Lecture 20. Rare Events

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Metastability and transition events

Consider the diffusion process defined by

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

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.

Schematics of metastability and transitions

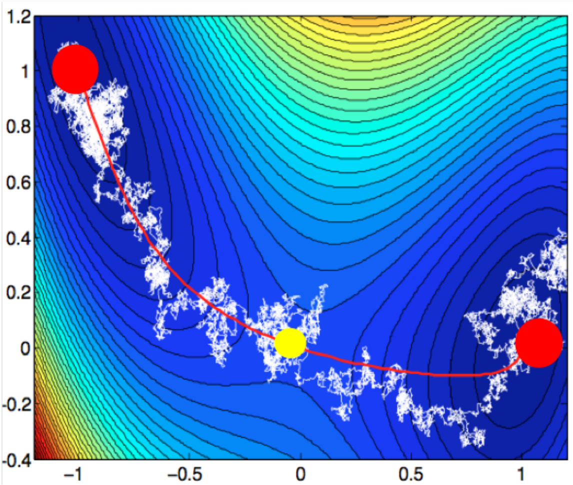

Figure: Schematics of the metastability phenomenon

Gradient system: ODE case

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- 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.

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- 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.

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- 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.

Metastability: 1D example

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$$B_- = \{x|\ x \leq 0\} \quad \text{and} \quad B_+ = \{x|\ x \geq 0\}.$$

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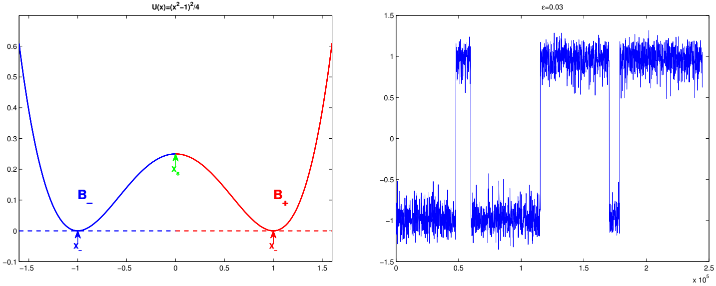
$$B_- = \{x |\ x \leq 0\} \quad \text{and} \quad B_+ = \{x |\ x \geq 0\}.$$
- Most of time, X_t wanders around x_+ or x_-. But after exponentially large time scales in $O(1/\varepsilon)$, X_t^ε hops between the regions B_+ and B_-, which manifests basic features of rare events.

Metastability: 1D example



(a) Potential function $U(x)$ (b) A typical trajectory of X_t

Figure: 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.

Metastability: key questions

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.

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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.

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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.

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- Consider the SDEs

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

  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.

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Law of Large Numbers

- Let $\boldsymbol{X}_t^0$ be the solution of the deterministic ODEs

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- It can be shown that for any fixed $T > 0$ and $\delta > 0$, we have the law of large numbers for the processes $\boldsymbol{X}^\varepsilon$

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

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- Further detailed analysis on the behavior of the pdf is studied below.

WKB analysis

- 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

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

  where $\boldsymbol{A}(\boldsymbol{x}) = \boldsymbol{\sigma}\boldsymbol{\sigma}^T(\boldsymbol{x}) = (a_{ij}(\boldsymbol{x}))$ is the diffusion matrix.

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- Collecting the leading order terms gives a time-dependent Hamilton-Jacobi equation

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

  where H is the Hamiltonian with the form

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

Hamilton-Jacobi Theory

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

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

where I_t is the action functional

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

and L is called the Lagrangian

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

where the norm $\|\boldsymbol{z}\|_{\boldsymbol{A}}^2 := \boldsymbol{z}^T \boldsymbol{A}^{-1} \boldsymbol{z}$.

Lagrangian and Hamiltonian

- The Lagrangian L is the dual of the Hamiltonian H in the sense of Legendre-Fenchel transform

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

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- The readers may be referred to
  H. Goldstein, *Classical mechanics*,
  V. I. Arnold, *Mathematical methods of classical mechanics*
  for more details about the variational derivations about the above connections.

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Implications of WKB results

- The WKB analysis 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.

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- This large deviation type estimate is even true in path space $C[0, T]$.

Large deviations on path space

First let us quote the large deviation result for the SDEs.

Theorem

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 $\boldsymbol{X}^\varepsilon$.

(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 $G \subset (C[0,T])^d$,*

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

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  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

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

  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.

Large deviations for SDEs

- Then let us consider the stochastic ODE

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

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  We are interested in the asymptotic behavior of the probability distribution P^ε induced by $\{X_t^\varepsilon\}$.
- 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 $dP^\varepsilon[\varphi]$ 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.

