Transition paths: zero-temperature limit

July 02, 2025

Reminder

1. **Exercises**: solve 8 – 10 questions. Submission deadline: **23.07.2025**
2. **Course project**: Select one topic to conduct numerical experiment, and write a short report. Submission deadline: **27.07.2025**
3. give a 10-15 min **presentation**. Date: 11.07.2025 or 18.07.2025.

Machine learning

1. Supervised learning

   Dataset contains features and labels: $\mathcal{D} = \{(x_n, y_n)\}_{n=1}^{N}$.

   1. Classification (pattern recognition)
   2. Regression

2. **Unsupervised learning**

   Data: $\mathcal{D} = \{x_n\}_{n=1}^{N}$.

   - clustering: k-means
   - discovering latent structure: PCA
   - generative modeling

Part 1: Transition paths

Brownian dynamics

Brownian dynamics

1. Brownian dynamics in $\mathbb{R}^d$

$$dX_t = -\nabla V(X_t)\, dt + \sqrt{2\epsilon} dB_t, \quad t \geq 0\,,$$

where $\epsilon > 0$ is a constant.

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2. Invariant probability density is

$$\pi(x) = \frac{1}{Z} \mathrm{e}^{-\frac{1}{\epsilon} V(x)}\,,$$

   where $Z = \int_{\mathbb{R}^d} \mathrm{e}^{-\frac{1}{\epsilon} V(x)} dx$ is a normalizing constant.

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2. Small perturbation of noise.
3. Related terminology:
   1. low-temperature regime
   2. zero-temperature limit

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where $X(t;x) : [0, +\infty) \times \mathbb{R}^d \to \mathbb{R}^d$ is the flow map of the ODE

$$\frac{dX(t;x)}{dt} = -\nabla V(X(t;x)), \quad X(0;x) = x.$$

Gradient system

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2. $\lim_{t\to\infty} X_t = a$, once $X_0 \in \Omega(a)$.

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1. Invariant probability density: $\pi(x) = \frac{1}{Z}\mathrm{e}^{-\frac{1}{\epsilon}V(x)}$.
2. When V has multiple local minima, each local minimum points will be visited infinitely many times.
3. For most of the time, the system is attracted to vicinity of local minimum points, but transitions happen occasionally.

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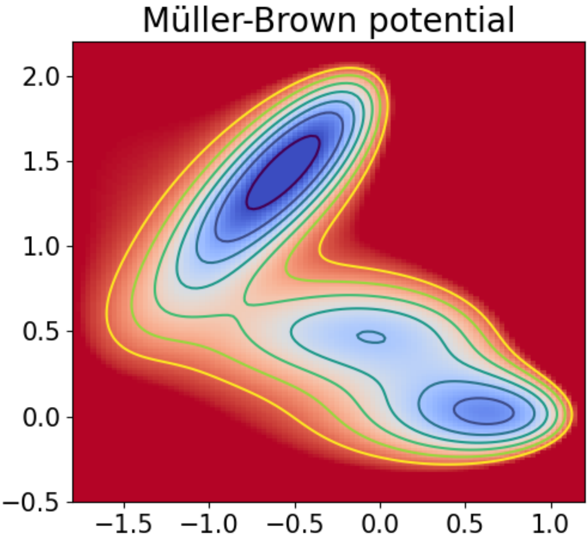
4. Numerical simulation of transitions becomes computationally challenging.
5. Goal: characterize transition events
   e.g. identify the most probable transition pathways.

Example



Part 2: Minimal energy path (MEP)

Wentzell-Freidlin theory and Large deviation theory

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3. Given $T > 0$, the space of transition paths:

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4. Action functional:

$$I_T(\varphi) = \frac{1}{4}\int_0^T \left|\dot{\varphi}(t) + \nabla V(\varphi(t))\right|^2 dt\,.$$

Similarly, on $[T_1, T_2]$, where $-\infty < T_1 < T_2 < +\infty$, the action functional is

$$I_{[T_1,T_2]}(\varphi) = \frac{1}{4}\int_{T_1}^{T_2} \left|\dot{\varphi}(t) + \nabla V(\varphi(t))\right|^2 dt\,,$$

among all paths which satisfy

$$\varphi(T_1) = a \text{ and } \varphi(T_2) = b.$$

Lower bound of action

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where $c = \arg\min_{x \in \partial\Omega(a) \cap \partial\Omega(b)} V(x)$.

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Therefore, the lower bound of action is ΔV.

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1. On the other hand, there exists a path φ, which satisfies

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$$\dot{\varphi}(t) = \begin{cases} \nabla V(\varphi(t)), & T_1 < t < T^*\,, \\ -\nabla V(\varphi(t)), & T^* < t < T_2\,. \end{cases}$$

   As $T_1 \to -\infty$, $T_2 \to +\infty$, the lower bound of the action will be achieved by this path.

