Understanding the metastable behavior of the McKean-Vlasov process

LSA — winter meeting

Ashot ALEKSIAN

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Toulouse School of Economics (TSE)

Metastability

Exit-time problem

McKean-Vlasov diffusion

Old and new results

Open questions

Metastability

An example

"Stochastic gradient descent":

$$X_{n+1} = X_n + \eta(-\nabla V(X_n) + \xi_n)$$

Itô Diffusion:

$$\begin{cases} \mathrm{d}X_t^\sigma = -\nabla V(X_t^\sigma)\,\mathrm{d}t + \sigma\,\mathrm{d}W_t\,, \\ X_0^\sigma = x_0. \end{cases}$$

Metastability

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Metastability

To describe the metastable phenomenon in a system, we need:

- metastable regimes

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- transition time between them

Linear diffusion

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V – multi-well potential, W – Brownian motion in $\mathbb{R}^d$, $\sigma > 0$ – noise parameter.

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- What are the metastable regimes?
- What are the transition times?
- What are the transition position?

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Alternatively, to describe metastability, we need:

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Let $G \subset \mathbb{R}^d$ be an open domain. We want to estimate the exit-time, i.e.:

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$$\tau_G^{\sigma} := \inf\{t > 0 : X_t^{\sigma} \in \partial G\}.$$

Assumptions :

- There is only one attractor a inside G
- G is bounded
- G is stable

Three approaches

1. PDE (potential-theoretic) approach

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3. The spectral approach

1. PDE (potential-theoretic) approach

A classical theorem:

$$u(x) := \mathsf{E}_x \left(f(X_{\tau_G^\sigma}) + \int_0^{\tau_G^\sigma} g(X_s^\sigma)\,\mathrm{d}s \right)$$

satisfies the Poisson equation in G:

$$\begin{aligned} L^\sigma u &= -g, \text{ in } G, \\ u &= f, \text{ on } \partial G, \end{aligned}$$

where $L^\sigma u := \frac{\sigma^2}{2}\Delta u - \nabla V \cdot \nabla u$.

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1. PDE (potential-theoretic) approach

Idea:

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Idea: Solve this PDE!

1. Kramers (1940) : solved it for a toy model with a double-well potential in $d = 1$ and get:

$$\mathrm{E}_{a_1}\tau_{a_2} = (1 + o(1))\frac{2\pi}{\sqrt{-V''(z^*)V''(a_1)}}\exp\left\{\frac{2(V(z^*) - V(a_1))}{\sigma^2}\right\}$$

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3. Bovier, Eckhoff, Gayrard and Klein (2001) : potential theory

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2. The pathwise approach

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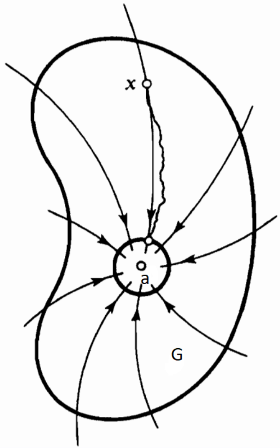

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Assumptions :

- $V \in \mathcal{C}^2(\mathbb{R}^d)$ et $V \geq 0$,
- G – bounded; $\overline{G}$ is stable under $-\nabla V$; a is the only attractor inside G

Theorem (Freidlin, Wentzell)

Let $H := \inf_{x \in \partial G} \{V(x) - V(a)\}$. *Then for any* $x \in G$ *and for any* $\delta > 0$

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- $\lim_{\sigma\to 0} \frac{\sigma^2}{2}\log \mathrm{E}_x \tau_G^\sigma = H.$

For any $N \subset \partial G$ *such that* $\inf_{z\in N}\{V(z) - V(a)\} > H$ *then also*

- $\lim_{\sigma\to 0} \mathrm{P}_x\left(X^\sigma_{\tau_G^\sigma} \in N\right) = 0.$

Comparison of the two approaches

In favour of the PDE approach:

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In favour of the pathwise approach:

1. works in the nonreversible case
2. gives more information (result in P, exit-position, exit trajectory, etc.)
3. I understand it better

McKean-Vlasov diffusion

McKean-Vlasov diffusion

$$\begin{cases} \mathrm{d}X_t^\sigma = \sigma\,\mathrm{d}W_t - \nabla V(X_t^\sigma)\,\mathrm{d}t - \nabla F * \mu_t^\sigma(X_t^\sigma)\,\mathrm{d}t, \\ \mu_t^\sigma = \mathcal{L}(X_t^\sigma), \\ X_0^\sigma = x_0 \in \mathbb{R}^d \text{ a.s.}; \end{cases}$$

1. $V : \mathbb{R}^d \to \mathbb{R}$ – **confinement potential**
2. $F : \mathbb{R}^d \to \mathbb{R}$ – **interaction potential**
3. $\mu_t^\sigma = \mathcal{L}(X_t^\sigma)$ – **the law of** X_t^σ
4. W – Brownian motion

A measure dependent diffusion

$$\begin{cases} \mathrm{d}X_t^{i,N} = \sigma\,\mathrm{d}W_t^i - \nabla V(X_t^{i,N})\,\mathrm{d}t - \frac{1}{N}\sum_{j=1}^N \nabla F(X_t^{i,N} - X_s^{j,N})\,\mathrm{d}t, \\ X_0^{i,N} = x_0 \in \mathbb{R}^d \text{ p.s.} \end{cases}$$

