Stability, cutoff phenomenon and Eyring-Kramers estimates for the Langevin dynamics

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Joint work with Seungwoo Lee[1] and Insuk Seo[1]

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with $F \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R}^d)$, $\gamma, \epsilon > 0$.

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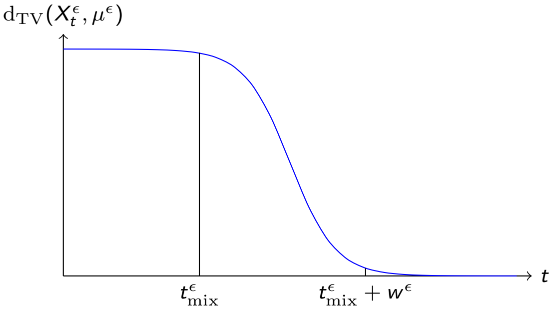
with $F \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R}^d)$, $\gamma, \epsilon > 0$.

Question: How fast does the convergence to the equilibrium distribution μ^ϵ happen?

Cutoff phenomenon



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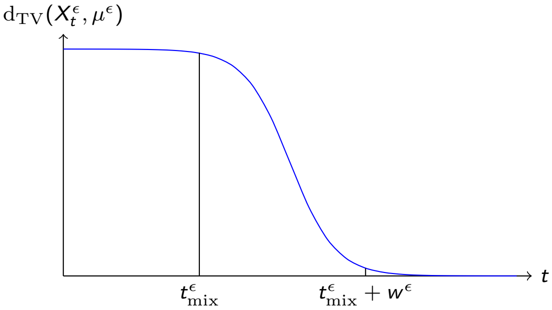

Cutoff if $w^\epsilon / t^\epsilon_{\mathrm{mix}} \underset{\epsilon \to 0}{\longrightarrow} 0$ and

$$\lim_{c \to +\infty} \limsup_{\epsilon \to 0} \mathrm{d_{TV}} \left(X^\epsilon_{t^\epsilon_{mix} + cw^\epsilon}, \mu_\epsilon \right) = 0,$$

$$\lim_{c \to -\infty} \liminf_{\epsilon \to 0} \mathrm{d_{TV}} \left(X^\epsilon_{t^\epsilon_{mix} + cw^\epsilon}, \mu_\epsilon \right) = 1.$$

Overdamped Langevin dynamics case

Let

$$\mathrm{d}X_t^\epsilon = -F(X_t^\epsilon)\mathrm{d}t + \sqrt{2\epsilon}\mathrm{d}B_t, \qquad X_0 = x.$$

Theorem (*G. Barrera, M. Jara* (2020))

Assume that there exist $\alpha > 0$ such that for all $y, q \in \mathbb{R}^d$,

$$DF(y)q \cdot q \geq \alpha |q|^2.$$

Then, there exist $\eta(x), \nu(x), T(x)$ such that cutoff is satisfied with

$$t_{\mathrm{mix}}^\epsilon = \frac{1}{2\eta(x)} \log\left(\frac{1}{2\epsilon}\right) + \frac{\nu(x)-1}{\eta(x)} \log\log\left(\frac{1}{2\epsilon}\right) + T(x), \quad w^\epsilon = \frac{1}{\eta(x)} + o(1).$$

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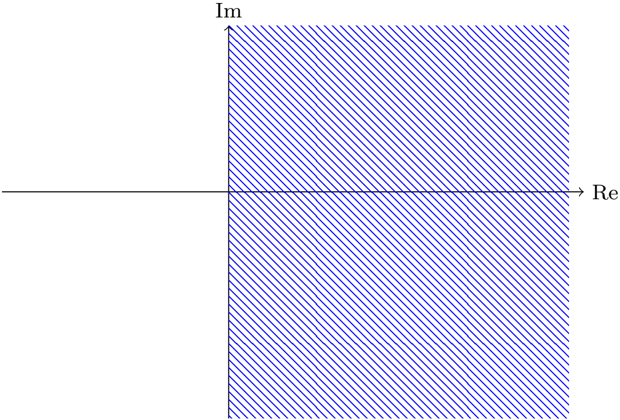
Extension to *Langevin* dynamics with global attractor at 0 ?

