Statistical mechanics and computation of large deviation rate functions

Metastability in systems of coupled multistable SDEs

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Interacting SDEs with noise

Example 1 [B, Fernandez, Gentz, Nonlinearity 2007]

- ▷ *N* particles on a circle $\mathbb{Z}/N\mathbb{Z}$
- Bistable local dynamics
- Ferromagnetic nearest neighbour coupling
- Independent noise on each site



$$dx_t^{i} = [x_t^{i} - (x_t^{i})^3] dt + \frac{\gamma}{2} [x_t^{i+1} - 2x_t^{i} + x_t^{i-1}] dt + \sqrt{2\varepsilon} dW_t^{i}$$

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Gradient system $dx_t = -\nabla V(x_t) dt + \sqrt{2\varepsilon} dW_t$ potential $V(x) = \sum_i U(x^i) + \frac{\gamma}{4} \sum_i (x^{i+1} - x^i)^2 \qquad U(\xi) = \frac{1}{4}\xi^4 - \frac{1}{2}\xi^2$

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Example 2 [B, Dutercq, JoTP 2015]: Same potential + constraint $\sum_{i} x^{i} = 0$

General gradient systems with noise

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

 $V:\mathbb{R}^{N}\rightarrow\mathbb{R}:$ confining potential, class \mathcal{C}^{2}

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Dynamics \sim markovian jump process on $\mathcal{G} = (\mathcal{X}_0, \mathcal{E}), \ \mathcal{E} \subset \mathcal{X}_1$



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ün	ganzjährig offen
u	Wintersperre

Pass	Land	Passhöhe (m.ü.M.)
Flüela	CH	2383
Albula	CH	2312
Julier	CH	2284
Maloja	CH	1815
Splügen	I - CH	2115
Reschen	A - I	1507
Ofen	CH	2149
Umbrail	CH - I	2502
Stilfserjoch	1	2757
Foscagno	1	2291
Bernina	CH - I	2323
Fla. di Livigno	1	2315
	Pass Flüela Albula Julier Maloja Splügen Reschen Ofen Umbrail Stilfserjoch Foscagno Bernina Fla. di Livigno	Pass Land Flüela CH Albula CH Julier CH Maloja CH Splügen I - CH Reschen A - I Ofen CH - I Sultiserjoch I Foscagno I Bernina CH - I Fla.d Litvigno I

Wentzell–Freidlin theory

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

Large-deviation rate function: $I_{[0,T]}(\varphi) = \frac{1}{2} \int_0^T \|\dot{\varphi}(t) - f(\varphi(t))\|^2 dt$

Noise-induxed exit from domain \mathcal{D} containing unique attractor x^*

Mean exit time:

 $\lim_{\varepsilon \to 0} 2\varepsilon \log \mathbb{E}^{x_0}[\tau] = \inf_{z \in \partial \mathcal{D}} \overline{V}(x^*, z) \qquad \overline{V}(x^*, z) = \inf_{T > 0} \inf_{\varphi: x^* \to z} I_{[0, T]}(\varphi)$

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Case of multiple attractors: $V^{(k)} = \min_{g \ W\text{-graph}, |W|=k} \sum_{(\alpha \to \beta) \in g} \overline{V}(\alpha, \beta)$ Small eigenval. λ_k of generator satisfy $-\lim_{\varepsilon \to 0} \varepsilon \log(|\lambda_k|) = V^{(k)} - V^{(k+1)}$ Efficient computation of λ_k : [Cameron and Vanden–Eijnden 2014]

Eyring–Kramers law for $dx_t = -\nabla V(x_t) dt + \sqrt{2\varepsilon} dW_t$

Definition: Communication height $H(x_i^*, x_j^*) = \inf_{\gamma: x_i^* \to x_j^*} \sup_t V(\gamma_t) - V(x_i^*)$ $= V(z_{ii}^*) - V(x_i^*)$