Rate functional

Based on the theorem above 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 $C[0,T]$.

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- 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

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

Minimum action path

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- 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

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

We have the following characterizations.

Minimum action/energy path

Lemma

The minimum action path φ of the Brownian dynamics is comprised of two parts defined through functions φ_1 and φ_2 as

$$\dot{\varphi}_1(s) = \nabla U(\varphi_1(s)), \quad \varphi_1(-\infty) = A, \varphi_1(\infty) = C,$$

$$\dot{\varphi}_2(s) = -\nabla U(\varphi_2(s)), \quad \varphi_2(-\infty) = C, \varphi_2(\infty) = B,$$

and the minimum action is achieved as

$$I^* = I_\infty(\varphi_1) + I_\infty(\varphi_2) = I_\infty(\varphi_1) = 2(U(C) - U(A)) = 2\Delta U_{AB}.$$

Minimum action path: Proof

Proof.

It is not difficult to convince oneself that the minimum in T is attained when $T = \infty$ since A, B and C are all critical points (see Exercise 13.1). To see why the minimization problem in is solved by the path defined above, we first note that

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

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

Minimum energy path (MEP)

- Thus the most probable transition path is then the combination of φ_1 and φ_2: φ_1 goes along the steepest *ascent* dynamics and therefore requires the action of the noise. φ_2 simply follows the steepest *descent* dynamics and therefore does not require the help from the noise.

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Paths that satisfy this equation are called the *minimum energy path* (MEP).

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

$$\big(\nabla U(\varphi)\big)^{\perp} = 0,$$

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

Minimum energy path (MEP)

Question: How to compute the MEP for complicate systems?

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- The equation looks quite reasonable. Is it really true that the trajectory will converge to the solution of the steady equation $(\nabla U(\boldsymbol{\varphi}))^{\perp} = 0$?
- The naive pseudo-steepest descent flow is not good for numerics!

String Method

- A modified form better for numerical implementation

$$\partial_t \boldsymbol{\varphi}(\alpha, t) = -(\nabla U(\boldsymbol{\varphi}))^{\perp} + r\hat{\boldsymbol{\tau}}, \qquad \boldsymbol{\varphi}(0) = A, \boldsymbol{\varphi}(1) = B.$$

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- $\boldsymbol{\varphi}(\alpha, t)$ is parametric curve of $\alpha \in (0,1)$, $\hat{\boldsymbol{\tau}} = \boldsymbol{\varphi}_\alpha / |\boldsymbol{\varphi}_\alpha|$, and

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$$(\nabla U(\boldsymbol{\varphi}))^{\perp} = \nabla U(\boldsymbol{\varphi}) - (\hat{\boldsymbol{\tau}} \otimes \hat{\boldsymbol{\tau}}) \cdot \nabla U(\boldsymbol{\varphi}).$$

- r is just a Lagrange multiplier to ensure the equi-arclength parameterization:

$$(|\boldsymbol{\varphi}_\alpha|)_\alpha = 0.$$

String Method

- A modified form better for numerical implementation

$$\partial_t \boldsymbol{\varphi}(\alpha, t) = -(\nabla U(\boldsymbol{\varphi}))^{\perp} + r\hat{\boldsymbol{\tau}}, \qquad \boldsymbol{\varphi}(0) = A, \boldsymbol{\varphi}(1) = B.$$

- $\boldsymbol{\varphi}(\alpha, t)$ is parametric curve of $\alpha \in (0, 1)$, $\hat{\boldsymbol{\tau}} = \boldsymbol{\varphi}_\alpha / |\boldsymbol{\varphi}_\alpha|$, and

$$(\nabla U(\boldsymbol{\varphi}))^{\perp} = \nabla U(\boldsymbol{\varphi}) - (\hat{\boldsymbol{\tau}} \otimes \hat{\boldsymbol{\tau}}) \cdot \nabla U(\boldsymbol{\varphi}).$$

- r is just a Lagrange multiplier to ensure the equi-arclength parameterization:

$$(|\boldsymbol{\varphi}_\alpha|)_\alpha = 0.$$

- Note that the term $r\hat{\boldsymbol{\tau}}$ is not necessary for the evolution of a continuous path $\boldsymbol{\varphi}$, and the equi-arclength parameterization can be also replaced by other choices. This is called *String Method* in the literature.

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   - Define $s_0 = 0$, $s_i = s_{i-1} + |\tilde{\boldsymbol{\varphi}}_i^n - \tilde{\boldsymbol{\varphi}}_{i-1}^n|$ for $i = 1, \ldots, N$, and $\tilde{\alpha}_i = s_i / s_N$.

