Lecture 3: SDEs

2025–05–07

2.4 Invariant distribution

Assume that the probability density $X_0 = x$ is $\pi(x)$, where $\pi(x)$ is positive and $\int_{\mathbb{R}^d} \pi(x)dx = 1$. Then the probability density of X_t satisfies the Fokker-Planck equation

$$\begin{aligned} &\frac{\partial p}{\partial t} = \mathcal{L}^\top p\,, \quad t > 0\,, \\ &p(x,0) = \pi(x)\,. \end{aligned} \tag{2.1}$$

Definition 1. π is an invariant density, if $p(\cdot,t) = \pi$ for all $t \geq 0$.

From (2.1), we know that π is (smooth) invariant density if and only if

$$\mathcal{L}^\top \pi = 0\,. \tag{2.2}$$

In many cases, the process X_t approaches equilibrium as $t \to +\infty$. This means that its probability density converges to some limiting probability density p_∞, i.e. $\lim\limits_{t\to+\infty} p(x,t) = p_\infty(x)$.

Definition 2. 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 $t = 0$.

Theorem 1 (Birkhoff ergodic theorem)**.** Assume X_t is ergodic with respect to the invariant density π. Let $f : \mathbb{R}^d \to \mathbb{R}$ be a measurable function such that $\int_{\mathbb{R}^d} |f(x)|\pi(x)dx < \infty$. Then, with probability one, we have

$$\lim_{T\to+\infty} \frac{1}{T}\int_0^T f(X_t)dt = \int_{\mathbb{R}^d} f(x)\pi(x)dx\,. \tag{2.3}$$

Theorem 1 allows us to estimate the mean value with respect to density π by computing time average along the trajectory of X_t.

2.5 Feynman-Kac formula

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

$$u(x,t) = \mathbb{E}\Big[\mathrm{e}^{-\int_t^T h(X_s)ds} g(X_T)\Big| X_t = x\Big], \quad x \in \mathbb{R}^d, \quad t \in [0,T]\,. \tag{2.4}$$

Proposition 1. The function u in (2.4) solves the PDE

$$\begin{aligned} &\frac{\partial u}{\partial t} + \mathcal{L}u = h, \quad 0 \leq t < T\,, \\ &u(x,T) = g\,, \quad t = T \end{aligned} \tag{2.5}$$

Proof. Let us first show that

$$u(x,t) = \mathbb{E}\Big[\mathrm{e}^{-\int_t^{t'} h(X_s)ds} u(X_{t'},t')\Big| X_t = x\Big], \quad \forall t \le t' \le T\,. \tag{2.6}$$

In fact, using (2.4), we have

$$\begin{aligned} u(x,t) =& \mathbb{E}\Big[\mathrm{e}^{-\int_t^{T} h(X_s)ds} g(X_T)\Big| X_t = x\Big] \\ =& \mathbb{E}\Big[\mathrm{e}^{-\int_t^{t'} h(X_s)ds} \mathrm{e}^{-\int_{t'}^{T} h(X_s)ds} g(X_T)\Big| X_t = x\Big] \\ =& \mathbb{E}\Big[\mathbb{E}\Big[\mathrm{e}^{-\int_t^{t'} h(X_s)ds} \mathrm{e}^{-\int_{t'}^{T} h(X_s)ds} g(X_T)\Big| X_{t'}\Big]\Big| X_t = x\Big] \\ =& \mathbb{E}\Big[\mathrm{e}^{-\int_t^{t'} h(X_s)ds} u(X_{t'},t')\Big| X_t = x\Big]\,. \end{aligned} \tag{2.7}$$

Applying Ito's formula, we obtain

$$\begin{aligned} d\mathrm{e}^{-\int_t^{t'} h(X_s)ds} =& -h(X_{t'})\mathrm{e}^{-\int_t^{t'} h(X_s)ds} dt' \\ du(X_{t'},t') =& \Big(\frac{\partial u}{\partial t} + \mathcal{L}u\Big)(X_{t'},t')dt' + \nabla u(X_{t'},t')^\top \sigma(X_{t'})dB_{t'} \end{aligned} \tag{2.8}$$

