Sharp spectral gap of adaptive Langevin dynamics.

Loïs Delande

Starting point

We consider a homogeneous Langevin process :

$$dX_t = \xi(X_t)dt + \sqrt{2h}\sigma(X_t)dB_t$$

Where :

- $(B_t)_t$ brownian motion on $\mathbb{R}^d$
- $\xi \ : \ \mathbb{R}^d \to \mathbb{R}^d$ vector field, drift coefficient
- σ matrix, diffusion coefficient
- h proportional to the system's temperature.

$$u(t,x) = \mathbb{E}(u_0(X_t)|X_0 = x) \implies \begin{cases} \partial_t u + \mathcal{L}u & = 0 \\ u_{|t=0} & = u_0 \end{cases}$$

With :

$$\mathcal{L} = -h \sum_{i,j} a_{i,j}\, \partial_{x_i}\, \partial_{x_j} - \sum_k \xi_k\, \partial_{x_k}, \quad (a_{i,j}) = \sigma\sigma^T \tag{1}$$

Exemples

→ Witten Laplacian :

$$\mathcal{L} = -h\Delta + \nabla V \cdot \nabla,$$

[Helffer, Klein, Nier '04], [Helffer, Sjöstrand '85].

→ Fokker-Planck :

$$\mathcal{L} = \partial_x V \cdot \partial_v - v \cdot \partial_x - h\Delta_v + v \cdot \partial_v,$$

[Herau, Hitrik, Sjöstrand '08], [Bony, Le Peutrec, Michel '22].

Sampling methods

On Fokker-Planck :

Theorem Lelievre, Rousset, Stoltz '10

For any initial condition X_0 and any bounded mesurable observable φ,

$$\lim_{T \to +\infty} \frac{1}{T} \int_0^T \varphi(X_t)dt = C^{-1} \int_{\mathbb{R}} \varphi(x,v) e^{-f(x,v)/h} dxdv$$

where $f(x,v) = V(x) + \frac{v^2}{2}$ *and* $C = \int_{\mathbb{R}} e^{-f(x,v)/h} dxdv.$

Uncertainty on $\nabla V \rightsquigarrow$ problems of precision in the simulations.

Our framework

[Leikmuhler, Sachs, Stoltz '20] :

$$P = H_0 + \nu Y + \gamma \mathcal{O} \tag{2}$$

$$\begin{cases} H_0 = v \cdot h\partial_x - \partial_x V \cdot h\partial_v, \\ Y = h(|v|^2 \partial_y - yv \cdot \partial_v) - dh(h\,\partial_y + \frac{y}{2}), \\ \mathcal{O} = -h^2 \Delta_v + \frac{|v|^2}{4} - h\frac{d}{2}. \end{cases} \tag{3}$$

- $\gamma, \nu > 0$,
- $(x, v, y) \in \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}$,
- $V : \mathbb{R}^d \to \mathbb{R}$ smooth.

$$f(x, v, y) = \frac{V(x)}{2} + \frac{|v|^2 + y^2}{4} \rightsquigarrow H_0(e^{-f/h}) = Y(e^{-f/h}) = \mathcal{O}(e^{-f/h}) = 0$$

The potential V

Assumption 1

V is Morse and there exists $C > 0$ and $K \subset \mathbb{R}^d$ compact such that $\forall x \in \mathbb{R}^d \setminus K$,

$$V(x) \ \geq \ -C, \quad |\nabla V(x)| \geq \frac{1}{C} \quad \text{and} \quad |\,\text{Hess}\, V(x)| \geq C.$$

$\rightsquigarrow$ V has a finite number of critical points, which are not degenerated.

We denote

- $\mathcal{U}$ the set of critical points
- $\mathcal{U}^{(0)}$ those of index 0, of cardinal n_0

Goal : Show that P has as many small eigenvalues as V has minima, and quantify the spectral gap.

