Metastabilité et loi de Kramers pour des diffusions dans des potentiels à selles non quadratiques

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Reversible diffusion

$\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$

- $V : \mathbb{R}^d \to \mathbb{R}$: potential, growing at infinity
- W_t: d-dim Brownian motion on $(\Omega, \mathcal{F}, \mathbb{P})$

Reversible w.r.t.
invariant measure:

$$\mu_\varepsilon(\mathrm{d}x) = \frac{\mathrm{e}^{-V(x)/\varepsilon}}{Z_\varepsilon}\,\mathrm{d}x$$

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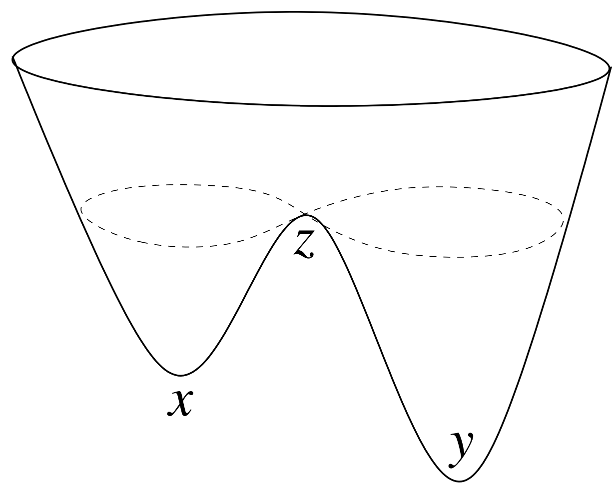

τ_y^x: first-hitting time of small ball $\mathcal{B}_\varepsilon(y)$, starting in x

"Eyring–Kramers law" (Eyring 1935, Kramers 1940)

- Dim 1: $\mathbb{E}[\tau_y^x] \simeq \dfrac{2\pi}{\sqrt{V''(x)|V''(z)|}}\,\mathrm{e}^{[V(z)-V(x)]/\varepsilon}$
- Dim$\geqslant 2$: $\mathbb{E}[\tau_y^x] \simeq \dfrac{2\pi}{|\lambda_1(z)|}\sqrt{\dfrac{|\det(\nabla^2 V(z))|}{\det(\nabla^2 V(x))}}\,\mathrm{e}^{[V(z)-V(x)]/\varepsilon}$

Towards a proof of Kramers' law

- Large deviations (Wentzell & Freidlin 1969):

$$\lim_{\varepsilon\to 0} \varepsilon \log(\mathbb{E}[\tau_y^x]) = V(z) - V(x)$$

- Analytic (Helffer, Sjöstrand 85, Miclo 95, Mathieu 95, Kolokoltsov 96,...): low-lying spectrum of generator
- Potential theory/variational (Bovier, Eckhoff, Gayrard, Klein 2004):

$$\mathbb{E}[\tau_y^x] = \frac{2\pi}{|\lambda_1(z)|}\sqrt{\frac{|\det(\nabla^2 V(z))|}{\det(\nabla^2 V(x))}}\,\mathrm{e}^{[V(z)-V(x)]/\varepsilon}\Big[1+\mathcal{O}(\varepsilon^{1/2}|\log\varepsilon|^{1/2})\Big]$$

and similar asymptotics for eigenvalues of generator
- Witten complex (Helffer, Klein, Nier 2004): full asymptotic expansion of prefactor
- Distribution of τ_y^x (Day 1983, Bovier *et al* 2005):

$$\lim_{\varepsilon\to 0} \mathbb{P}\Big\{\tau_y^x > t\mathbb{E}[\tau_y^x]\Big\} = \mathrm{e}^{-t}$$

The question

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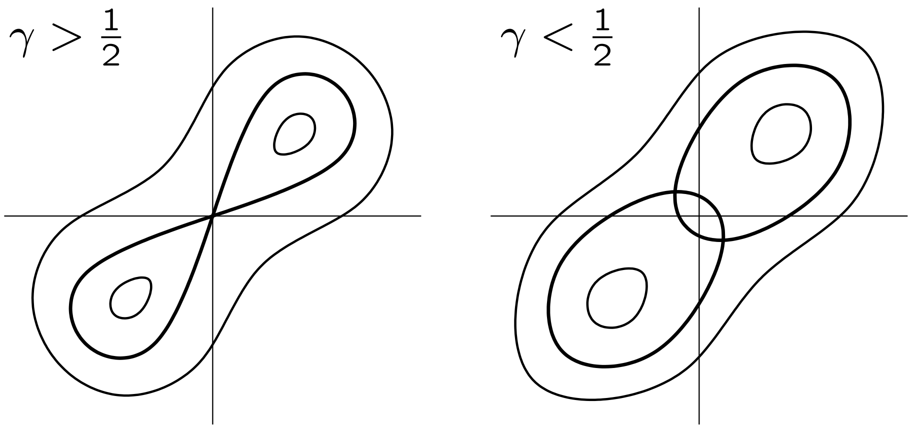
Dependence on parameter $\Rightarrow$ Bifurcations

