Lecture 19 Rare Events: I *

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1 Metastability and transition events

Consider the diffusion process defined by

$$d\boldsymbol{X}_t^\varepsilon = -\nabla U(\boldsymbol{X}_t^\varepsilon)dt + \sqrt{\varepsilon}d\boldsymbol{W}_t \tag{1}$$

where $\boldsymbol{W}_t$ is the standard multi-dimensional Wiener process, $U(\boldsymbol{x})$ is assumed to be a smooth Morse function, i.e. the critical points of U are non-degenerate in the sense that the Hessian matrices at the critical points are non-degenerate. When $\varepsilon = 0$, for generic initial conditions, the solution of this ODEs converges to a local minimum of the potential function U. For each local minimum, the set of initial conditions from which the solutions of the ODEs converge to that local minimum is the *basin of attraction* of that local minimum. The whole configuration space is then divided into the union of the different basins of attraction. The boundaries of the basins of the attraction are the separatrices, which are themselves invariant sets of the deterministic dynamics. In particular, each local minimum is stable under the dynamics.

When ε is positive but small, on $O(1)$ time scale, the picture just described still pretty much holds. In particular, with overwhelming probability, the solution to the SDEs will stay within the basin of attraction of a local minimum. However, as we discuss below, on exponentially large time scales in $O(1/\varepsilon)$, the solution will hop over from one basin of attraction to another, giving rise to a noise-induced instability. Such hopping events are the rare events we are interested in.

The above picture can be best illustrated in the following one dimensional example (see Figure

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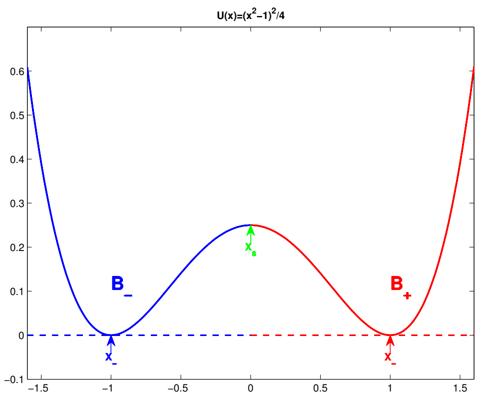
1) with the double-well potential

$$U(x) = \frac{1}{4}(x^2 - 1)^2. \tag{2}$$

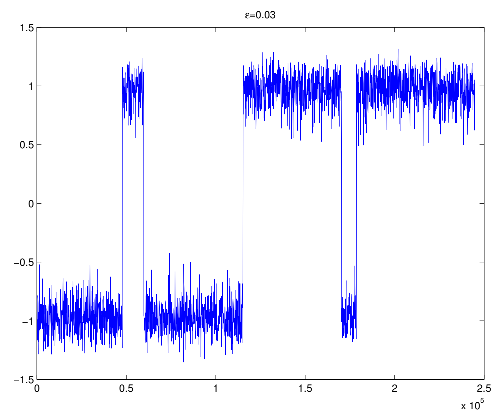
The potential U has two local minima at $x_+ = 1$ and $x_- = -1$, and one saddle at $x_s = 0$. x_s is also called the transition state between x_+ and x_-. Thus we have two basins of attraction

$$B_- = \{x|\ x \le 0\} \quad \text{and} \quad B_+ = \{x|\ x \ge 0\}.$$

Most of time, X_t wanders around x_+ or x_-. But after exponentially large time scales in $O(1/\varepsilon)$, X_t^ε hops between the regions B_+ and B_-, which manifests basic features of rare events.



(a) Potential function $U(x)$



(b) A typical trajectory of X_t

Figure 1: Illustration of rare events in the 1D double-well potential. Left panel: The symmetric double-well potential with two metastable states at $x_+ = 1$ and $x_- = -1$. Right panel: A specific trajectory of X_t, which wanders around x_+ or x_- and hops after a sufficiently long time.

In physical terms, the local minima or the basin of attractions are called metastable states. Obviously, when we discuss metastability, the key issue is that of the time scale. In rare event studies, one is typically concerned about the following three key questions:

1. What is the most probable transition path and how to compute it? When the dimension of X_t^ε is bigger than 1, this becomes a meaningful question.