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With such implementation, the boundary states can be chosen close to A and B instead of knowing their exact locations.

Illustration of String Method

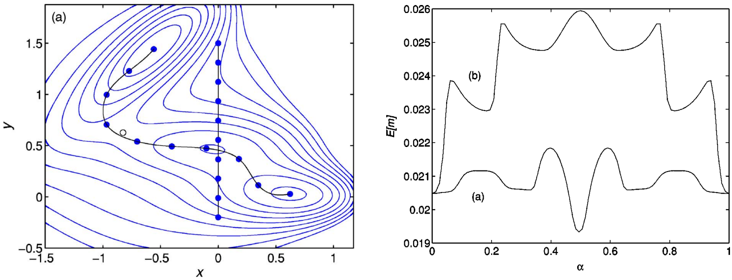

Figure: Applied to Mueller potential (left) and micromagnetic switching (right).

- Left panel: The calculated MEP and initial string (the vertical straight line).
- Right panel: Magnetic energy along two transition paths found by string method with different initial values.
- The path (a) costs lower action than path (b).

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Assume that $U(x)$ has two local minima at $x_A = -1$, $x_B = 1$ and a local maximum, also a saddle point, at $x_C = 0$. Consider diffusion in domain $D = [a, b]$ with reflecting and absorbing boundaries at a and b, respectively.

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- Then we derive equation for $\tau(x)$ using the probability remaining in $[a, b)$.

Equation for Mean First Passage Time

- The probability remaining in $[a, b)$ at time t has the form

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- Applying $\mathcal{L}$ to both sides, we get

$$\begin{aligned}\mathcal{L}\tau(x) &= \int_0^\infty \mathcal{L}R(x,t)dt = \int_0^\infty \int_a^b \partial_t p(y,t|x,0)dydt \\ &= \int_a^b p|_{t=\infty} - p|_{t=0}dy = -\int_a^b \delta(x-y)dy = -1.\end{aligned}$$

Mean First Passage Time (MFPT)

- From the boundary conditions for the backward equation, we have $R(x,t)|_{x=b} = 0$ and $\partial_x R(x,t)|_{x=a} = 0$, which implies the boundary conditions for $\tau(x)$:

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- It has the solution

$$\tau(x) = \frac{1}{\epsilon}\int_x^b e^{\frac{U(y)}{\varepsilon}} \int_a^y e^{-\frac{U(z)}{\varepsilon}} dz dy.$$

MFPT in Zero-Temperature Limit

- Take $a \to -\infty$, $b \to x_B$ and $x = x_A$, thus obtain

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- Define the function $F(y,z) = U(y) - U(z)$ on the domain

$$S = \{(y,z) : y \in [x_A, x_B] \text{ and } z \in (-\infty, y] \text{ for any } y\}.$$

We have

$$\max_{(y,z)\in S} F(y,z) = \Delta U_{AB} = U(x_C) - U(x_A)$$

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- With Laplace asymptotics in the 2D domain S, we have

$$\tau(x) \approx \tau(x_A) \sim \frac{2\pi}{\sqrt{|U''(x_C)|U''(x_A)}} e^{\frac{\Delta U_{AB}}{\varepsilon}}$$

  for any $x \leq x_C - \delta_0$, where δ_0 is a positive constant. We implicitly require that $U''(x_A)$ and $|U''(x_C)|$ are positive.

1D Transition Rates

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- The derivations also tell that the length of transition times does not heavily depends on where the particle starts from.
- In the considered case, we naturally define the transition rate

$$k_{AB} = \frac{1}{\tau(x_A)} = \frac{\sqrt{|U''(x_C)|U''(x_A)}}{2\pi} \exp\left(-\frac{\Delta U_{AB}}{\varepsilon}\right).$$

  This is the celebrated Kramers reaction rate formula in the Brownian dynamics case, which is also called Arrhenius's law of reaction rates.

Multi-dimensional Transition Rates

- In the multi-dimensional case with index-one saddle point x_C, one can also derive the reaction rate asymptotics

$$k_{AB} = \frac{\sqrt{|\lambda_s|}}{2\pi} \sqrt{\frac{\det H_A}{\det H_C^{\perp}}} \exp\left(-\frac{\Delta U_{AB}}{\varepsilon}\right).$$

  for the Brownian dynamics, where $\lambda_s < 0$ is the unique negative eigenvalue of the Hessian $H_C = \nabla^2 U(\boldsymbol{x}_C)$, $H_A = \nabla^2 U(\boldsymbol{x}_A)$, $H_C^{\perp}$ is the restriction of H_C on the $(d-1)$-dimensional stable manifold at $\boldsymbol{x}_C$.