FU course: Mathematical Strategies for Complex Stochastic Dynamics

Lecture 3

May 07, 2025

Course Information

Tentative plan for grading:

1. **Solve problems**: Each week, I will provide questions/problems. You choose one of them to solve. In total, $8-10$ questions shall be solved.
2. **1 short report**: I provide 3-4 topics for numerical experiment. Select 1 topic to conduct numerical experiement, and write a short report.
   - length: no requirement. 4-6 pages recommended.
   - problem description and goal
   - method and algorithm
   - details about numerical experiment
3. give a 5-10 min presentation.

Two persons can work together.

Last week (1)

- Ito's integration: $\int_0^T f(t)dB_t = \lim_{N\to+\infty} \sum_{n=0}^{N-1} f(t_n)(B_{t_{n+1}} - B_{t_n})$.

$$\mathbb{E}\Big(\int_0^T f(t)dB_t\Big) = 0, \quad \mathbb{E}\Big(\int_0^T f(t)dB_t\Big)^2 = \int_0^T f^2(t)dt\,. \tag{1}$$

$$(dB_t)^2 = dt\,, \text{ or}\,, \; dB_t dB_s = \delta(t-s)dt\,.$$

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- SDEs: $dX_t = f(X_t)\,dt + \sigma(X_t)dB_t$.

$$\mathcal{L}g = f\cdot\nabla g + \frac{1}{2}\sum_{i,j=1}^{d}(\sigma\sigma^\top)_{ij}\frac{\partial^2 g}{\partial x_i \partial x_j}\,, \quad \mathcal{L}^\top g = -\mathrm{div}(fg) + \frac{1}{2}\sum_{i,j=1}^{d}\frac{\partial^2\big((\sigma\sigma^\top)_{ij}g\big)}{\partial x_i\partial x_j}\,.$$

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- Ito's lemma: $dg(X_t) = \mathcal{L}g(X_t)dt + \sigma(X_t)g'(X_t)dB_t$.

Last week (2)

- Semigroup: $(T_t g)(x) = \mathbb{E}\big[g(X(t))|X(0) = x\big]$.

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- Fokker-Planck equation $\frac{\partial p}{\partial t} = \mathcal{L}^\top p$.
- Brownian motion: $dX_t = dB_t$, $\mathcal{L} = \mathcal{L}^\top = \frac{1}{2}\Delta$, heat equation.

Density under ODE

Consider the ODE

$$\frac{dx(t)}{dt} = f(x(t), t)\,, \quad t \in [0, T]\,, \tag{3}$$

where the prob. density of $x(0)$ is $p_0(x)$. Let $p(x, t)$ be the density of $x(t)$ at $t \in [0, T]$.

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Lemma

The density p satisfies the continuity equation

$$\begin{aligned} &\frac{\partial p}{\partial t} + div(fp) = 0\,, \quad \forall\, t \in (0, T] \\ &p(x, 0) = p_0\,. \end{aligned} \tag{4}$$

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Remark

With $\mathcal{L}_t g = f \cdot \nabla g$, $\mathcal{L}_t^\top g = -\mathrm{div}(fg)$, *we can write* (4) *as* $\frac{\partial p}{\partial t} = \mathcal{L}_t^\top p$.

Invariant distribution and ergodicity

Invariant distribution

Assume the probability density $X_0 = x$ is $\pi(x)$. Then the probability density of X_t satisfies the Fokker-Planck equation

$$\begin{aligned} &\frac{\partial p}{\partial t} = \mathcal{L}^\top p\,, \quad t > 0\,, \\ &p(x,0) = \pi(x)\,. \end{aligned} \tag{5}$$

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Therefore, π is (smooth) invariant density if and only if

$$\mathcal{L}^\top \pi = 0\,. \tag{6}$$

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Definition

X_t is **ergodic** with respect to an invariant density π, if $p(x, t)$ converges to π as $t \to +\infty$ starting from any density $p(x, 0)$ at time $t = 0$.

Convergence to equilibrium

Theorem (Birkhoff ergodic theorem)

Assume X_t is ergodic with respect to the invariant density π. Let $g : \mathbb{R}^d \to \mathbb{R}$ be a measuable function such that $\int_{\mathbb{R}^d} |g(x)|\pi(x)dx < \infty$. Then, with probability one, we have

$$\lim_{T \to +\infty} \frac{1}{T} \int_0^T g(X_t)dt = \int_{\mathbb{R}^d} g(x)\pi(x)dx\,. \tag{7}$$

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Remark

Theorem above allows to compute the mean $\int_{\mathbb{R}^d} f(x)\pi(x)dx$ by simulating SDEs.

Euler-Maruyama scheme

SDE:

$$dX_t = f(X_t)dt + \sigma(X_t)dB_t \tag{8}$$

Discretized scheme

$$x_{n+1} = x_n + f(x_n)h + \sqrt{h}\sigma(x_n)\eta_n \,, \quad n = 0, 1, 2, \cdots . \tag{9}$$

Estimator:

$$\int_{\mathbb{R}^d} g(x)\pi(x)dx \approx \frac{1}{N}\sum_{n=1}^{N} g(x_n) \tag{10}$$

Euler-Maruyama scheme

Algorithm Euler-Maruyama scheme

$n = 0$, $h = \frac{T}{N}$.
while $n < N$ **do**
  generate $\eta_n \sim \mathcal{N}(0, 1)$.
  $x_{n+1} = x_n + f(x_n)h + \sqrt{h}\sigma(x_n)\eta_n$.
  $n \leftarrow n + 1$.
end while