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = -F(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sqrt{2\epsilon}\mathrm{d}B_t, \end{cases}$$

Stability of the dynamical system

$$\frac{\mathrm{d}X_t}{\mathrm{d}t} = -F(X_t), \quad X_0 = x.$$

$$(X_t)_{t\geq 0} \textit{ locally stable} \iff \exists \alpha > 0, \text{ such that } |x| \leq \alpha \Rightarrow |X_t| \underset{t\to\infty}{\longrightarrow} 0$$
$$\iff \mathrm{Sp}_{\mathbb{C}}(DF(0)) \subset \{a + ib, a > 0, b \in \mathbb{R}\}.$$



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$$(q_t, p_t)_{t\geq 0} \textit{ locally stable} \iff \exists \alpha > 0, \text{ such that } |x| \leq \alpha \Rightarrow |(q_t, p_t)| \underset{t\to\infty}{\longrightarrow} 0$$

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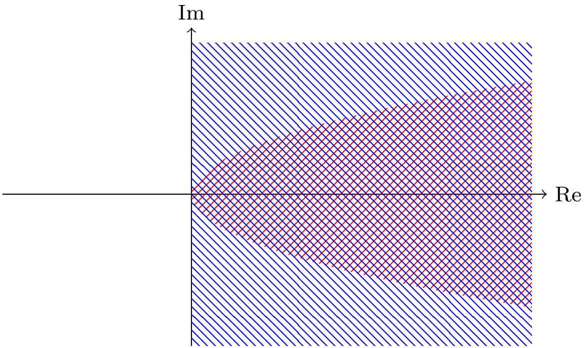

Remark: $\forall q \in \mathbb{R}^d$, $F(q) \cdot q \geq \alpha |q|^2$ not enough to guarantee stability!

Stability condition

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = -F(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t, \end{cases}$$

Theorem (Global stability)

Assume that

$$F(q) = \nabla U(q) + \ell(q),$$

with U non-negative. Besides, there exists $\alpha > 0$, $\beta \in (0, \gamma)$ *such that*

$$F(q) \cdot q \geq \alpha(|q|^2 + U(q)) + \frac{|\ell(q)|^2}{\beta^2}.$$

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Then, there exist $C, \lambda > 0$ such that

$$|(q_t, p_t)| \leq C|(q_0, p_0)|\mathrm{e}^{-\lambda t}.$$

Linear case

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where F is a constant normal matrix ($FF^T = F^T F$). Then,

$$\text{Stability} \iff S + \frac{A^2}{\gamma^2} \text{ is definite positive,}$$

where $S = \frac{1}{2}(F + F^T)$, $A = \frac{1}{2}(F - F^T)$.

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Conclusion: Almost sharp condition!

Cutoff in the underdamped setting

Theorem

Assume F satisfies the previous condition then there exist $\eta(x), \nu(x), T(x)$ such that cutoff is satisfied for the underdamped Langevin dynamics starting from $x \in \mathbb{R}^{2d}$ with cutoff time $t^{\epsilon}_{\mathrm{mix}}$ and window w^{ϵ}:

$$t^{\epsilon}_{\mathrm{mix}} = \frac{1}{2\eta(x)} \log\left(\frac{1}{2\epsilon}\right) + \frac{\nu(x)-1}{\eta(x)} \log\log\left(\frac{1}{2\epsilon}\right) + T(x), \quad w^{\epsilon} = \frac{1}{\eta(x)} + o(1).$$

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- *Lyapunov matrix equation*

$$\begin{pmatrix} 0 & -DF(0)^T \\ I_d & -\gamma I_d \end{pmatrix} \Sigma + \Sigma \begin{pmatrix} 0 & I_d \\ -DF(0) & -\gamma I_d \end{pmatrix} = -\begin{pmatrix} 0 & 0 \\ 0 & I_d \end{pmatrix}.$$

Eyring-Kramers estimates for the Langevin dynamics

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = -\nabla U(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sqrt{2\gamma\epsilon}\mathrm{d}B_t, \end{cases}$$

where $\gamma, \epsilon > 0$.