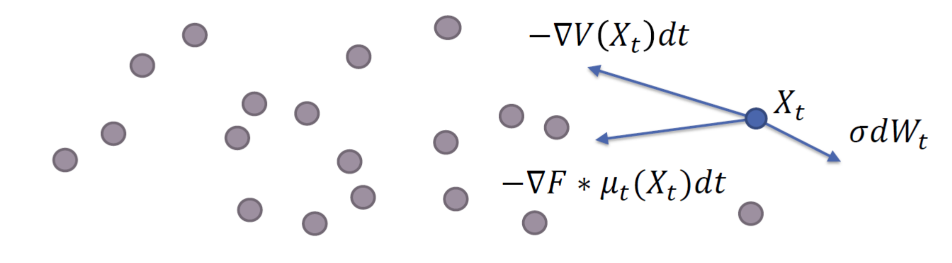
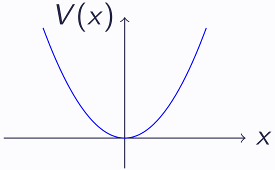


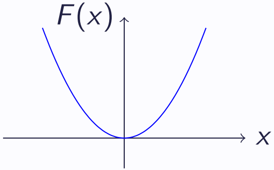
Figure 1: Dynamic of $X^{i,N}$

Old and new results

Some previous results

1. Convex-Convex case : [HIP08] – Kramers' type law





Techniques: LDP, remake of the Freidlin-Wentzell theory (the pathwise approach)

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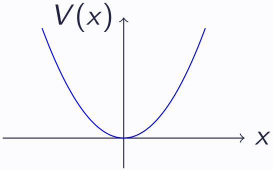
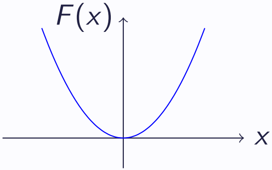
2. Convex-Convex case : [Tug16] – Kramers' type law





Techniques : control of the law, coupling method

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But what about the general case? e.g.:

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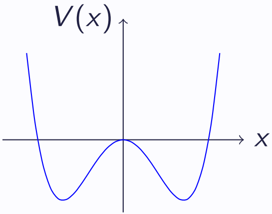

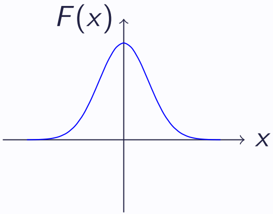

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The idea was:

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The idea was:

1. Convexity of the confinement => control of the law ($\mu_t^\sigma \approx \delta_a$)
2. Convexity => closeness with the coupled process Y^σ:

$$\mathrm{d}X_t^\sigma = -\nabla V(X_t^\sigma)\,\mathrm{d}t - \nabla F * \mu_t^\sigma(X_t^\sigma)\,\mathrm{d}t + \sigma\,\mathrm{d}W_t$$
$$\mathrm{d}Y_t^\sigma = -\nabla V(Y_t^\sigma)\,\mathrm{d}t - \nabla F * \delta_a(Y_t^\sigma)\,\mathrm{d}t + \sigma\,\mathrm{d}W_t$$

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The new idea is:

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How to approach this problem

The new idea is:

1. ~~Convexity of the confinement~~. But, before the exit-time, we are in the domain of attraction G. Thus, $\mu_t^\sigma \approx \delta_a$ should be true *at least until the exit-time*
2. ~~Convexity~~. But both Y^σ and X^σ spend most of the time around a. Thus, we still expect that they are close.

$$
\begin{aligned}
\mathrm{d}X_t^\sigma &= -\nabla V(X_t^\sigma)\,\mathrm{d}t - \nabla F * \mu_t^\sigma(X_t^\sigma)\,\mathrm{d}t + \sigma\,\mathrm{d}W_t \\
\mathrm{d}Y_t^\sigma &= -\nabla V(Y_t^\sigma)\,\mathrm{d}t - \nabla F * \delta_a(Y_t^\sigma)\,\mathrm{d}t + \sigma\,\mathrm{d}W_t
\end{aligned}
$$

New result

Assumptions:

1. V and F are regular
2. $G \subset \mathbb{R}^d$ is a regular, bounded domain
3. $a \in G$ is the unique (*inside* G) attractor of $-\nabla V$
4. $\overline{G}$ is stable under $-\nabla V - \nabla F(\cdot - a)$.

Theorem ([AT24])

Under the assumptions above, we have:

1. *Kramers' type law: for all $\delta > 0$:*

$$\lim_{\sigma \to 0} \mathrm{P}\left[\exp\left\{\frac{2}{\sigma^2}(H-\delta)\right\} \leq \tau_G^\sigma \leq \exp\left\{\frac{2}{\sigma^2}(H+\delta)\right\}\right] = 1$$

2. *Exit location : for all closed $N \subset \partial G$ such that $\inf_{z \in N} W_a(z) > H$, we have:*

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Results

Theorem ([AT24])

Under the assumptions above, we have:

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Question: where is $\mathrm{E}_x(\tau_G^\sigma)$?

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1. Generalization of the process (in particular, diffusion term)
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4. Prefactors ?

Thank you for your attention !

References i

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