2. Where is the transition state, i.e. the neighboring saddle point, for a transition event starting from a metastable state? Presumably the saddle points can be identified from the eigenvalue

analysis of the Hessian of U. However, when the dimension is high and the landscape of U is complex, it is not trivial.

3. How large is the typical transition time from a metastable state? Answer of this question helps understanding the stability of a metastable state, which corresponds to the key time scale issue.

We will present some recent methodologies in the literature to answer these questions.

2 WKB Analysis

Consider the SDEs

$$d\boldsymbol{X}_t^\varepsilon = \boldsymbol{b}(\boldsymbol{X}_t^\varepsilon)dt + \sqrt{\varepsilon}\boldsymbol{\sigma}(\boldsymbol{X}_t^\varepsilon) \cdot d\boldsymbol{W}_t, \qquad \boldsymbol{X}_0^\varepsilon = \boldsymbol{y} \in \mathbb{R}^d. \tag{3}$$

We assume that the standard Lipschitz and uniform ellipticity conditions on $\boldsymbol{b}$ and $\boldsymbol{\sigma}$ hold and denote the transition pdf by $p_\varepsilon(\boldsymbol{x}, t|\boldsymbol{y})$. We are interested in the behavior of its solution for small ε. Let $\boldsymbol{X}_t^0$ be the solution of the deterministic ODEs

$$\dot{\boldsymbol{X}}_t^0 = \boldsymbol{b}(\boldsymbol{X}_t^0), \qquad \boldsymbol{X}_0^0 = \boldsymbol{y}.$$

It can be shown that (cf. [3] for reference) for any fixed $T > 0$ and $\delta > 0$, we have the law of large numbers for the processes $\boldsymbol{X}^\varepsilon$

$$\lim_{\varepsilon \to 0} \mathbb{P}\left(\max_{t \in [0,T]} |\boldsymbol{X}_t^\varepsilon - \boldsymbol{X}_t^0| > \delta \right) = 0.$$

This implies that for any open set $B \subset \mathbb{R}^d$, we have

$$\lim_{\varepsilon \to 0} \int_B p_\varepsilon(\boldsymbol{x}, t|\boldsymbol{y}) d\boldsymbol{x} = \begin{cases} 1, & \text{if } \boldsymbol{X}_t^0 \in B, \\ 0, & \text{otherwise,} \end{cases}$$

or equivalently $\lim_{\varepsilon \to 0} p_\varepsilon(\boldsymbol{x}, t|\boldsymbol{y}) = \delta(\boldsymbol{x} - \boldsymbol{X}_t^0)$.

Inspired by the form of probability distribution function of Brownian dynamics, we insert the

Wentzel-Kramers-Brillouin (WKB) ansatz

$$p_\varepsilon(\boldsymbol{x}, t|\boldsymbol{y}) \sim \exp\left(-\varepsilon^{-1}\phi(\boldsymbol{x}, t|\boldsymbol{y})\right)$$

into the forward Kolmogorov equation associated with the SDEs (3)

$$\frac{\partial p_\varepsilon}{\partial t} = -\nabla \cdot (\boldsymbol{b}(\boldsymbol{x})p_\varepsilon) + \frac{\varepsilon}{2}\nabla^2 : (\boldsymbol{A}(\boldsymbol{x})p_\varepsilon). \tag{4}$$

where $\boldsymbol{A}(\boldsymbol{x}) = \boldsymbol{\sigma}\boldsymbol{\sigma}^T(\boldsymbol{x}) = (a_{ij}(\boldsymbol{x}))$ is the diffusion matrix. Collecting the leading order terms gives a time-dependent Hamilton-Jacobi equation

$$\frac{\partial \phi}{\partial t} = H(\boldsymbol{x}, \nabla_{\boldsymbol{x}}\phi), \tag{5}$$

where H is the Hamiltonian with the form

$$H(\boldsymbol{x}, \boldsymbol{p}) = \boldsymbol{b}^T(\boldsymbol{x})\boldsymbol{p} + \frac{1}{2}\boldsymbol{p}^T\boldsymbol{A}(\boldsymbol{x})\boldsymbol{p} = \sum_i b_i p_i + \frac{1}{2}\sum_{ij} a_{ij}p_i p_j. \tag{6}$$