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In 1D, given x_n, we have

$$x_{n+1} \sim \mathcal{N}\Big(x_n + f(x_n)h, \sigma(x_n)^2 h\Big).$$

Connections between SDEs and PDEs

Feynman-Kac

Given $g, h : \mathbb{R}^d \to \mathbb{R}$. Let us define

$$u(x,t) = \mathbb{E}\left[\mathrm{e}^{-\int_t^T h(X_s)ds} g(X_T) \middle| X_t = x\right], \quad x \in \mathbb{R}^d, \quad t \in [0,T]. \tag{11}$$

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Proposition

The function u in (11) *solves the PDE*

$$\begin{aligned} \frac{\partial u}{\partial t} + \mathcal{L}u = h, \quad 0 \le t < T, \\ u(x,T) = g, \quad t = T \end{aligned} \tag{12}$$

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Proof.

- Show $u(x,t) = \mathbb{E}\left[\mathrm{e}^{-\int_t^{t'} h(X_s)ds} u(X_{t'}, t') \middle| X_t = x\right]$, for $t \le t' \le T$.
- Apply Ito's formula to $\mathrm{e}^{-\int_t^{t'} h(X_s)ds} u(X_{t'}, t')$.

□

Exit time

Consider a bounded domain $D \subseteq \mathbb{R}^d$. Define

$$\omega(x) = \mathbb{E}\left[g(X_{\tau_D}) + \int_0^{\tau_D} h(X_s) ds \middle| X_0 = x \right], \quad x \in D. \tag{13}$$

where

$$\tau_D = \inf\{t \geq 0, X_t \in \partial D\} \tag{14}$$

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Proof.

Apply Ito's formula to the solution to (15) up to time $t = \tau_D$. □

Concrete SDEs

Brownian dynamics

- $V : \mathbb{R}^d \to \mathbb{R}$ is smooth, and $\beta > 0$ is a constant.

$$dX_t = -\nabla V(X_t)\, dt + \sqrt{2\beta^{-1}} dB_t\,, \quad t > 0$$

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- Its generator is

$$\mathcal{L}g = -\nabla V \cdot \nabla g + \frac{1}{\beta}\Delta g\,.$$

- The adjoint of $\mathcal{L}$ is

$$\mathcal{L}^\top g = \mathrm{div}(\nabla V g) + \frac{1}{\beta}\Delta g\,.$$

Brownian dynamics

Definition (Boltzmann distribution)

$$\pi(x) = \frac{1}{Z} \mathrm{e}^{-\beta V(x)}, \quad x \in \mathbb{R}^d, \tag{16}$$

where $Z = \int_{\mathbb{R}^d} \mathrm{e}^{-\beta V(x)}\, dx$, such that $\int_{\mathbb{R}^d} \pi(x) dx = 1$.

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Proposition

The probability density π *in* (16) *is invariant under the Brownian dynamics*

$$dX_t = -\nabla V(X_t)\, dt + \sqrt{2\beta^{-1}} dB_t\,, \quad t > 0\,.$$

Ornstein-Unlenbeck process

When $V(x) = \frac{\kappa|x|^2}{2}$, the Brownian dynamics is

$$dX_t = -\kappa X_t \, dt + \sqrt{2\beta^{-1}} dB_t \,, \quad t > 0 \tag{17}$$

The invariant density is

$$\pi(x) = \frac{1}{Z} \mathrm{e}^{-\frac{\beta\kappa|x|^2}{2}} \,. \tag{18}$$

Langevin dynamics

- $V : \mathbb{R}^d \to \mathbb{R}$ is smooth, and $\beta, \gamma > 0$ is a constant.

$$
\begin{aligned}
dQ_t =& P_t dt \\
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- It corresponds to $dX_t = f(X_t)dt + \sigma(X_t)dB_t$ with $x = (q, p) \in \mathbb{R}^{2d}$, and

$$\begin{aligned} f(q,p) =& \big(p, -\nabla V(q) - \gamma p\big)^\top \in \mathbb{R}^{2d}, \\ \sigma =& \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{2\gamma\beta^{-1}} I_d \end{pmatrix} \in \mathbb{R}^{2d\times 2d} \,. \end{aligned} \tag{19}$$

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- In physics notation:

$$\frac{d^2 Q_t}{dt^2} = -\nabla V(Q_t)\, dt - \gamma \frac{dQ_t}{dt} dt + \sqrt{2\gamma\beta^{-1}} \frac{dB_t}{dt} \,.$$

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- Its adjoint is

$$\begin{aligned} \mathcal{L}^\top g &= -\operatorname{div}_q(pg) + \operatorname{div}_p(\nabla V g) + \gamma \operatorname{div}_p(pg) + \frac{\gamma}{\beta} \Delta_p g \\ &= -p \cdot \nabla_q g + \nabla V \cdot \nabla_p g + \gamma \operatorname{div}_p\Big(pg + \beta^{-1} \nabla_p g\Big) \,. \end{aligned}$$

Langevin dynamics

Definition (Hamiltonian)

Define the Hamiltonian

$$H(q, p) = V(q) + \frac{|p|^2}{2} . \quad (20)$$

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Proposition

The probability density $Z_1^{-1}\mathrm{e}^{-\beta H}$ is invariant under Langevin dynamics, where $Z_1 = \int_{\mathbb{R}^{2d}} \mathrm{e}^{-\beta H} dqdp$.

Questions?