Therefore,

$$\begin{aligned} & d\Big(\mathrm{e}^{-\int_t^{t'} h(X_s)ds} u(X_{t'},t')\Big) \\ =& d\Big(\mathrm{e}^{-\int_t^{t'} h(X_s)ds}\Big) u(X_{t'},t') + \Big(\mathrm{e}^{-\int_t^{t'} h(X_s)ds}\Big) du(X_{t'},t') \\ =& \mathrm{e}^{-\int_t^{t'} h(X_s)ds}\Big[\Big(-h(X_{t'}) + \frac{\partial u}{\partial t} + \mathcal{L}u\Big)(X_{t'},t')dt' + \nabla u(X_{t'},t')^\top \sigma(X_{t'})dB_{t'}\Big]\,. \end{aligned} \tag{2.9}$$

Integrating and taking expectation, we get

$$\begin{aligned} & \mathbb{E}\Big[\int_t^{t'} \mathrm{e}^{-\int_t^{s'} h(X_s)ds}\Big(-h(X_{s'}) + \frac{\partial u}{\partial t} + \mathcal{L}u\Big)(X_{s'},s')ds'\Big| X_t = x\Big] \\ =& \mathbb{E}\Big[\mathrm{e}^{-\int_t^{t'} h(X_s)ds} u(X_{t'},t')\Big| X_t = x\Big] - u(x,t) \\ =& 0\,, \end{aligned} \tag{2.10}$$

where the last equality follows from (2.6).

Since the above equality is true for all $t' \in [t,T]$, taking $t' = t$, we conclude that u solves the PDE (2.5). The terminal condition in (2.5) follows directly from (2.4). $\square$

Let us now consider a bounded domain $D \subseteq \mathbb{R}^d$. Define

$$\omega(x) = \mathbb{E}\Big[g(X_{\tau_D}) + \int_0^{\tau_D} h(X_s)ds\Big| X_0 = x\Big]\,, \quad x \in D\,. \tag{2.11}$$

where

$$\tau_D = \inf\{t \ge 0, X_t \in \partial D\} \tag{2.12}$$

is the exit time from D.

Proposition 2. The function ω in (2.11) solves the PDE

$$\begin{aligned} \mathcal{L}\omega &= -h\,, \quad \text{in } D \\ \omega &= g\,, \quad \text{on } \partial D\,. \end{aligned} \tag{2.13}$$

Proof. Assume that ω is the solution to (2.13) and $X_0 = x$. Applying Ito's formula, we have

$$\omega(X_t) - \omega(x) = \int_0^\top \mathcal{L}\omega(X_s)ds + \int_0^\top \nabla\omega(X_s)^\top \sigma(X_s)dB_s\,. \tag{2.14}$$

Choosing $t = \tau_D$ and taking expectation in the identity above, we get

$$\begin{aligned} \omega(x) =& \mathbb{E}\Big(\omega(X_{\tau_D}) - \int_0^{\tau_D} \mathcal{L}\omega(X_s)ds \Big| X_0 = x\Big) \\ =& \mathbb{E}\Big(g(X_{\tau_D}) + \int_0^{\tau_D} h(X_s)ds \Big| X_0 = x\Big) \end{aligned} \tag{2.15}$$

□

2.6 Brownian dynamics and Langevin equation

Let $V : \mathbb{R}^d \to \mathbb{R}$ be a smooth function. We consider the Brownian dynamics

$$dX_t = -\nabla V(X_t)\,dt + \sqrt{2\beta^{-1}}dB_t\,, \quad t > 0 \tag{2.16}$$

where $\beta > 0$ is a constant.