We will call $\boldsymbol{p}$ the momentum variable for its formal correspondence in classical mechanics [1,4]. The solution of this equation can be characterized by the variational principle:

$$\phi(\boldsymbol{x}, t|\boldsymbol{y}) = \inf_{\boldsymbol{\varphi}} \left\{ I_t[\boldsymbol{\varphi}] : \boldsymbol{\varphi} \text{ is absolutely continuous in } [0,t] \text{ and } \boldsymbol{\varphi}(0) = \boldsymbol{y}, \boldsymbol{\varphi}(t) = \boldsymbol{x} \right\}, \tag{7}$$

where I_t is the action functional

$$I_t[\boldsymbol{\varphi}] = \int_0^t L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}})ds \tag{8}$$

and L is called the Lagrangian

$$L(\boldsymbol{x}, \boldsymbol{z}) = \frac{1}{2}\|\boldsymbol{z} - \boldsymbol{b}(\boldsymbol{x})\|^2_{\boldsymbol{A}} \tag{9}$$

where the norm $\|\boldsymbol{z}\|^2_{\boldsymbol{A}} := \boldsymbol{z}^T\boldsymbol{A}^{-1}\boldsymbol{z}$. The Lagrangian L is the dual of the Hamiltonian H in the sense of Legendre-Fenchel transform

$$L(\boldsymbol{x}, \boldsymbol{z}) = \sup_{\boldsymbol{p}}\{\boldsymbol{p} \cdot \boldsymbol{z} - H(\boldsymbol{x}, \boldsymbol{p})\}.$$

The readers may be referred to [1, 4] for more details about the variational derivations about the above connections.

3 Large Deviations and Transition Paths

The WKB analysis in Chapter 2 has given us the intuition that the probability

$$\mathbb{P}(\boldsymbol{X}_t^\varepsilon \in B) \asymp \exp(-\varepsilon^{-1}C) \quad \text{as } \varepsilon \to 0,$$

where B is an open set, and the symbol $\asymp$ means exponential equivalence, i.e. we have $\lim_{\varepsilon\to 0} \varepsilon \ln A_\varepsilon/B_\varepsilon = 1$ if $A_\varepsilon \asymp B_\varepsilon$. The constant C will be positive if $\boldsymbol{x}(t) \notin B$, and 0 otherwise. Indeed this large deviation type estimate is rigorously true, and even hold for the SDEs (3) in path space $C[0, T]$.

First let us quote the large deviation result for the SDEs [2, 5].

Theorem 1. *Under the condition that $\boldsymbol{b}(\boldsymbol{x})$ and $\boldsymbol{\sigma}(\boldsymbol{x})$ is bounded and Lipschitz, and $\boldsymbol{A}(\boldsymbol{x})$ is uniformly elliptic, we have that for any $T > 0$, the following large deviation estimates for $\boldsymbol{X}^\varepsilon$ defined in* (3) *hold.*

(i) Upper bound. For any closed set $F \subset (C[0, T])^d$,

$$\limsup_{\varepsilon\to 0} \varepsilon \ln \mathbb{P}(\boldsymbol{X}^\epsilon \in F) \leq -\inf_{\boldsymbol{\varphi}\in F} I_T[\boldsymbol{\varphi}].$$

(ii) Lower bound. For any open set $G \subset (C[0, T])^d$,

$$\liminf_{\varepsilon\to 0} \varepsilon \ln \mathbb{P}(\boldsymbol{X}^\epsilon \in G) \geq -\inf_{\boldsymbol{\varphi}\in G} I_T[\boldsymbol{\varphi}].$$

Here $I_T[\boldsymbol{\varphi}]$ is the rate functional defined in (8)-(9) *if $\boldsymbol{\varphi}$ is absolutely continuous with square integrable $\dot{\boldsymbol{\varphi}}$ and satisfies $\boldsymbol{\varphi}(0) = \boldsymbol{y}$, otherwise $I_T[\boldsymbol{\varphi}] = \infty$.*