Definition: Metastable hierarchy $x_1^* \prec x_2^* \prec \cdots \prec x_n^* \Leftrightarrow \exists \theta > 0: \forall k$ $H_k := H(x_k^*, \{x_1^*, \dots, x_{k-1}^*\})$ $\leq \min_{i < k} H(x_i^*, \{x_1^*, \dots, x_{i-1}^*, x_{i+1}^*, \dots, x_k^*\}) - \theta$



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Theorem: Eyring–Kramers law [Bovier,Eckhoff,Gayrard,Klein 2004] $\tau_k = \text{first-hitting time of nbh of } \{x_1^*, \dots, x_k^*\} \qquad \lambda_k = k^{\text{th}} \text{ ev of generator}$ $\mathbb{E}^{x_k^*}[\tau_{k-1}] = \frac{2\pi}{|\lambda_-(z_k^*)|} \sqrt{\frac{|\det \nabla^2 V(z_k^*)|}{\det \nabla^2 V(x_k^*)}} e^{H_k/\varepsilon} [1 + \mathcal{O}_{\varepsilon}(1)] \simeq |\lambda_k|^{-1}$

Potential landscape for Example 1

$$V(x) = \sum_{i \in \mathbb{Z}/N\mathbb{Z}} U(x^{i}) + \frac{\gamma}{4} \sum_{i \in \mathbb{Z}/N\mathbb{Z}} (x^{i+1} - x^{i})^{2} \qquad U(\xi) = \frac{1}{4}\xi^{4} - \frac{1}{2}\xi^{2}$$

 $\gamma = 0: \ \mathcal{X} = \{-1, 0, 1\}^N$, $\mathcal{X}_0 = \{-1, 1\}^N$, $\mathcal{X}_1 = \{x \in \mathcal{X}: \text{ one } x^i = 0\}$

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Theorem [BFG, Nonlinearity 2007] No bifurcation for $0 \le \gamma \le \gamma^*(N)$ where $\gamma^*(N) > \frac{1}{4} \quad \forall N \ge 2$

 $V_{\gamma}(z_{\gamma}^{*}) = V_{0}(z_{0}^{*}) + \gamma(\# \text{ interfaces}) + \cdots$ Ising-like dynamics





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Theorem [BFG, Nonlinearity 2007]

$$\gamma > \frac{1}{2\sin^2(\pi/N)} \Leftrightarrow \mathcal{X}_0 = \{\pm(1,\ldots,1)\}, \ \mathcal{X}_1 = \{0\} \Leftrightarrow \text{Synchronization}$$



++++++++

Transition to synchronization

Symmetry group $G = D_N \times \mathbb{Z}_2 = \langle r, s, c \rangle$ $r(x) = (x^2, x^3, \dots, x^N, x^1)$ $s(x) = (x^N, x^{N-1}, \dots, x^1)$ c(x) = -x

 \mathcal{X} partitionned into group orbits $O_x = \{gx : g \in G\}$ Stabilizer: $G_x = \{g \in G : gx = x\}$ $\Rightarrow |O_x||G_x| = |G|$

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Problem: no metastable hierarchy \Rightarrow Usual Eyring–Kramers law invalid

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Question 3:

What happens when $\gamma \sim N^2$ and $N \to \infty$ in example 1? One expects convergence to Allen–Cahn SPDE

$$\partial_t u(t,x) = \frac{\gamma}{N^2} \Delta u(t,x) + u(t,x) - u(t,x)^3 + \sqrt{2\varepsilon} \xi(t,x)$$

where ξ is space-time white noise

Is there an Eyring-Kramers law for such SPDEs?