Space of quasimodes :

$$F_h = \text{span}\{f_{\mathbf{m}}, \mathbf{m} \in \mathcal{U}^{(0)}\}$$

where

$$f_{\mathbf{m}}(x, v, y) = \chi_{\mathbf{m}}(x) e^{(-f(x,v,y) - f(\mathbf{m}))/h}$$

with $\chi_{\mathbf{m}}$ cutoffs around $\mathbf{m}$ with disjoint support.

Hypocoercivity estimates

Theorem 1

$\exists h_0, c_0, c_1, c > 0$ such that $\forall h \in]0, h_0]$, $\forall \gamma, \nu > 0$, $\forall u \in D(P) \cap F_h^{\perp}$, we have

$$\|(P - z)u\|_{L^2} \geq c_1 g(h) \|u\|_{L^2}$$

uniformily w.r.t $z \in \mathbb{C}$ such that $\mathrm{Re}(z) \leq c_0 g(h)$, where

$$g(h) = h \min\left(\nu^2 h\gamma, \frac{1}{\gamma}, \frac{\gamma}{\nu^2 h}, \frac{\nu^2 h}{\gamma}\right). \tag{4}$$

Resolvent estimate

Theorem 2

$\exists h_0, c_0, c_1, c, c' > 0$, such that $\forall h \in]0, h_0]$, $\forall \gamma, \nu > 0$, and any $0 < c_0' < c_1$, we have

$$\sigma(P) \cap \{\mathrm{Re}\, z \leq c_0 g(h)\} = \{\lambda(\mathbf{m}, h), \mathbf{m} \in \mathcal{U}^{(0)}\}$$

$$\forall \mathbf{m} \in \mathcal{U}^{(0)}, \ |\lambda(\mathbf{m}, h)| \leq c' e^{-c'/h}$$

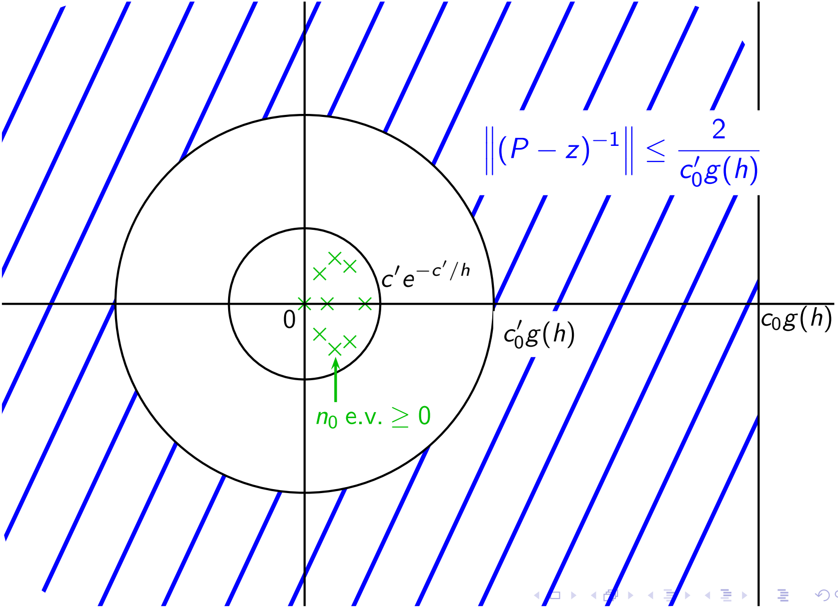
Moreover

$$\forall |z| > c_0' g(h), \mathrm{Re}\, z \leq c_0 g(h), \ \left\|(P - z)^{-1}\right\|_{L^2} \leq \frac{2}{c_0' g(h)},$$

where $g(h)$ defined in (4) satisfies

$$g(h) > e^{-\frac{c_f}{2h}}, \text{ with some } c_f > 0.$$

Visually ?