Example: $V_\gamma(x_1, x_2) = U(x_1) + U(x_2) + \frac{\gamma}{2}(x_1 - x_2)^2$

$$U(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2$$

Rotation of $\pi/4$: $\widehat{V}_\gamma(y_1, y_2) = -\frac{1}{2}y_1^2 - \frac{1-2\gamma}{2}y_2^2 + \frac{1}{8}(y_1^4 + 6y_1^2y_2^2 + y_2^4)$

$\det \nabla^2 \widehat{V}_\gamma(0,0) = \frac{1-2\gamma}{4}$: Pitchfork bifurcation at $\gamma = \frac{1}{2}$



Definition of saddles

▷ Communication height $\overline{V}(x,y) = \inf_{\gamma:x\to y} \sup_{t\in[0,|\gamma|]} V(\gamma(t))$

▷ For $A, B \subset \mathbb{R}^d$: $\overline{V}(A,B) = \inf_{x\in A, y\in B} \overline{V}(x,y)$

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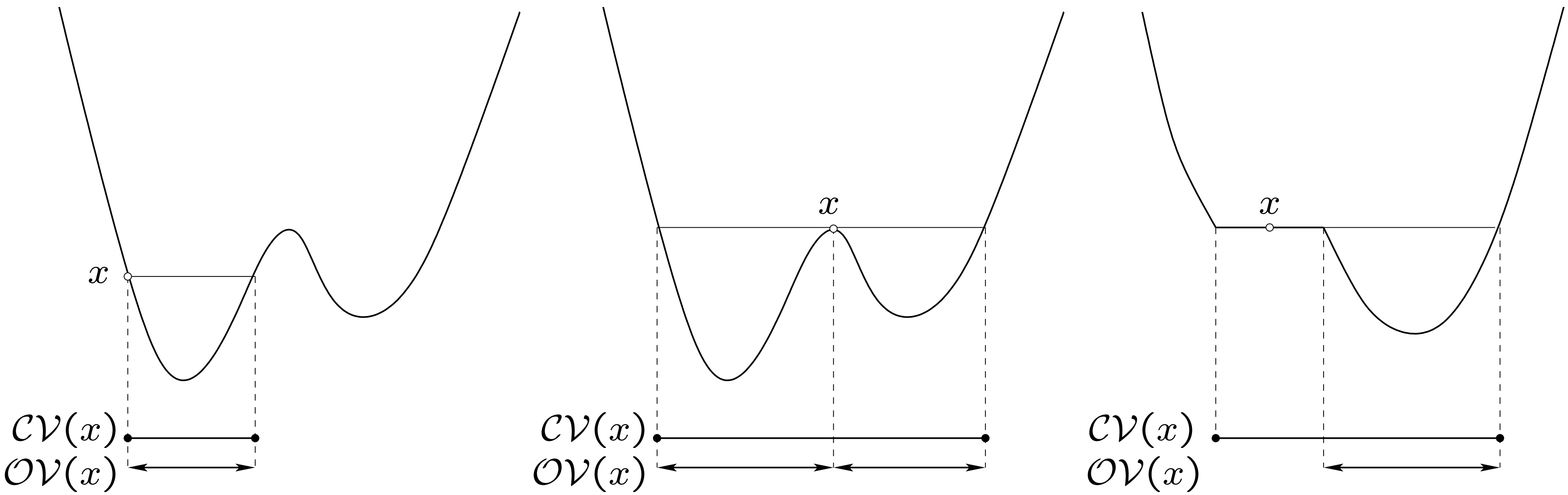

- ▷ Closed valley: $\mathcal{CV}(x) = \{y \in \mathbb{R}^d \colon \overline{V}(x,y) = V(x)\}$
- ▷ Open valley: $\mathcal{OV}(x) = \{y \in \mathcal{CV}(x) \colon V(y) < V(x)\}$

Definition of saddles

Definition: z is a saddle if $\exists \varepsilon > 0$ s.t.

