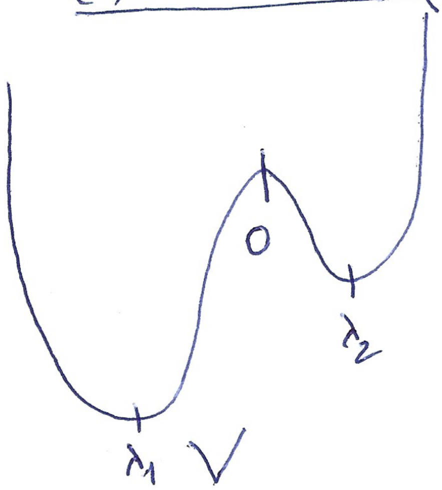
When metastability meets non-linearity

I) Metastability

(a) Motivation (Why?)



$$\mu_\beta(dx) = Z_\beta^{-1} \exp(-\beta V) \; ; \quad \beta > 0$$
$$\beta \gg 1 .$$

- Sampling of μ_β.
- Optimization of V.

Goals of the game :

* molecular dynamics
 ↳ protein folding
 ↳ configurational isomerism

* machine learning
 ↳ training of neural networks

* statistics
 ↳ likelihood maximum estimator.

(b) Definition (What?)

we use $\quad X_t = X_0 + \sqrt{\frac{2}{\beta}}\, B_t - \int_0^t \nabla V(X_s)\,ds .$

Then $\displaystyle \int \varphi(x)\,\mu_\beta(dx) = \lim_{T\to\infty} \frac{1}{T}\int_0^T \varphi(X_t)\,dt$

$\left(= \lim_{T\to\infty} \mathbb{E}\left[\varphi(X_T)\right] \text{ also} \right).$

What is the rate? The rate is bad $\Leftrightarrow$ metastability.

(c) Different approaches (How?)

* Log-Sob inequalities: - see PhD dissertation of Lise MAURIN for example (non-conservative case).
- see Lelièvre book.

* quasi-stationary distribution : - see Lelièvre works.

* Eyring-Kramers Formula :

We consider $X_t = X_0 + \sqrt{\frac{2}{\beta}} B_t - \int_0^t \nabla V(X_s)\, ds$.

$\tau(\beta) := \inf\{t \geq 0 : X_t \notin D\}$, $D =]-\infty; 0[$ on the graph.

(Remark : * β^{-1} is sometimes replaced by $\frac{\sigma^2}{2}$ or $\frac{\varepsilon}{2}$ or ε)

Eyring-Kramers is :
(or Arrhenius
or Kramers,
or Kramers' type)

$\tau(\beta) \asymp \exp(+\beta H)$

$\Leftrightarrow \beta^{-1} \log(\tau(\beta)) \xrightarrow[\beta \to \infty]{} \cancel{\exp(+\beta H)}\ H$

for some $H > 0$.

(d) Our approach (Who?)

E-K formula that is related to exit-time.

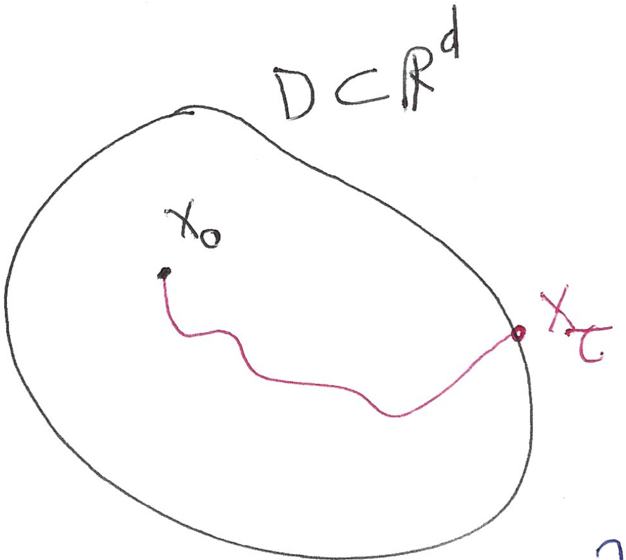
Techniques : * Large deviations principles. (F-W theory)

* Potential theory (see the works of Bovier et al)

II) Freidlin-Wentzell theory

(a) Large deviations for processes

$X = (X_t)_{t \geq 0}$ stochastic process : - Diffusion
- Jump process
- PDMP
- ....



$\tau := \inf\{t \geq 0 : X_t \notin D\}$

questions : * Exit-time : τ ? $\mathcal{L}(\tau)$? $\mathbb{E}(\tau)$?

* Exit-location : X_τ ? $\mathcal{L}(X_\tau)$? $X_\tau \notin D$?