Quick reminder on the Witten Laplacian

Potential $W : \mathbb{R}^d \to \mathbb{R}$

$\hookrightarrow$ semiclassical Laplacian $\Delta_W = -h^2\Delta + |\nabla W|^2 - h\Delta W$

Denoting $\delta_W = h\nabla + \nabla W = e^{-W/h} \circ h\nabla \circ e^{W/h}$ we obtain

- $\Delta_W = \delta_W^* \delta_W \ \rightsquigarrow \ \sigma(\Delta_W) \subset \mathbb{R}_+$
- $0 \in \sigma(\Delta_W) \iff e^{-W/h} \in L^2(\mathbb{R}^d)$

Under Assumption 1, $\exists c, \varepsilon > 0$, such that $\forall h \in]0, h_0]$,

$$\sharp\sigma(\Delta_W) \cap [0, ce^{-c/h}] = n_0 \quad \text{and} \quad \sigma(\Delta_W) \cap \,]ce^{-c/h}, \varepsilon h[\, = \emptyset.$$

Auxiliary hypocoercive operator

$\rightarrow$ Let $Z = H_0 + \nu Y$, Π_ρ projector onto $\operatorname{Ker}\mathcal{O}$ we denote

$$A = (h\min(1,\nu^2 h) + h^{-1}(Z\Pi_\rho)^*(Z\Pi_\rho))^{-1}(Z\Pi_\rho)^*$$

$$\rightsquigarrow A = \Pi_\rho A = A(1-\Pi_\rho)$$

[Dolbeault, Mouhot, Schmeiser '15]

Proposition

- $(Z\Pi_\rho)^*(Z\Pi_\rho) = dh(\Delta_{\frac{v}{2}} + 2\nu^2 h\Delta_{\frac{y^2}{4}})\Pi_\rho = dhB\Pi_\rho$
- $\forall u \in F_h^\perp$, $\langle B\Pi_\rho u, u\rangle \geq c_0 h\min(1,\nu^2 h)\|\Pi_\rho u\|^2$

Outline of proof :

- $H_0\Pi_\rho = v\cdot\delta_x\Pi_\rho$ and $Y\Pi_\rho = (|v|^2 - dh)\delta_y\Pi_\rho$
- Assumption 1 $\rightsquigarrow \Delta_{\frac{v}{2}}, \Delta_{\frac{y^2}{4}} \geq ch$

Proposition

$\exists C, \delta_0, h_0 > 0$ such that $\forall h \in]0, h_0]$, $\forall \gamma, \nu > 0$, $\forall u \in D(P) \cap F_h^\perp$, we have

$$\mathrm{Re}\, \langle Pu, (1 + \delta(h)(A + A^*))u \rangle_{L^2} \geq Cg(h)\|u\|_{L^2}^2$$

where $\delta(h) = \delta_0 \dfrac{g(h)}{h}$.

Outline of proof :

$$\begin{aligned}
&\mathrm{Re}\langle Pu, (1 + \delta(h)(A + A^*))u \rangle \\
&\qquad \geq \gamma h \|(1 - \Pi_\rho)u\|^2 + \delta\, \mathrm{Re}\langle Pu, (A + A^*)u \rangle \\
&\qquad \geq \gamma h \|(1 - \Pi_\rho)u\|^2 + \delta c_0' h \|\Pi_\rho u\|^2 \\
&\qquad\qquad + \delta\, \mathrm{Re}(\langle AZ(1 - \Pi_\rho)u, u \rangle + \gamma \langle A\mathcal{O}u, u \rangle + \langle Zu, Au \rangle) \\
&\qquad \geq \gamma h \|(1 - \Pi_\rho)u\|^2 + \delta c_0' h \|\Pi_\rho u\|^2 \\
&\qquad\qquad - \delta(\|\Pi_\rho AZ\| + \|\Pi_\rho AO\|)\, \|(1 - \Pi_\rho)u\|\, \|\Pi_\rho u\| \\
&\qquad\qquad - \delta\, \|Z\Pi_\rho A\|\, \|(1 - \Pi_\rho)u\|^2
\end{aligned}$$