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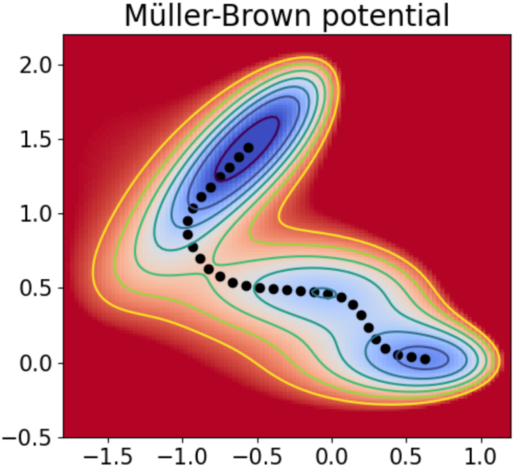
$\Longrightarrow$ MEP is the **most probable** transition path when $\epsilon \to 0$.

Example



Part 3: String method

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while keeping $|\dot{\varphi}(s)|$ to be uniform, i.e, $|\dot{\varphi}(s)| \equiv C$, where $C > 0$.

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3. Therefore, φ is a MEP.

Algorithm

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1. Update:
$$\varphi_i^* = -\tau \nabla V(\varphi_i^k) + \varphi_i^k, \quad i = 0, 1, 2, \cdots, N,$$
where τ is the step-size.

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$$\varphi_i^{k+1} = \frac{L_{j+1}^* - L_i}{L_{j+1}^* - L_j^*}\varphi_j^* + \frac{L_i - L_j^*}{L_{j+1}^* - L_j^*}\varphi_{j+1}^*,$$

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   where $L_j^* < L_i \leq L_{j+1}^*$, $L_0^* = L_0 = 0$, and

$$L_i^* = \frac{\sum_{j=0}^{i-1} |\varphi_{j+1}^* - \varphi_j^*|}{\sum_{j=0}^{N-1} |\varphi_{j+1}^* - \varphi_j^*|}\,, \quad L_i = \frac{i}{N}, \quad i = 1, \cdots, N\,.$$

Example

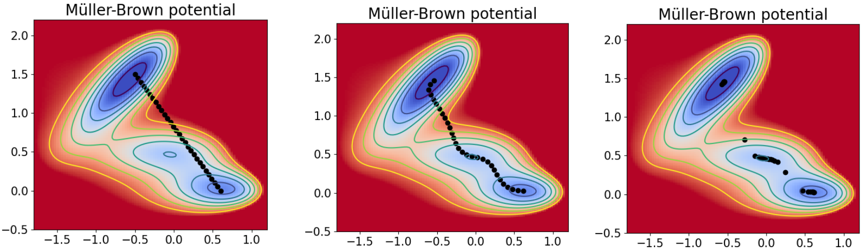

Figure: Left: init path. Middle: path after 30 iterations. Right: path after 30 iterations without reparametrization.

Part 4: Computing saddle point

Saddle point

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=& \frac{1}{4}\int_{T_1}^{T^*} \left|\dot{\varphi}(t) - \nabla V(\varphi(t))\right|^2 dt + \frac{1}{4}\int_{T^*}^{T_2} \left|\dot{\varphi}(t) + \nabla V(\varphi(t))\right|^2 dt \\
&+ \int_{T_1}^{T^*} \dot{\varphi}(t) \cdot \nabla V(\varphi(t))\, dt \\
\geq& \int_{T_1}^{T^*} \dot{\varphi}(t) \cdot \nabla V(\varphi(t)) dt \\
=& V(\varphi(T^*)) - V(\varphi(T_1)) \\
\geq& V(c) - V(a) =: \Delta V,
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where

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c = \underset{x\in\partial\Omega(a)\cap\partial\Omega(b)}{\arg\min} V(x).
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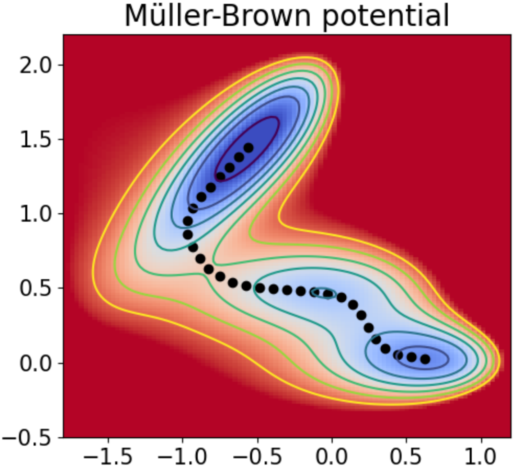
2. It tells whether the transition occurs or not.

Example



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Hence, c is a stable stationary point under (2).

Gentlest Ascent Dynamics (GAD)

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1. Both the saddle point and the unstable direction are updated.
2. It requires computing Hessian of V.