The proof of Theorem 1 is beyond the scope of this book. However we will give a formal derivation by path integral approach. It is straightforward that the one-dimensional SDE

$$dX_t^\varepsilon = \sqrt{\varepsilon} dW_t, \qquad X_0 = 0$$

has solution $X_t^\varepsilon = \sqrt{\varepsilon} W_t$. Using the path integral representation, the probability distribution induced by $\{X_t^\varepsilon\}$ on $C[0,T]$ can be formally written as

$$dP^\varepsilon[\varphi] = Z^{-1} \exp\left(-\frac{1}{2\varepsilon}\int_0^T |\dot\varphi(s)|^2 ds\right) D\varphi = Z^{-1} \exp\left(-\frac{1}{\varepsilon} I_T[\varphi]\right) D\varphi \tag{10}$$

Note that $I_T[\varphi]$ can be $+\infty$ if φ is not absolutely continuous and square integrable or does not satisfy the corresponding initial condition. Then let us consider the stochastic ODE

$$dX_t^\varepsilon = b(X_t^\varepsilon)dt + \sqrt{\varepsilon}\sigma(X_t^\varepsilon)dW_t, \qquad X_0 = y.$$

We are interested in the asymptotic behavior of the probability distribution P^ε induced by $\{X_t^\varepsilon\}$. To understand how the action functional I_T has the form (8)-(9), we can reason formally as follows. From the SDE we have $\dot W_t = (\sqrt{\varepsilon})^{-1}\sigma^{-1}(X_t^\varepsilon)(\dot X_t^\varepsilon - b(X_t^\varepsilon))$. Hence

$$\int_0^T \dot W_t^2 dt = \varepsilon^{-1} \int_0^T |\sigma^{-1}(X_t^\varepsilon)(\dot X_t^\varepsilon - b(X_t^\varepsilon)|^2 dt.$$

From the distribution (10) induced by $\sqrt{\varepsilon} W_t$, we obtain

$$dP^\varepsilon[\varphi] = Z^{-1} \exp\left(-\frac{1}{\varepsilon} I_T[\varphi]\right) D\varphi,$$

where $I_T[\varphi]$ is finite if φ is absolutely continuous with square integrable $\dot\varphi$ and satisfies $\varphi(0) = y$, and $I_T[\varphi] = \infty$ otherwise.

Based on Theorem 1 and Varadhan's lemma, we have the asymptotics

$$-\varepsilon \log P^\varepsilon(\mathcal{B}) \sim \inf_{\varphi\in\mathcal{B}} I_T[\varphi], \quad \varepsilon \to 0$$

for a reasonable set $\mathcal{B}$ in $C[0,T]$. This motivates a natural characterization of the most probable transition paths in the limit $\varepsilon \to 0$. Given a set of path $\mathcal{B}$ in $C[0,T]$ we can define the optimal path in $\mathcal{B}$ as the path $\varphi^\star$ that has the maximum probability or minimal action

$$\inf_{\varphi\in\mathcal{B}} I_T(\varphi) = I_T(\varphi^\star),$$

if this minimization problem has a solution. Such a path is called a *minimum (or least) action path.*

The minimum action path has special features in case that $\boldsymbol{b}(\boldsymbol{x}) = -\nabla U(\boldsymbol{x})$ and $\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{I}$. Assume that A and B are two neighboring metastable states of U separated by the saddle point C. Define $\mathcal{B} = \{\boldsymbol{\varphi} : \boldsymbol{\varphi} \in (C[0,T])^d, \boldsymbol{\varphi}(0) = A, \boldsymbol{\varphi}(T) = B\}$. We are interested in the minimum action path $\boldsymbol{\varphi} \in \mathcal{B}$ and let the transition time T to be free

$$\inf_{T>0} \inf_{\boldsymbol{\varphi}(0)=A, \boldsymbol{\varphi}(T)=B} I_T[\boldsymbol{\varphi}]. \tag{11}$$

We have the following characterizations.

