I) Metastability

(a) Motivation (Why?)

\[ \mu_\beta(\mathbf{x}) = \frac{1}{Z_\beta} \exp(-\beta V); \quad \beta > 0 \]

- Sampling of \( \mu_\beta \).
- 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 \( X_T = X_0 + \sqrt{\frac{2}{\beta}} B_T - \frac{1}{T} \int_0^T \nabla V(X_0) \, dt \).

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

\( = \lim_{T \to \infty} E [\varphi(X_T)] \) also.

What is the rate? The rate is bad \( \iff \) 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 \[ X_t = X_0 + \sqrt{\frac{2}{\beta}} B_t - \int_0^t \nabla V(X_s) \, ds \]
  \[ \tau(\beta) := \inf \{ t > 0 : X_t \notin \mathbb{D} \} \quad \mathbb{D} = \mathbb{J}_\infty, 0 \mathbb{J} \text{ on the graph} \]

  (Remark: \( \beta^4 \) is sometimes replaced by \( \frac{\sigma^2}{2} \) or \( \frac{\epsilon}{2} \) or \( \epsilon \))

  Eyring-Kramers is: \[ \tau(\beta) \asymp \exp(\beta H) \]

  \[ \beta^4 \log(\tau(\beta)) \to H \]

  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.)
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: \( \tau \) ? \( \mathbb{P}(\tau) \) ? \( \mathbb{E}(\tau) \) ?
- Exit-location: \( X_\tau \) ? \( \mathbb{P}(X_\tau) \) ? \( X_\tau \notin D \) ?

If \( X \) is a linear diffusion:

\[ X_t^\circ = x_0 + \sigma M_t + \int_0^t a(x_\circ) \, ds \]

we introduce:

\[ X_t = x_0 + \xi + \int_0^t a(x_\circ) \, ds \]

\[ \Rightarrow \forall \tau > 0 : \lim_{\sigma \to 0} \mathbb{E} \left[ \sup_{[0,\tau]} \| X_t^\circ - X_t \|^2 \right] = 0 \]

That implies:

\[ \lim_{\sigma \to 0} \mathbb{P} \left( \sup_{[0,\tau]} \| X_t^\circ - X_t \| > s \right) = 0 , \forall \tau, s \]
Assumptions:

- \( \forall x \in D, \; \Psi_t(x) \in D \; \forall t \geq 0 \).
- \( \forall x \in D, \; \Psi_t(x) \rightarrow \Delta_0 \).

\[ \Psi_t(x) = x + \int_0^t a(\Psi_t(\sigma)) \, d\sigma. \]

(There are two other assumptions)

For any \( T > 0 \), we put:

\[ I_T^{\Psi_0}(\Psi) := \frac{1}{T} \int_0^T \| \dot{\Psi}_t - a(\Psi_t) \|_2 \, dt \quad \text{if } \Psi_0 = \Delta_0 \]

and \( \Psi_t \), A.C.

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

\[ q_T(z) := \inf_{T > 0} \inf_{\Psi} I_T^{\Psi_0}(\Psi). \]

Then:

\[ H := \inf_{z \in \mathbb{R}^d} q_T(z). \]

We assume \( H < \infty \).

Remark:

\[ H = \inf_{\Delta \in D} V - \inf_{D} V, \quad \text{if } a = -\nabla V. \]

(b) General result

\[ \mathbb{P} - \lim_{\sigma \to 0} \frac{\sigma^2}{2} \log(\zeta_D(\sigma)) = H \quad \text{that is } \quad \forall s > 0 \]

\[ \lim_{\sigma \to 0} \mathbb{P}\left( e^{\frac{\sigma^2}{2}(H-s)} < \zeta_D(\sigma) < e^{\frac{\sigma^2}{2}(H+s)} \right) = 1. \]
(c) Example

\[ H = V(0) - V(\lambda_0). \]

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

\[ \Rightarrow \quad \mathcal{C}_D(\sigma) = e^{\frac{1}{2\sigma^2}}. \]

III) Non-linear Diffusions

(a) System of particles (high dimension)

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

\[ X^{i,N}_t = X_0^i + \sigma B_t^i - \int_0^t \nabla V(X^{i,N}_s) \, ds - \frac{1}{N} \sum_{j=0}^{N-1} \int_0^t \nabla F_i(X^{j,N}_s \cdot X^{i,N}_s) \, ds \]

\( i \in \{1, \ldots, N\}, \quad N \gg 1, \quad \sigma > 0 \)

\( (X^i_0) \): iid

\( (B^i_t) \): B.M. \( \mathbb{1} \) and \( \mathbb{1} \) from \( (X^i_0) \).

\( V \): confining potential; \( F \): interacting one.