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Remark: Guarantees positive recurrence, tightness on the stationary distribution.

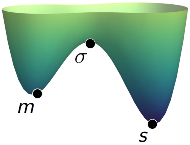

Figure: Double well potential.

Issues:

- No reversibility.
- No ellipticity (hypoelliptic).

Main result

Let μ^ϵ be the stationary distribution of the Langevin process

$$\mathrm{d}\mu^\epsilon = \frac{1}{Z_\epsilon}\mathrm{e}^{-V(q,p)/\epsilon}\mathrm{d}\boldsymbol{q}\mathrm{d}\boldsymbol{p},$$

where $V(q,p) = U(q) + |p|^2/2$.

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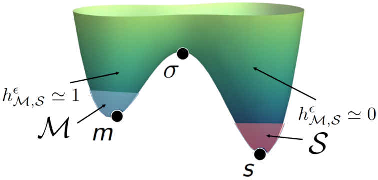
Theorem (Eyring-Kramers estimates)

Let $\mathbb{H}^m$ (resp. $\mathbb{H}^\sigma$) be the Hessian matrices of V at m (resp. σ). Then,

$$E_m(\tau_{\mathcal{S}}) = (1 + o_\epsilon(1)) \frac{2\pi}{\lambda^\sigma} \sqrt{\frac{-\det \mathbb{H}^\sigma}{\det \mathbb{H}^m}} \exp\left(\frac{U(\sigma) - U(m)}{\epsilon} \right),$$

where $-\lambda^\sigma$ is the unique negative eigenvalue of $\mathbb{H}^m \begin{pmatrix} 0 & I_d \\ -I_d & \gamma I_d \end{pmatrix}$ and $\mathcal{S} = \mathcal{B}(s, \epsilon)$.

Scheme of proof



Potential theory approach.

$$\boxed{E_{\nu}(\tau_{\mathcal{S}}) = \frac{1}{C_{\epsilon}(\mathcal{M},\mathcal{S})} \int_{\mathbb{R}^{2d}} h^{\epsilon,*}_{\mathcal{M},\mathcal{S}} \mathrm{d}\mu^{\epsilon}.}$$

Estimates:

- $E_{\nu}(\tau_{\mathcal{S}}) = E_m(\tau_{\mathcal{S}}) + o_{\epsilon}(1)$.
- $\int_{\mathbb{R}^{2d}} h^{\epsilon,*}_{\mathcal{M},\mathcal{S}}(x)\mathrm{d}\mu^{\epsilon}(x) = (1 + o_{\epsilon}(1))Z_{\epsilon}^{-1}(2\pi\epsilon)^d e^{-U(m)/\epsilon} \frac{1}{\sqrt{\det \mathbb{H}^m}}$.
- $C_{\epsilon}(\mathcal{M}_{\epsilon}, \mathcal{S}_{\epsilon}) = (1 + o_{\epsilon}(1))Z_{\epsilon}^{-1}(2\pi\epsilon)^d e^{-U(\sigma)/\epsilon} \frac{\lambda^{\sigma}}{2\pi} \frac{1}{\sqrt{-\det \mathbb{H}^{\sigma}}}$.

Scheme of proof

Difficulties

- $\nu_{\mathrm{eq}} := \nabla h^{\epsilon,*}_{\mathcal{M},\mathcal{S}}(x) \cdot n_{\partial\mathcal{M}}(x)\mu^{\epsilon}(x)\sigma(\mathrm{d}x)$ well defined ?
- $\mathrm{Cap}(\mathcal{M},\mathcal{S}) := \epsilon \int_{(\mathcal{M}\cup\mathcal{S})^c} |\nabla_p h^{\epsilon,*}_{\mathcal{M},\mathcal{S}}(x)|^2 \mathrm{d}\mu^{\epsilon}(x)$ well defined ?

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- Build ν which satisfies the averaged estimate (no clear link with the equilibrium measure ν_{eq}).

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Remark: Analogous work regarding the spectral gap by Bony, Le Peutrec, Michel (2022)