1. $\mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(z)$ non-empty and not path-connected
2. $(\mathcal{OV}(z) \cap \mathcal{B}_\varepsilon(z)) \cup \{z\}$ path-connected

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Let z be a saddle. Then

- ▷ $V \in \mathcal{C}^1 \Rightarrow \nabla V(z) = 0$
- ▷ $V \in \mathcal{C}^2 \Rightarrow \nabla^2 V(z)$ has at least 1 ev $\leqslant 0$ and at most 1 ev < 0
- ▷ $V \in \mathcal{C}^2, \nabla V(z) = 0, \det \nabla^2 V(z) \neq 0$
  $\Rightarrow z$ saddle iff $\nabla^2 V(z)$ has exactly 1 ev < 0

Nonquadratic saddle: $\det \nabla^2 V(z) = 0$
e.g. $\nabla^2 V(z)$ has ev $\lambda_1 < 0 = \lambda_2 < \lambda_3 \leqslant \dots \leqslant \lambda_d$

Classification of nonquadratic saddles

Assume $V \in \mathcal{C}^4$ and $\nabla^2 V(0)$ has ev $\lambda_1 < 0 = \lambda_2 < \lambda_3 \leqslant \dots \leqslant \lambda_d$

$$V(x) = -\frac{1}{2}|\lambda_1| x_1^2 + \frac{1}{2}\sum_{j=3}^{d} \lambda_j x_j^2 + \sum_{1 \leqslant i \leqslant j \leqslant k \leqslant d} V_{ijk} x_i x_j x_k + \dots$$

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Normal form: There exists polynomial $g(y) = \mathcal{O}(\|y\|^2)$ s.t.

$$V(y + g(y)) = -\frac{1}{2}|\lambda_1| y_1^2 + \frac{1}{2}\sum_{j=3}^{d} \lambda_j y_j^2 + C_3 y_2^3 + C_4 y_2^4 + \dots$$

($C_3 = V_{111}$, C_4 explicitly known)

Proposition:

- $C_3 \neq 0$ or $C_4 < 0 \Rightarrow z = 0$ is not a saddle
- $C_3 = 0$ and $C_4 > 0 \Rightarrow z = 0$ is a saddle
- $C_3 = C_4 = 0 \Rightarrow$ depends on higher-order terms

Potential theory

Consider first Brownian motion $W_t^x = x + W_t$

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Fact 1: $w_A(x) = \mathbb{E}[\tau_A^x]$ satisfies

$$\Delta w_A(x) = 1 \qquad x \in A^c$$
$$w_A(x) = 0 \qquad x \in A$$

$G_{A^c}(x, y)$ Green's function $\Rightarrow w_A(x) = \int_{A^c} G_{A^c}(x, y)\, \mathrm{d}y$

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Fact 2: $h_{A,B}(x) = \mathbb{P}[\tau_A^x < \tau_B^x]$ satisfies

$$\begin{aligned} \Delta h_{A,B}(x) &= 0 \qquad & x \in (A \cup B)^c \\ h_{A,B}(x) &= 1 \qquad & x \in A \\ h_{A,B}(x) &= 0 \qquad & x \in B \end{aligned}$$

$\Rightarrow h_{A,B}(x) = \int_{\partial A} G_{B^c}(x,y)\,\rho_{A,B}(\mathrm{d}y)$

$\rho_{A,B}$: "surface charge density" on ∂A

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Key observation: let $C = \mathcal{B}_\varepsilon(x)$, then

$$\begin{aligned} \int_{A^c} h_{C,A}(y)\,\mathsf{d}y &= \int_{A^c} \int_{\partial C} G_{A^c}(y,z) \rho_{C,A}(\mathsf{d}z)\,\mathsf{d}y \\ &= \int_{\partial C} w_A(z) \rho_{C,A}(\mathsf{d}z) \simeq w_A(x)\,\mathsf{cap}_C(A) \end{aligned}$$

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$$\Rightarrow \qquad \mathbb{E}[\tau_A^x] = w_A(x) \simeq \frac{\int_{A^c} h_{\mathcal{B}_\varepsilon(x),A}(y)\,\mathrm{d}y}{\mathrm{cap}_{\mathcal{B}_\varepsilon(x)}(A)}$$

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Variational representation: Dirichlet form

$$\operatorname{cap}_A(B) = \int_{(A\cup B)^c} \|\nabla h_{A,B}(x)\|^2\,\mathrm{d}x = \inf_{h\in\mathcal{H}_{A,B}} \int_{(A\cup B)^c} \|\nabla h(x)\|^2\,\mathrm{d}x$$

($\mathcal{H}_{A,B}$: set of sufficiently smooth functions satisfying b.c.)