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

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

\[ N \to \infty : \quad X^{i,N}_t \to X^{i,\infty}_t \quad (\text{in some sense}). \]

\[ (X^{i,\infty}_t = X^i_0 + \sigma \cdot B^i_t - \int_0^t \nabla V(X^{i,\infty}_s) \, ds - \int_0^t \nabla F_i \cdot M^{i,\infty}_s (X^{i,\infty}_s) \, ds \]

\[ M^{i,\infty}_t = \mathcal{C} \left( X^{i,\infty}_t \right) \]
This limit is the "propagation of chaos".

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

$X_t = X_0 + \sigma B_t - \int_0^t \left( \frac{X_0^4}{4} + \alpha X_0^2 - \alpha F(X_0) \right) ds$.

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

Some names: McKean (66/67); BRTV (98); BRL (98); BCCP (98); CMV (03, 08); CEM (08); H2P (08); HT (10); T (13); DT (15, 18) ...

(c) Increasing the exit-time

Result of HIP in APP 08.

$V, F$ convexes

$\frac{\sigma^2}{2} \log (\tau_D(s)) \xrightarrow{\sigma \to 0} \hat{H} := \inf_{\tau_D} \left( V + F \times S_{\tau_D} - V(\tau_D) \right)$.

$Idea: \exists! \text{ inv. } P$ - 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 $\gamma_t^\sigma = X_t^\sigma + \sigma (B_t - B_t^\tau) - \int_t^\tau V'(X_t^\sigma) ds - \int_0^\tau \nabla F(X_t^\sigma - \lambda_0) ds$.

Where $\tau$ is s.t. $\lambda_0 (X_{\tau}) \leq \lambda_0$. 
Reducing exit-time with repulsive interaction

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

(a) Equation + Assumptions

\[\begin{align*}
\left\{ \begin{array}{l}
     dX^\sigma_t = a(X^\sigma_t) \, dt + b(X^\sigma_t, \mu^\sigma_t) \, dt + \sigma \, M \, dB_t \\
     \mu^\sigma_t = \int_0^t m^\sigma_0 \, R(t, ds) \\
    m^\sigma = \infty(X^\sigma_t)
    \end{array} \right. \\

\end{align*} \]

- \(a: \mathbb{R}^d \rightarrow \mathbb{R}^d\) locally Lipschitz.
- \(b: \mathbb{R}^d \times \mathbb{P}(\mathbb{R}^d) \rightarrow \mathbb{R}^d\) globally Lipschitz.
- \(3 - y^j ; a(y) - a(y^j) + 3 - y^j: b(y, \mu) - b(y^j, \nu) \leq -p y_j^2 + k W_2^2(\mu, \nu)\) with \(0 \leq k < p\).
- \(R(t, [0, t_0]) \rightarrow 0\) as \(t \rightarrow \infty\).
- \(\exists! \, \delta_0 \in \mathbb{R}^d\) s.t. \(a(\delta_0) + b(\delta_0, S_{\delta_0}) = 0\).

- \(D \subseteq \mathbb{R}^d\) is open.
- \(a\) is Lipschitz on an enlargement of \(D\).
- \(m^\sigma_0 = m_0\) and \(\text{supp}(m_0) \subseteq \overline{B(\delta_0, \rho)} \subseteq D\). \(\rho\) is not small.

And:
- One can approximate \(D\) by \(D_{\sigma_5} \subseteq D \subseteq D_{\sigma_5}\) with:
  \[\begin{align*}
  \tau_{X^\sigma_t, D_{\sigma_5}} &\leq \frac{2}{\sigma_5^2} H_{\sigma_5} \quad \text{and} \quad \tau_{X^\sigma_t, D_{\sigma_5}} \leq \frac{2}{\sigma_5^2} H_{\sigma_5} \\
  \text{where} &\quad H_{\sigma_5} < H < H_{\sigma_5} \rightarrow H.
  \end{align*} \]

[Image 0x0 to 595x842]
Here, $X_T^\sigma = \xi_0 + \int_0^T a(X_s^\sigma) ds + \int_0^T b(X_s^\sigma, S_s) ds + \sigma M B_t$.

(a) Theorem

\[ \frac{\sigma^2 \log \left( \frac{C_D(\omega)}{\sigma} \right)}{\sigma} \xrightarrow{\sigma \to 0} P \xrightarrow{\sigma \to 0} H = \lim_{\sigma \to 0} H_{\sigma} = \lim_{\sigma \to 0} H_{\alpha, \xi} \]  

(c) Global strategy

When $T$ is large enough: $\mu_T^\sigma \approx S_{\alpha_0}$

$\Rightarrow X_T^\sigma \approx \xi_0$.

$\Rightarrow X_{T+T}^\sigma \approx \xi_0 + \sigma M B_t + \int_T^{T+T} a(X_s^\sigma) ds + \int_T^{T+T} b(X_s^\sigma, S_s) ds$.

We know the exit-time of this last diffusion.

$\Rightarrow$ we have the one of $(X^\sigma)$.

IV) Perspectives

$L$ System of particles

$L$ Nonconvexity of $V$

$L$ ABF method.