Double well case

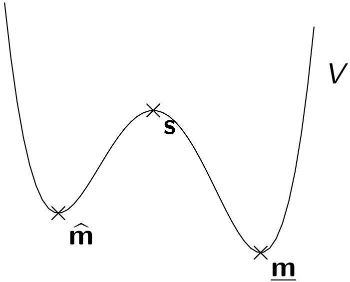


Figure – Typical representation of a double well Morse function

Sharp estimates

Theorem 3

Assume that $\mathcal{U}^{(0)} = \{\underline{\mathbf{m}}, \widehat{\mathbf{m}}\}$*, where* $\underline{\mathbf{m}}$ *is the unique minimum of* V*,* $\mathcal{U}^{(1)} = \{\mathbf{s}\}$ *and* $\gamma, \nu > 0$ *are fixed.* $\exists h_0, c > 0$*, such that* $\forall h \in]0, h_0]$*, we have counting with multiplicities,*

$$\sigma(P) \cap \{\operatorname{Re} z \leq ch^2\} = \{0, \lambda\},$$

with

$$\lambda = z(\widehat{\mathbf{m}}) h e^{-(V(\mathbf{s}) - V(\widehat{\mathbf{m}}))/h}(1 + O(\sqrt{h})),$$

$$z(\widehat{\mathbf{m}}) = \frac{\mu(\mathbf{s})(\det \operatorname{Hess} V(\widehat{\mathbf{m}}))^{\frac{1}{2}}}{2\pi |\det \operatorname{Hess} V(\mathbf{s})|^{\frac{1}{2}}}$$

where $\mu(\mathbf{s}) = \frac{1}{2}(-\gamma + \sqrt{\gamma^2 + 4\eta}) > 0$ *with* η *the sole negative eigenvalue of* $\operatorname{Hess} V(\mathbf{s})$*.*

Gaussian quasimodes

[Bony, Le Peutrec, Michel '22] : gaussian quasimodes $u = \chi_h e^{-(f-f(\mathbf{m}))/h}$ where

$$\chi_h(x,v,y) = \int_0^{\ell(x,v,y,h)} \zeta(s/\tau) e^{-s^2/2h} ds$$

<u>Goal :</u> determine $\ell \sim \sum_{j\geq 0} \ell_j h^j$ in order to get $\|Pu\| = O(h^3)\sqrt{\lambda}$

$\hookrightarrow \ell = \ell_0 + \ell_1 h$

One can show that

$$Pu = h(w + r) e^{-\left(f - f(\mathbf{m}) + \frac{\ell^2}{2}\right)/h}, \tag{5}$$

with $r \equiv 0$ for X near $\mathbf{s}$ and where

$$P = -h \operatorname{div} \circ A \circ h\nabla + \frac{1}{2}(b \cdot h\nabla + h \operatorname{div} \circ b) + c$$

$\rightsquigarrow w = w_0 + w_1 h + O(h^2)$ with

$$\begin{cases} w_0 = (b^0 + 2A\nabla f) \cdot \nabla \ell_0 + A\nabla \ell_0 \cdot \nabla \ell_0 \ \ell_0, \\ w_1 = (b^0 + 2A(\nabla f + \ell_0 \nabla \ell_0)) \cdot \nabla \ell_1 + A\nabla \ell_0 \cdot \nabla \ell_0 \ \ell_1 + R_1 \end{cases}$$

Need : $w_0 = O(X^4)$ and $w_1 = O(X^2)$. Hence we set

$\ell_0(X) = \xi \cdot X + \ell_{0,2}(X) + \ell_{0,3}(X)$, $\xi \in \mathbb{R}^d$ TBD

$\ell_1(X) = \ell_{1,0} + \ell_{1,1}(X)$ with $\ell_{k,j} \in \mathcal{P}^j_{hom}$