Q1: Markovian jump processes with symmetries

Generator L: transition rates $L_{ij} = \frac{c_{ij}}{m_i} e^{-h_{ij}/\varepsilon}$, $c_{ij} = c_{ji}$ $\forall i, j \in \mathcal{X}_0$ Assumptions

- ▷ Reversibility: $m_i e^{-V_i/\varepsilon} L_{ij} = m_j e^{-V_j/\varepsilon} L_{ji}$ $\forall i, j \in \mathcal{X}_0$
- ▷ Symmetry: $L_{ij} = L_{g(i)g(j)}$ $\forall g \in G$, (G, *) a finite group i.e. $\pi(g)L = L\pi(g)$ where $\pi(g)_{ab} = 1_{\{g(a)=b\}}$ permutation matrix
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Main observation: π is a representation: $\pi(g * h) = \pi(g)\pi(h) \forall g, h \in G$ Representation theory of finite groups: $\pi = \bigoplus_{p=0}^{r-1} \alpha^{(p)} \pi^{(p)}$ where $\pi^{(p)}$: irreducible representations of G

$$P^{(p)}L = LP^{(p)}$$
 $p = 0, ..., r - 1$

where $P^{(p)}$: projector on im $\pi^{(p)} \Rightarrow$ each subspace $P^{(p)}\mathbb{C}^n$ invariant for LEach restricted generator satisfies an asymmetric Eyring–Kramers law

Q1: Modified Eyring–Kramers law

Trivial representation: $\pi^{(0)}(g) = 1 \forall g \Rightarrow m \text{ ev } (m = \# \text{ orbits})$

Theorem [B, Dutercq, J Theor Proba 2015]

 $k \leq m$, initial distribution μ uniform on each $A_i, i \geq k$ $\tau_{k-1} =$ first-hitting time of $A_1 \cup A_2 \cup \cdots \cup A_{k-1}$ $G_a := \{g : g(a) = a\}$

$$\mathbb{E}^{\mu}[\tau_{k-1}] = \frac{|\mathcal{G}_{a_i} \cap \mathcal{G}_{a_j}|}{|\mathcal{G}_{a_k}|} \frac{m_{a_k}}{c_{a_i a_j}} e^{H_k/\varepsilon} \left[1 + \mathcal{O}(e^{-\theta/\varepsilon})\right] = \frac{1 + \mathcal{O}(e^{-\theta/\varepsilon})}{\lambda_k^{(0)}}$$

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Other representations: Similar result for process on set of active orbits \Rightarrow clustering of eigenvalues: $\lambda_k^{(p)} = C_k^{(p)} e^{-H_k/\varepsilon}$

$$\xrightarrow{\mathcal{O}(\varepsilon)}_{H_3} \xrightarrow{\mathcal{O}(\varepsilon)}_{H_2} \xrightarrow{\mathcal{O}(\varepsilon)}_{H_1} \rightarrow -\varepsilon \log(-\lambda)$$

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Case of diffusions: similar results [S. Dutercq, PhD thesis, 2015]

Q2: Eyring–Kramers law for nonquadratic saddles

Facts from potential theory: $A, B \subset \mathbb{R}^d$, $\tau_A = \inf\{t > 0 \colon x_t \in A\}$ Committor function: $h_{A,B}(x) = \mathbb{P}^x\{\tau_A < \tau_B\}$

Capacity:
$$\operatorname{cap}(A, B) = \int_{(A \cup B)^c} \|\nabla h_{A,B}(x)\|^2 e^{-V(x)/\varepsilon} dx$$

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

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Theorem: [B & Gentz, MPRF 2010]

▷ Saddle in 0, separating A and B ▷ $V(x) = -u_1(x_1) + u_2(x_2, ..., x_q) + \frac{1}{2} \sum_{j=q+1}^d \lambda_j x_j^2 + \cdots, \quad \lambda_j > 0$ $\operatorname{cap}(A, B) = \varepsilon \frac{\int e^{-u_2(x_2, ..., x_q)/\varepsilon} dx_2 \dots dx_q}{\int e^{-u_1(x_1)/\varepsilon} dx_1} \prod_{j=q+1}^d \sqrt{\frac{2\pi\varepsilon}{\lambda_j}} \left[1 + \mathcal{O}((\varepsilon |\log \varepsilon|)^{\alpha})\right]$

