck equation**
- The density function of \( \mu \) solves equation
  \[
  \mathcal{L}^* u = \frac{1}{2} \epsilon^2 \sum_{i,j=1}^{N} (a_{ij} u)_{ij} - \nabla \cdot (fu) = 0,
  \]
- where \( A = \{a_{ij}\}_{i,j=1}^{d} = \sigma\sigma^T \).
Numerical example: Rossler Attractor
Numerical example: Rossler Attractor + noise
How to compute invariant density function?

**Numerical PDE approach**

Discretize steady-state Fokker-Planck equation

\[
\frac{1}{2} \epsilon^2 \sum_{i,j=1}^{N} (a_{ij}u)_{ij} - \nabla \cdot (fu) = 0.
\]

**Problem: What’s the boundary condition?**

- Sufficiently large numerical domain.
- Use large deviations. Zero boundary.
- Find least square solution.
- High computational cost in general.
How to compute invariant density function?

**Monte Carlo method**
- Divide the domain into many bins $B_1, \cdots, B_N$.
- Run a long SDE trajectory.
- Count samples in each bin. Estimate density.
- Works for arbitrary numerical domain.

**Problem: accuracy**
- Not many sample points in each bin. High relative error.
- Solution looks “furry” even with large number of samples.
Numerical example: Gradient flow + rotation

Equation

\[
\begin{align*}
\frac{dX_t}{dt} &= (Y_t - 4X_t(X_t^2 + Y_t^2 - 1))dt + dW_t \\
\frac{dY_t}{dt} &= (-X_t - 4Y_t(X_t^2 + Y_t^2 - 1))dt + dW_t
\end{align*}
\]

Invariant probability density function

\[
\rho(x, y) = \frac{1}{K}e^{-2(x^2+y^2-1)^2},
\]

\(K\) is a normalizing constant.
Deterministic vector field
Sample density function from Monte Carlo
Solution: Data-driven PDE solver (low dimensional version)

Setting

- \( i = 1, \cdots, N \) grid points. Solution vector \( \mathbf{u} = (u_1, \cdots, u_N) \).
- \( A\mathbf{u} = 0 \): Linear relation from numerical PDE scheme.
- No boundary condition. \( A \) is not a full matrix.

\[
\begin{align*}
(\frac{-1}{h} f_1 + \frac{\epsilon}{2h^2}) u_1 - \frac{\epsilon}{h^2} u_2 + (\frac{1}{h} f_3 + \frac{\epsilon}{2h^2}) u_3 &= 0 \\
(\frac{1}{h} f_2 + \frac{\epsilon}{2h^2}) u_2 - \frac{\epsilon}{h^2} u_3 + (\frac{1}{h} f_4 + \frac{\epsilon}{2h^2}) u_4 &= 0 \\
(\frac{-1}{h} f_3 + \frac{\epsilon}{2h^2}) u_3 - \frac{\epsilon}{h^2} u_4 + (\frac{1}{h} f_5 + \frac{\epsilon}{2h^2}) u_5 &= 0
\end{align*}
\]
Solution: Data-driven PDE solver (low dimensional version)

Use Monte Carlo data

- \( \mathbf{v} = (v_1, \cdots, v_N) \) is obtained from Monte Carlo simulation.
- Use \( \mathbf{v} \) as a reference for the variational problem

\[
\begin{align*}
\min & \quad \| \mathbf{u} - \mathbf{v} \|^2 \\
\text{subject to} & \quad A\mathbf{u} = \mathbf{0}
\end{align*}
\]

Least norm solution

- Let \( \mathbf{d} = -A\mathbf{v} \).
- \( \mathbf{u}^* = \mathbf{v} + A^T(AA^T)^{-1}\mathbf{d} \) is called the least norm solution to the variational problem.
Solution: Data-driven PDE solver (low dimensional version)

- The PDE solver does not rely on the boundary condition now.
- High resolution profile for interested area.
- Still need to solve large linear system.

**Mechanism**
- $v - u^{ext}$ is a random vector.
- Optimization problem projects $v - u^{ext}$ to $\text{Ker}(A)$.
- Projection reduces $u^* - u^{ext}$.
Error Analysis

Proposition (with M. Dobson and J. Zhai)

Consider $N \times N$ mesh. Assume entries of $\mathbf{v} - \mathbf{u}^{\text{ext}}$ be i.i.d. random variables with zero mean and variance $\zeta^2$. Assume the PDE solver has error $O(N^{-p})$. We have

$$\mathbb{E}[\|u - u^{\text{ext}}\|_{L^2}] \leq O(N^{-1/2}\zeta) + O(N^{-p}),$$

where $\| \cdot \|_{L^2}$ is the $L^2$ numerical integral with respect to grid points.