If X is a linear diffusion :

$$X_t^\sigma = x_0 + \sigma B_t + \int_0^t a(X_s^\sigma)\, ds .$$

we introduce : $X_t^0 = x_0 + \cancel{\phi} + \int_0^t a(X_s^0)\, ds$.

$$\Rightarrow \forall T > 0 : \lim_{\sigma \to 0} \mathbb{E}\left[\sup_{[0;T]} \| X_t^\sigma - X_t^0 \|^2\right] = 0 .$$

that implies $\lim_{\sigma \to 0} \mathbb{P}\left(\sup_{[0;T]} \| X_t^\sigma - X_t^0 \| > \delta\right) = 0$, $\forall T, \delta$.

<u>Assumptions</u> : • $\forall x \in D$, $\varphi_t(x) \in D$ $\forall t \geq 0$.

•• $\forall x \in D \cup \partial D$, $\varphi_t(x) \longrightarrow z_0$.

$$\varphi_t(x) = x + \int_0^t a(\varphi_s(x))\, ds.$$

(There are two other assumptions)

For any $T > 0$, we put:

$$I_{z_0}^T(\varphi) := \frac{1}{4} \int_0^T \| \dot{\varphi}_t - a(\varphi_t) \|^2 \, dt \quad \text{if } \varphi_0 = z_0 \text{ and } (\varphi_t)_t \text{ A.C.}$$

For any $z \in \mathbb{R}^d$, we consider:

$$q(z) := \inf_{T \geq 0} \inf_{\varphi} I_{z_0}^T(\varphi).$$

Then: $H := \inf_{z \in \partial D} q(z)$. We assume $H < \infty$.

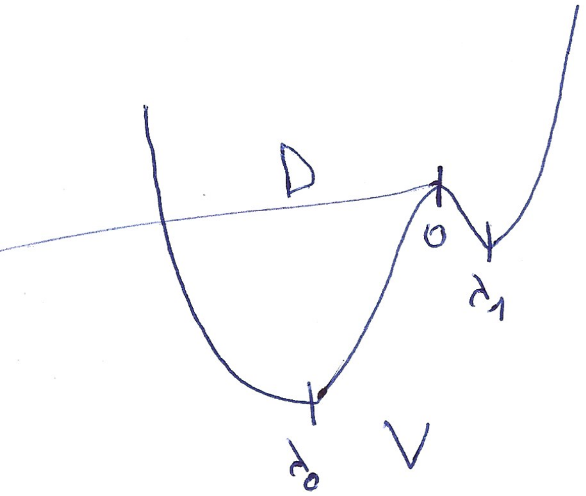
<u>Remark</u>: $H = \inf_{\partial D} V - \inf_{D} V$, if $a = -\nabla V$.

<u>(b) General result</u>

$\mathbb{P}\text{-}\lim \frac{\sigma^2}{2} \log(\tau_D(\sigma)) = H$ that is $\forall \delta > 0$

$$\lim_{\sigma \to 0} \mathbb{P}\left(e^{\frac{2}{\sigma^2}(H-\delta)} < \tau_D(\sigma) < e^{\frac{2}{\sigma^2}(H+\delta)} \right) = 1.$$

(c) Example



$H = V(0) - V(\lambda_0)$.

If $V(x) = \frac{x^4}{4} - \frac{x^2}{2}$, $D = \mathbb{R}_-^*$ then $H = \frac{1}{4}$.

$\Rightarrow$ $\boxed{\tau_D(\sigma) \asymp e^{\frac{1}{2\sigma^2}}}$.

III) Non-linear Diffusions

(a) System of particles (high dimension)

Kac (1959): simplification of kinetic Vlasov equation on plasmas:

$$X_t^{i,N} = X_0^i + \sigma B_t^i - \int_0^t \nabla V(X_s^{i,N})\,ds - \frac{1}{N}\sum_{j=1}^N \int_0^t \nabla F(X_s^{i,N} - X_s^{j,N})\,ds$$

$i \in [\![1, N]\!]$, $N \gg 1$, $\sigma > 0$

$(X_0^i)_i$ iid

$(B^i)_i$ B.M. $\perp\!\!\!\perp$ and $\perp\!\!\!\perp$ from $(X_0^i)_i$.

V: confining potential; F: interacting one.

Remark: Of course, we can consider kinetic and non-conservative case.

(b) Self-Stabilizing Diffusions (non-linearity)

$N \longrightarrow \infty$: $X^{1,N} \longrightarrow X^{1,\infty}$ (in some sense).

$$\begin{cases} X_t^{1,\infty} = X_0^1 + \sigma B_t^1 - \int_0^t \nabla V(X_s^{1,\infty})\,ds - \int_0^t \nabla F * m_s^{1,\infty}(X_s^{1,\infty})\,ds \\ m_t^{1,\infty} = \mathcal{L}(X_t^{1,\infty}) \end{cases}$$

This limit is the "propagation of chaos".