Lemma 2. *The minimum action path* $\boldsymbol{\varphi}$ *of the Brownian dynamics is comprised of two parts defined through functions* $\boldsymbol{\varphi}_1$ *and* $\boldsymbol{\varphi}_2$ *as*

$$\dot{\boldsymbol{\varphi}}_1(s) = \nabla U(\boldsymbol{\varphi}_1(s)), \quad \boldsymbol{\varphi}_1(-\infty) = A, \boldsymbol{\varphi}_1(\infty) = C, \tag{12}$$

$$\dot{\boldsymbol{\varphi}}_2(s) = -\nabla U(\boldsymbol{\varphi}_2(s)), \quad \boldsymbol{\varphi}_2(-\infty) = C, \boldsymbol{\varphi}_2(\infty) = B, \tag{13}$$

and the minimum action is achieved as

$$I^* = I_\infty(\boldsymbol{\varphi}_1) + I_\infty(\boldsymbol{\varphi}_2) = I_\infty(\boldsymbol{\varphi}_1) = 2(U(C) - U(A)) = 2\Delta U_{AB}. \tag{14}$$

Proof. It is not difficult to convince oneself that the minimum in T in (11) is attained when $T = \infty$ since A, B and C are all critical points (see Exercise 1). To see why the minimization problem in (11) is solved by the path defined above, we first note that

$$I_\infty[\boldsymbol{\varphi}_1] = 2\Delta U_{AB}, \quad I_\infty[\boldsymbol{\varphi}_2] = 0. \tag{15}$$

In addition, for any path $\boldsymbol{\varphi}$ connecting A and a point $\tilde{C}$ on the separatrix that separates the basins of attraction of A and B, we have

$$\begin{aligned} I_\infty[\boldsymbol{\varphi}] &= \frac{1}{2}\int_{\mathbb{R}} (\dot{\boldsymbol{\varphi}} - \nabla U, \dot{\boldsymbol{\varphi}} - \nabla U)dt + 2\int_{\mathbb{R}} \dot{\boldsymbol{\varphi}} \cdot \nabla U dt \\ &\geq 2\int_{\mathbb{R}} \dot{\boldsymbol{\varphi}} \cdot \nabla U dt = 2(U(\tilde{C}) - U(A)) \geq 2\Delta U_{AB} \end{aligned}$$

since C is the minimum of U on the separatrix. Combing the result above we obtain the minimum

$I^* = 2\Delta U_{AB}$. $\square$

Thus the most probable transition path is then the combination of $\boldsymbol{\varphi}_1$ and $\boldsymbol{\varphi}_2$: $\boldsymbol{\varphi}_1$ goes along the steepest *ascent* dynamics and therefore requires the action of the noise. $\boldsymbol{\varphi}_2$ simply follows the steepest *descent* dynamics and therefore does not require the help from the noise. Putting them together we obtain the characterization for the most probable transition path of Brownian dynamics

$$\dot{\boldsymbol{\varphi}}(s) = \pm\nabla U(\boldsymbol{\varphi}(s)). \tag{16}$$

Paths that satisfy this equation are called the *minimum energy path* (MEP). One can write (16) as:

$$\Big(\nabla U(\boldsymbol{\varphi})\Big)^{\perp} = 0, \tag{17}$$

where $(\nabla U(\boldsymbol{\varphi}))^{\perp}$ denotes the component of $\nabla U(\boldsymbol{\varphi})$ normal to the curve described by $\boldsymbol{\varphi}$.

Exercises

1. Prove that for absolutely continuous $\boldsymbol{\varphi}$ on $[0,T]$, the variational minimization

$$\inf_{T>0} \inf_{\boldsymbol{\varphi}(0)=\boldsymbol{y},\boldsymbol{\varphi}(T)=\boldsymbol{x}} I_T[\boldsymbol{\varphi}] = \inf_{\boldsymbol{\varphi}(0)=\boldsymbol{y},\boldsymbol{\varphi}(\infty)=\boldsymbol{x}} I_\infty[\boldsymbol{\varphi}],$$

where $I_T[\boldsymbol{\varphi}]$ is defined in (8)-(9), and $\boldsymbol{x}$ is a stationary point, i.e. $\boldsymbol{b}(\boldsymbol{x}) = \mathbf{0}$.

References

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