Its generator is

$$\mathcal{L}g = -\nabla V \cdot \nabla g + \frac{1}{\beta}\Delta g\,. \tag{2.17}$$

And the adjoint of $\mathcal{L}$ is

$$\mathcal{L}^\top g = \mathrm{div}(\nabla V g) + \frac{1}{\beta}\Delta g = \mathrm{div}(\nabla V g + \beta^{-1}\nabla g)\,. \tag{2.18}$$

Definition 3 (Boltzmann distribution)**.** The density of Boltzmann distribution is

$$\pi(x) = \frac{1}{Z}\mathrm{e}^{-\beta V(x)}, \quad x \in \mathbb{R}^d, \tag{2.19}$$

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

Proposition 3. The probability density π in (2.19) is invariant under the Brownian dynamics.

Proof. Using (2.18), it is easy to see that

$$\mathcal{L}^\top \pi = Z^{-1}\mathrm{div}(\nabla V \mathrm{e}^{-\beta V(x)} + \beta^{-1}\nabla \mathrm{e}^{-\beta V(x)}) = 0.$$

Therefore, π is invariant. $\square$

In fact, under certain conditions on V, the process X_t is ergodic with respect to the Boltzmann distribution.

Example (Ornstein-Unlenbeck process)**.** When $V(x) = \frac{\kappa|x|^2}{2}$. The SDE is

$$dX_t = -\kappa X_t \, dt + \sqrt{2\beta^{-1}} dB_t \,, \quad t > 0 \tag{2.20}$$

The invariant density is

$$\pi(x) = \frac{1}{Z} \mathrm{e}^{-\frac{\beta\kappa|x|^2}{2}} \,. \tag{2.21}$$

Next, let us consider the Langevin dynamics:

$$\begin{aligned} dQ_t =& P_t dt \\ dP_t =& -\nabla V(Q_t)\, dt - \gamma P_t dt + \sqrt{2\gamma\beta^{-1}} dB_t \,. \end{aligned} \tag{2.22}$$

This corresponds to the SDE in the general form with

$$x = (q,p) \in \mathbb{R}^{2d}, \quad f(q,p) = \big(p, -\nabla V(q) - \gamma p\big)^\top \in \mathbb{R}^{2d}, \quad \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{2\gamma\beta^{-1}} I_d \end{pmatrix} \in \mathbb{R}^{2d \times 2d} \,. \tag{2.23}$$

The generator is

$$\mathcal{L} g = p \cdot \nabla_q g - \nabla V \cdot \nabla_p g - \gamma p \cdot \nabla_p g + \frac{\gamma}{\beta} \Delta_p g \,. \tag{2.24}$$

Its adjoint is

$$\begin{aligned} \mathcal{L}^\top g =& -\mathrm{div}_q(pg) + \mathrm{div}_p(\nabla V g) + \gamma \mathrm{div}_p(pg) + \frac{\gamma}{\beta}\Delta_p g \\ =& -p \cdot \nabla_q g + \nabla V \cdot \nabla_p g + \gamma \mathrm{div}_p \Big(pg + \beta^{-1} \nabla_p g\Big) \,. \end{aligned} \tag{2.25}$$

Definition 4 (Hamiltonian)**.** Define the Hamiltonian

$$H(q,p) = V(q) + \frac{|p|^2}{2} \,. \tag{2.26}$$

Proposition 4. The probability density $Z_1^{-1} \mathrm{e}^{-\beta H}$ is invariant under the Langevin dynamics (2.22), where $Z_1 = \int_{\mathbb{R}^{2d}} \mathrm{e}^{-\beta H} dq dp$ is the normalizing constant.

Proof. Using (2.25) and (2.26), we compute

$$\mathcal{L}^\top \mathrm{e}^{-\beta H} = -p \cdot \nabla_q \mathrm{e}^{-\beta H} + \nabla V \cdot \nabla_p \mathrm{e}^{-\beta H} + \gamma \mathrm{div}_p \Big(p \mathrm{e}^{-\beta H} + \beta^{-1} \nabla_p \mathrm{e}^{-\beta H} \Big) = 0 \,.$$

$\square$