Example: $d=1$, $V(x) = \frac{x^4}{4} - \frac{x^2}{2}$ and $F(x) = \frac{\alpha}{2}x^2$, $\alpha > 0$.

$$\Rightarrow \quad X_t = X_0 + \sigma B_t - \int_0^t \left(X_s^3 + (\alpha - 1) X_s - \alpha \mathbb{E}(X_s) \right) ds.$$

Interpretation as (economical) agent in a system where many interacts.

Some names: McKean (66/67); BRTV (98); BRV (98)
BCCP (98); CMV (03, 06); CGM (08); HIP (08).
HT (10); T (13); DT (15, 18) ...

(c) Increasing the exit-time

Result of HIP in AAP 08.

V, F convexes

$$\Rightarrow \quad \frac{\sigma^2}{2} \log(\tau_D(\sigma)) \xrightarrow[\sigma \to 0]{\mathbb{P}} \hat{H} := \inf_{\partial D} \left(V + F * \delta_{a_0} \right) - V(a_0).$$
$$> H.$$

Idea: - $\exists !$ inv. $\mathbb{P}$.
- reconstructing F-W theory and adapting.

Result of T12 in EJP

Using propagation of chaos $\Rightarrow$ same result.

Result of T16 in ECP $\Rightarrow$ same result (again).

Coupling with $Y_t^\sigma = X_T^\sigma + \sigma (B_t - B_T) - \int_T^t \nabla V(Y_s^\sigma) ds$
$$- \int_T^t \nabla F(Y_s^\sigma - a_0) ds,$$

where T is s.t. $\mathcal{L}(X_T^\sigma) \simeq \delta_{a_0}$.

IV) Reducing exit-time with repulsive interaction

(Joint work with PECDR, HD, PM, MT)

(a) Equation + Assumptions

$$\begin{cases} dX_t^\sigma = a(X_t^\sigma)\,dt + b(X_t^\sigma, \mu_t^\sigma)\,dt + \sigma M\,dB_t \\ \mu_t^\sigma = \int_0^t m_s^\sigma R(t, ds) \; ; \; m_t^\sigma = \mathcal{L}(X_t^\sigma). \end{cases}$$

- $a : \mathbb{R}^d \to \mathbb{R}^d$ locally Lipschitz.
- $b : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}^d$ globally Lipschitz.
- $\langle z - y \, ; \, a(z) - a(y) \rangle + \langle z - y \, ; \, b(z, \mu) - b(y, \nu) \rangle$
  $\leq -\rho |z - y|^2 + k\, W_2^2(\mu ; \nu)$ with $0 \leq k < \rho$.
- $R(t, [0, t_0]) \xrightarrow[t\to\infty]{} 0$.

$\Rightarrow \exists !\, \lambda_0 \in \mathbb{R}^d$ s.t. $a(\lambda_0) + b(\lambda_0, \delta_{\lambda_0}) = 0$

- $D \subsetneq \mathbb{R}^d$ is open.
- a is Lipschitz on an enlargement of D.
- $m_0^\sigma = m_0$ and $\mathrm{Supp}(m_0) \subset \mathbb{B}(\lambda_0, r) \subset D$. r is <u>not</u> small.

And:

- One can approximate D by $D_{i,\xi} \subset D \subset D_{e,\xi}$

with: $\tau_{\tilde{X}^\sigma, D_{i,\xi}} \asymp e^{\frac{2}{\sigma^2} H_{i,\xi}}$ and $\tau_{\tilde{X}^\sigma, D_{e,\xi}} \asymp e^{\frac{2}{\sigma^2} H_{e,\xi}}$

where $\overset{\nearrow H}{H_{i,\xi}} < H < H_{e,\xi} \longrightarrow H$.

Here, $\tilde{X}_t^\sigma = \delta_0 + \int_0^t a(\tilde{X}_s^\sigma)\,ds + \int_0^t b(\tilde{X}_s^\sigma, \delta_{\delta_0})\,ds + \sigma M B_t$.

(b) Theorem

$$\frac{\sigma^2}{2} \log(\tau_D(\sigma)) \xrightarrow[\sigma \to 0]{\mathbb{P}} H = \lim_{\xi \to 0} H_{i,\xi} = \lim_{\xi \to 0} H_{e,\xi}.$$

(c) Global strategy

When T is large enough: $\mu_T^\sigma \simeq \delta_{\delta_0}$

$\Rightarrow X_T^\sigma \simeq \delta_0$.

$$\Rightarrow X_{T+t}^\sigma \simeq \delta_0 + \sigma M B_t + \int_T^{T+t} a(X_s^\sigma)\,ds + \int_T^{T+t} b(X_s^\sigma, \delta_{\delta_0})\,ds$$

We know the exit-time of this last diffusion

$\longrightarrow$ we have the one of (X^σ).

V) Perspectives

- ↳ System of particles
- ↳ Nonconvexity of V
- ↳ ABF method.