$\hookrightarrow w_0 = w_{0,1} + w_{0,2} + w_{0,3}$, and $w_1 = w_{1,0} + w_{1,1}$ with $w_{k,j} \in \mathcal{P}^j_{hom}$

$$\begin{cases} w_{0,1} = \Lambda\xi \cdot X + A\xi \cdot \xi \ \xi \cdot X, \\ w_{0,j} = (\Upsilon X \cdot \nabla + \mu)\ell_{0,j} + R_{0,j} \quad j \in \{2,3\}, \end{cases}$$

Eikonal equation

$\rightarrow$ $w_{0,1}$: Eigenvalue problem for Λ, $A \geq 0$ so we need a negative one.

$$\Lambda = \begin{pmatrix} 0 & -\operatorname{Hess}_{\mathbf{s}} V & 0 \\ \mathrm{Id} & \gamma \,\mathrm{Id} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

When solved, we obtain $A\xi \cdot \xi = \mu = \frac{1}{2}(-\gamma + \sqrt{\gamma^2 + 4\eta}) > 0$ where η is the unique negative eigenvalue of $\operatorname{Hess} V(\mathbf{s})$.

$\rightarrow$ $w_{0,j}, j \geq 2$: Show that $\mathcal{L} = \Upsilon X \cdot \nabla + \mu$ is invertible on $\mathcal{P}^j_{hom}$

[Bony, Le Peutrec, Michel '22]

$$\hookrightarrow \quad \sigma(\Upsilon) \subset \{\operatorname{Re} z \geq 0\} \Rightarrow \sigma(\Upsilon X \cdot \nabla) \subset \{\operatorname{Re} z \geq 0\}.$$

$$\begin{cases} w_{1,0} = \mu\ell_{1,0} + b^1 \cdot \xi - \operatorname{div} A\nabla\ell_{0,2}, \\ w_{1,1} = \mathcal{L}\ell_{1,1} + R_{1,1}. \end{cases}$$

$$\rightsquigarrow \quad Pu = hO(X^4 + X^2 h + h^2)e^{-(f - f(\mathbf{m}) + \frac{\ell^2}{2})/h}. \tag{6}$$

→ Geometric constructions around $\mathbf{s}, \underline{\mathbf{m}}, \widehat{\mathbf{m}}$ and associated cutoffs :

Definition

We define our quasimode the following way

$$\begin{cases} \psi_{\underline{\mathbf{m}}}(X) = 2e^{-\frac{f - f(\underline{\mathbf{m}})}{h}}, \; \varphi_{\underline{\mathbf{m}}} = \frac{\psi_{\underline{\mathbf{m}}}}{\|\psi_{\underline{\mathbf{m}}}\|}, \\ \psi_{\widehat{\mathbf{m}}}(X) = \theta(X)(\chi_\ell(X) + 1)e^{-\frac{f - f(\widehat{\mathbf{m}})}{h}}, \; \varphi_{\widehat{\mathbf{m}}} = \frac{\psi_{\widehat{\mathbf{m}}}}{\|\psi_{\widehat{\mathbf{m}}}\|}. \end{cases}$$

Recalling $\chi_\ell(x, v, y) = c_h^{-1} \int_0^{\ell(x,v,y,h)} \zeta(s/\tau)e^{-s^2/2h} ds.$

Interaction matrix

Proposition

For $\tau > 0$ *then* $\delta > 0$ *small enough,* $\exists c > 0$ *such that* $\forall \mathbf{m}, \mathbf{m}' \in \mathcal{U}^{(0)} = \{\widehat{\mathbf{m}}, \underline{\mathbf{m}}\}$ *and* $h > 0$ *small,*

i) $\langle \varphi_{\mathbf{m}}, \varphi_{\mathbf{m}'} \rangle = \delta_{\mathbf{m},\mathbf{m}'} + O(e^{-c/h})$,