Error concentration

- Empirical performance is better.
- Error concentrates at the boundary of domain.
- Most principal angles between $\text{Ker}(A)$ and $\Theta_D$ are small.
Block data-driven solver

- Data-driven solver does not rely on boundary.
- Divide a large $N^d$ domain into $(N/M)^d$ blocks with size $M$.
- Original cost: $N^{pd}$. New cost: $M^{(p-1)d}N^d$.
- Empirically $M$ (block size) can be as small as 20 – 30.
- Most error term concentrates at block boundaries.
- Very efficient for 3D and 4D problems.
Interface error and correction

- Visible interface error occurs on the interface of blocks.
- Error mainly concentrates at boundary points.
- Method 1: Small overlap (1 – 4 grids) between blocks.
- Method 2: “Half block shift” to cover all interfaces.

**Figure:** Black: blocks. Red: Overlapping numerical domain. Green: Half step shift.
Solution without any treatment
Solution with 2-grid overlap
Solution after half-block shift
3D example: Rossler attractor

Rossler equation

\[
\begin{align*}
    dx &= (-y - z) \, dt + \varepsilon \, dW_t^x \\
    dy &= (x + ay) \, dt + \varepsilon \, dW_t^y \\
    dz &= (b + z(x - c)) \, dt + \varepsilon \, dW_t^z
\end{align*}
\]
Solution on “slices”
Projection of solution
High-dimensional data-driven solver

1. Discretization does not work for high dimensional problems.
2. Higher dimension: approximate the solution by an artificial neural network $\hat{u}$.
3. $v = (v_1, \cdots, v_N)$ from Monte Carlo simulation.
4. New optimization problem
   \[ \min \| u - v \|^2 + \| A u \|^2 \]
5. What is artificial neural network?
Artificial neural network (ANN)

1. ANN is a way to approximate functions $y = \mathcal{NN}(x, \theta)$
2. Parameter $\theta$ are coupling weights between neurons
3. Adjust $\theta$ such that $y = \mathcal{NN}(x, \theta)$ approximates $y = f(x)$
4. Minimize a loss function $L(\theta)$ over a training set $(x_1, y_1), (x_2, y_2), \cdots$
High-dimensional data-driven solver

1. Two loss functions: $\mathcal{L}_1 = \|\hat{u} - v\|$, $\mathcal{L}_2 = \|\mathcal{L}^*\hat{u}\|^2$.
2. Different training sets for $\mathcal{L}_1$ and $\mathcal{L}_2$.
3. Train two loss functions alternatively to avoid adjusting their weights.
4. $v$ is usually a very rough approximation in high dimension. Very high spatially uncorrelated noise.
Example 1: 4D ring

\[
\begin{align*}
    dX_t &= (-4X_t(X^2_t + Y^2_t + Z^2_t + S^2_t - 1) + Y_t) \, dt + \sigma \, dW^X_t, \\
    dY_t &= (-4Y_t(X^2_t + Y^2_t + Z^2_t + S^2_t - 1) - X_t) \, dt + \sigma \, dW^Y_t, \\
    dZ_t &= (-4Z_t(X^2_t + Y^2_t + Z^2_t + S^2_t - 1)) \, dt + \sigma \, dW^Z_t, \\
    dS_t &= (-4S_t(X^2_t + Y^2_t + Z^2_t + S^2_t - 1)) \, dt + \sigma \, dW^S_t,
\end{align*}
\]

Invariant density

\[
u(x, y, z, s) = \frac{1}{K} \exp(-2(x^2 + y^2 + z^2 + s^2 - 1)^2).
\]

concentrate near a 4D sphere.
Example 1: 4D ring
Example 2: Stochastic heat equation

Consider a discrete stochastic heat equation

\[ dU_i = (U_{i-1} + U_{i+1} - 2U_i)dt + dW_t^{(i)} \]

for \( i = 1, \cdots, N \). Assume \( U_0 = U_N = 0 \). Invariant probability density given by Lyapunov equation.

1. Neural network works well when \( N = 10 \)
2. Neural network is not enough (128 hidden neurons) when \( N = 20 \).
Example 2: Stochastic heat equation

\[(X^{(1)}, X^{(2)})\text{ slice from 10D distribution}
\]
\[\text{narrow first hidden layer}\]

\[(X^{(1)}, X^{(2)})\text{ slice from 20D distribution}
\]
\[\text{narrow first hidden layer}\]

\[(X^{(1)}, X^{(2)})\text{ slice from 10D distribution}
\]
\[\text{wide first hidden layer}\]

\[(X^{(1)}, X^{(2)})\text{ slice from 20D distribution}
\]
\[\text{wide first hidden layer}\]
Power-law ergodicity

1. Find a small set $C$
2. Recall that power law tail of $\eta_C$ is preserved in both $\eta_\alpha$ and the first simultaneous coupling.
3. Simulate the first passage time $\eta_C$
4. If $\sup_{x \in C} E_x[\eta_C^\beta] < \infty$, the speed of contraction is $\sim n^{-\beta}$.
5. Use extreme value theory to verify the bounded supreme if $C$ has high dimension.

Ref: H. Xu and Y. Li, 2017, JSP
Geometric ergodicity

Definition

$X_t$: Markov process with transition kernel $P$ and invariant probability measure $\pi$.