Potential theory

General case: $\mathrm{d}x_t = -\nabla V(x_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$

Generator: $\Delta \mapsto \varepsilon\Delta - \nabla V \cdot \nabla$

Then

$$\mathbb{E}[\tau_A^x] = w_A(x) \simeq \frac{\int_{A^c} h_{\mathcal{B}_\varepsilon(x),A}(y)\,\mathrm{e}^{-V(y)/\varepsilon}\,\mathrm{d}y}{\mathrm{cap}_{\mathcal{B}_\varepsilon(x)}(A)}$$

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Rough a priori bounds on h show that if x potential minimum,

$$\int_{A^c} h_{\mathcal{B}_\varepsilon(x),A}(y)\,\mathrm{e}^{-V(y)/\varepsilon}\,\mathrm{d}y \simeq \frac{(2\pi\varepsilon)^{d/2}\,\mathrm{e}^{-V(x)/\varepsilon}}{\sqrt{\det(\nabla^2 V(x))}}$$

Main result

Assume

- $z = 0$ saddle, A, B in different components of $\mathcal{OV}(z)$
- Normal form $V(y) = -u_1(y_1) + u_2(y_2) + \frac{1}{2}\sum_{j=3}^{d} \lambda_j y_j^2 + \dots$
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Theorem: For some known $\alpha > 0$ depending on growth cond.

$$\mathrm{cap}_A(B) = \varepsilon \frac{\int_{-\infty}^{\infty} \mathrm{e}^{-u_2(y_2)/\varepsilon} \, \mathrm{d}y_2}{\int_{-\infty}^{\infty} \mathrm{e}^{-u_1(y_1)/\varepsilon} \, \mathrm{d}y_1} \prod_{j=3}^{d} \sqrt{\frac{2\pi\varepsilon}{\lambda_j}} \Big[1 + \mathcal{O}((\varepsilon|\log\varepsilon|)^{\alpha})\Big]$$

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Proof:

▷ Upper bound: Use $h(y) = f(y_1)$ in Dirichlet form, f solution of $\varepsilon f''(y_1) - u_1'(y_1) f'(y_1) = 0$ with b.c. $f(\pm\delta(\varepsilon)) = 0, 1$

▷ Lower bound: Bound Dirichlet form below by restricting domain, taking only 1st component of gradient and use for b.c. a priori bound on $h_{A,B}$

Applications

1. Quartic case: $V(y) = -\frac{1}{2}|\lambda_1|y_1^2 + C_4 y_2^4 + \frac{1}{2}\sum_{j=3}^{d} \lambda_j y_j^2 + \dots$

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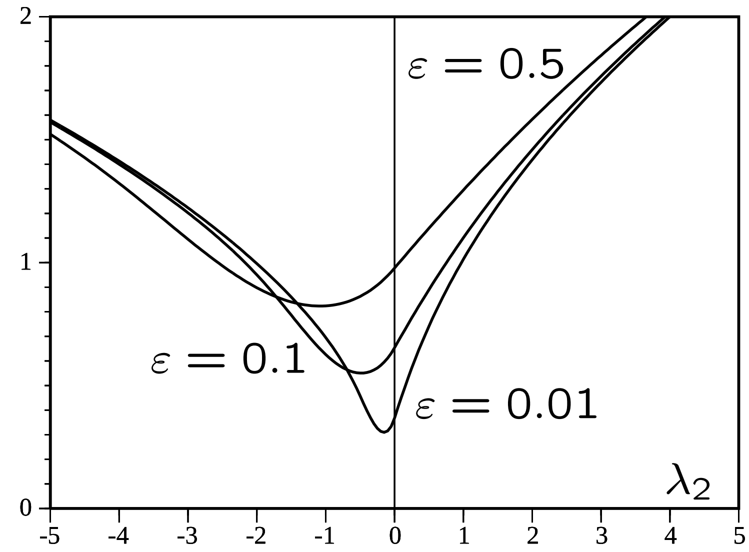
$$\mathbb{E}[\tau_y^x] = 2\pi\sqrt{\frac{(\lambda_2+\sqrt{2\varepsilon C_4})\lambda_3\dots\lambda_d}{|\lambda_1|\det(\nabla^2 V(x))}}\frac{\mathrm{e}^{\overline{V}(x,y)/\varepsilon}}{\Psi_+(\lambda_2/\sqrt{2\varepsilon C_4})}\Big[1+R(\varepsilon)\Big]$$

for $\lambda_2 > 0$, where

$\Psi_+(\alpha) = \sqrt{\frac{\alpha(1+\alpha)}{8\pi}}\,\mathrm{e}^{\alpha^2/16}\,K_{1/4}\Big(\frac{\alpha^2}{16}\Big)$

$\lim_{\alpha\to+\infty}\Psi_+(\alpha) = 1$

Similar expression for $\lambda_2 < 0$ involving $I_{\pm 1/4}$



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References

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- N. B. and Barbara Gentz, *The Eyring–Kramers law for potentials with non-quadratic saddles*, `hal-00294931` (2008)