ii) $\langle P\varphi_{\mathbf{m}}, \varphi_{\mathbf{m}} \rangle = he^{-2S(\mathbf{m})/h} \dfrac{\mu(s)}{2\pi} \dfrac{D_{\mathbf{m}}}{D_{\mathbf{s}}}(1 + O(\sqrt{h}))$

iii) $\|P\varphi_{\mathbf{m}}\|^2 = O(h^4)\langle P\varphi_{\mathbf{m}}, \varphi_{\mathbf{m}} \rangle$

iv) $\|P^*\varphi_{\mathbf{m}}\|^2 = O(h)\langle P\varphi_{\mathbf{m}}, \varphi_{\mathbf{m}} \rangle$

Denoting $D_{x^*} = |\det \mathrm{Hess}_{x^*}(f)|^{1/2}$, $S(\widehat{\mathbf{m}}) = f(\mathbf{s}) - f(\widehat{\mathbf{m}})$ and $S(\underline{\mathbf{m}}) = +\infty$.

Outline of proof : Laplace method and the use of
$P\psi_{\mathbf{m}} = \sqrt{h}O(X^4 + X^2h + h^2)e^{-(f - f(\mathbf{m}) + \frac{\ell^2}{2})/h}$.

We denote $\tilde{\lambda} = \langle P\,\varphi_{\widehat{\mathbf{m}}}, \varphi_{\widehat{\mathbf{m}}}\rangle$ and we obtain

$$\mathrm{Mat}_e P_{|\,\mathrm{span}(e)} = \begin{pmatrix} 0 & 0 \\ 0 & \tilde{\lambda}(1 + O(\sqrt{h})) \end{pmatrix},$$

where $e = (\varphi_{\underline{\mathbf{m}}}, e_1)$ is an orthonormal basis of the space of eigenvectors associated to the small eigenvalues $\{0, \lambda\}$.

What's next ?

We consider $P = X + N$ acting on $(x, v) \in \mathbb{R}^{d+d'}$ with

$$\begin{cases} X = \alpha(x,v) \cdot h\partial_x + \beta(x,v) \cdot h\partial_v + \frac{h}{2}(\mathrm{div}_x\,\alpha + \mathrm{div}_v\,\beta), \\ N = -h^2\Delta_v + 4|\Sigma^T\Sigma v|^2 - 2hTr(\Sigma^T\Sigma). \end{cases}$$

- Δ_v : Laplacian acting on v only,
- α, β smooth,
- $\Sigma \in \mathcal{M}_{d'}(\mathbb{R})$ fixed matrix,
- $X(e^{-f/h}) = N(e^{-f/h}) = 0,\ f(x,v) = V(x) + |\Sigma v|^2,\ V$ not Morse.

Bibliography

J.-F. Bony, D. Le Peutrec, and L. Michel, *Eyring-Kramers law for Fokker-Planck type differential operators.*
arXiv:2201.01660.

J. Dolbeault, C. Mouhot, and C. Schmeiser, *Hypocoercivity for linear kinetic equations conserving mass*, Trans. Amer. Math. Soc., 367 (2015), pp. 3807–3828.

B. Helffer, M. Klein, and F. Nier, *Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach*, Mat. Contemp., 26 (2004), pp. 41–85.

B. Helffer and J. Sjöstrand, *Puits multiples en mécanique semi-classique. IV. Étude du complexe de Witten*, Comm. Partial Differential Equations, 10 (1985), pp. 245–340.

F. Hérau, M. Hitrik, and J. Sjöstrand, *Tunnel effect for Kramers-Fokker-Planck type operators : return to equilibrium and applications*, Int. Math. Res. Not. IMRN, (2008).

B. Leimkuhler, M. Sachs, and G. Stoltz, *Hypocoercivity properties of adaptive langevin dynamics*, SIAM Journal on Applied Mathematics, 80 (2020), pp. 1197–1222.

T. Lelièvre, M. Rousset, and G. Stoltz, *Free energy computations*, Imperial College Press, 2010.
A mathematical perspective.