$X_t$ is geometrically ergodic with rate $r$ if

$$\lim_{t \to \infty} \frac{1}{t} \log \| P^t(x, \cdot) - \pi \|_{TV} = -r$$

Importance

- $r$ is the spectral gap for reversible $X_t$.
- Interplay of deterministic dynamics and noise.
- Difficult to estimate for non-gradient case. Most rigorous results are not sharp.
Recall: coupling lemma

**Coupling lemma**

- Let \((X_t^{(1)}, X_t^{(2)})\) be a coupling such that if \(X_t^{(1)} = X_t^{(2)}\), then \(X_s^{(1)} = X_s^{(2)}\) for all \(s > t\).
- \(\tau_C = \inf \{ X_t = Y_t \}\) is the coupling time.
- \[ \|\mu P^t - \nu P^t\|_{TV} \leq 2P_{\mu, \nu}[\tau_C > t]. \]
- There exists an optimal coupling such that the equality holds.
**Upper and lower bound**

### Lower bound

Estimate $r_l$ such that

$$
\mathbb{P}[\tau_C > t] \approx e^{-r_l t}.
$$

$r_l < r$ is a lower bound of geometric ergodicity rate.

### Upper bound

Construct disjoint sets $(A_t, B_t)$. Run coupling $(\mathcal{X}_t, \mathcal{Y}_t)$ with $\mathcal{X}_0 \in A_0$ and $\mathcal{Y}_0 \in B_0$.

$$
\xi_C = \min \left\{ \inf_t \{\mathcal{X}_t \notin A_t\}, \inf_t \{\mathcal{Y}_t \notin B_t\} \right\}, \quad \mathbb{P}[\xi_C > t] \approx e^{-r_u t}
$$

$r < r_u$ is an upper bound of geometric ergodicity rate.
How to couple numerically

Let \((X_t^{(1)}, X_t^{(2)})\) be a coupling.

- Independent. \(X_t^{(1)}\) and \(X_t^{(2)}\) are independent until coupling.
- Synchronous. Use the “same noise”.
- Reflection. Use “mirroring” random terms.
- Maximal coupling. Compare density function when
  \[|X_t^{(1)} - X_t^{(2)}| \ll 1.\]
Example 1: SIR model

SIR model with degenerate noise

\[ dS = (\alpha - \beta SI - \mu S)dt + \sigma SdW_t \]
\[ dI = (\beta SI - (\mu + \rho + \gamma)I)dt + \sigma IdW_t, \]

Non-degenerate invariant probability measure if
\[ \frac{\alpha \beta}{\mu} - (\mu + \rho + \gamma - \frac{\sigma^2}{2}) > 0. \] Rigorous proof only gives faster-than-power-law ergodicity (Yin et al. 2016 SIADS).

How to couple?

- Synchronous coupling until \( |X_t^{(1)} - X_t^{(2)}| \ll 1 \)
- Compute probability density function for two steps.
- Use maximal coupling.
SIR model
Example 2: Coupled FitzHugh-Nagumo oscillators

50 coupled neurons.

\[
du_i = \left( \frac{u}{\mu} - \frac{u^3}{3\mu} - \frac{1}{\sqrt{\mu}} v + \frac{d_u}{\mu} (u_{i+1} + u_{i-1} - 2u_i) + \frac{w}{\mu} (\bar{u} - u_i) \right) dt + \frac{\sigma}{\sqrt{\mu}} dW^1_t
\]

\[
dv_i = \left( \frac{1}{\sqrt{\mu}} u + \frac{a}{\sqrt{\mu}} \right) dt + \frac{\sigma}{\sqrt{\mu}} dW^2_t.
\]

- \(i = 1, \cdots, 50\)
- \(d_u\): nearest-neighbor coupling strength. \(w\): mean field coupling strength.
- \(\bar{u}\): average membrane potential.
Example 2: Coupled FitzHugh-Nagumo oscillators

- $\omega = 0.4$, $\mu = 0.05$, $\sigma = 0.6$
- Change nearest-neighbor coupling strength $du$.
- Reflection coupling until $|X_t - Y_t| \ll 1$
- Compare probability density functions and use maximal coupling.
- Numerical result: higher $du$ gives more coherent evolution, and slower rate of geometric ergodicity.
- Heuristically, strong synchronization makes two trajectories harder to couple.
Coupled Fitzhugh-Nagumo oscillators
Coupling method is data-driven. No spatial discretization.

Coupling speed versus noise magnitude depends on the deterministic dynamics.

Important application: classification of high dimensional potential landscape.

Ongoing work: *Can you hear the shape of a landscape?*
Selected Reference

- Li, Y. *A data-driven method for the steady state of randomly perturbed dynamics*, Communications in Mathematical Sciences, 17(4), 1045-1059, 2019

- Dobson, M., Li, Y. and Zhai, J. *An efficient data-driven solver for Fokker-Planck equations: algorithm and analysis*, Communications in Mathematical Sciences, accepted


- Li, Y., Wang, S. *Numerical computations of geometric ergodicity for stochastic dynamics*, Nonlinearity 33(12), 6935, 2020

- Li, Y., Xu, H. *Numerical Simulation of Polynomial-Speed Convergence Phenomenon* Journal of Statistical Physics, 169(4), 2017
Thank you