with α related to growth of u_1 and u_2





for $\lambda_2 > 0$ where $\Psi_+(\alpha) = \sqrt{\frac{\alpha(1+\alpha)}{8\pi}} e^{\alpha^2/16} K_{1/4}(\frac{\alpha^2}{16})$ $\lim_{\alpha \to +\infty} \Psi_+(\alpha) = 1$ $\lim_{\alpha \to 0} \Psi_+(\alpha) = \frac{\Gamma(1/4)}{2^{5/4}\pi^{1/2}} \simeq 0.860$ Similar expression for $\lambda_2 < 0$

with $\Psi_{-}(\alpha)$ involving $I_{\pm 1/4}$

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$$\partial_t u_t(x) = \partial_{xx} u_t(x) + f(u_t(x)) + \sqrt{2\varepsilon} \xi(t, x)$$
 e.g. $f(u) = u - u^3$

 $x \in [0, L]$ with periodic or Neumann b.c.

$$u_t(x) = \frac{1}{\sqrt{L}} \sum_{k \in \mathbb{Z}} z_k(t) e^{i\pi kx/L} \quad \Rightarrow \quad dz_t = -\nabla V(z_t) dt + \sqrt{2\varepsilon} dW_t$$
$$V = \int_0^L \left[\frac{1}{2} u'^2 - \frac{1}{2} u^2 + \frac{1}{4} u^4 \right] dx = \frac{1}{2} \sum_{k \in \mathbb{Z}} \lambda_k |z_k|^2 + \frac{1}{4L} \sum_{\sum k_i = 0} z_{k_1} z_{k_2} z_{k_3} z_{k_4}$$

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$$\begin{aligned} u_t(x) &= \frac{1}{\sqrt{L}} \sum_{k \in \mathbb{Z}} z_k(t) e^{i\pi kx/L} \quad \Rightarrow \quad \mathrm{d}z_t = -\nabla V(z_t) \,\mathrm{d}t + \sqrt{2\varepsilon} \,\mathrm{d}W_t \\ V &= \int_0^L \left[\frac{1}{2} u'^2 - \frac{1}{2} u^2 + \frac{1}{4} u^4 \right] \mathrm{d}x = \frac{1}{2} \sum_{k \in \mathbb{Z}} \lambda_k |z_k|^2 + \frac{1}{4L} \sum_{\sum k_i = 0} z_{k_1} z_{k_2} z_{k_3} z_{k_4} \\ \text{Initial cond } u_{\mathrm{in}} \simeq -1. \text{ Target } u_+ \equiv 1, \ \tau_+ = \inf\{t > 0: \|u_t - u_+\|_\infty\} < \rho \\ \text{Transition state: } (\beta = 1 \text{ for Neumann b.c. } \beta = 2 \text{ for periodic b.c.}) \end{aligned}$$

$$u_{\rm ts}(x) = \begin{cases} u_0(x) \equiv 0 & \text{if } L \leqslant \beta \pi \\ u_1(x) \ \beta \text{-kink stationary sol.} & \text{if } L > \beta \pi \end{cases} \quad \text{with ev } \lambda_k = (\frac{\beta k \pi}{L})^2 - 1$$

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 e.g. $f(u) = u - u^3$

 $x \in [0, L]$ with periodic or Neumann b.c.

$$\begin{aligned} u_t(x) &= \frac{1}{\sqrt{L}} \sum_{k \in \mathbb{Z}} z_k(t) e^{i\pi kx/L} \quad \Rightarrow \quad \mathrm{d}z_t = -\nabla V(z_t) \,\mathrm{d}t + \sqrt{2\varepsilon} \,\mathrm{d}W_t \\ V &= \int_0^L \left[\frac{1}{2} u'^2 - \frac{1}{2} u^2 + \frac{1}{4} u^4 \right] \,\mathrm{d}x = \frac{1}{2} \sum_{k \in \mathbb{Z}} \lambda_k |z_k|^2 + \frac{1}{4L} \sum_{\sum k_i = 0} z_{k_1} z_{k_2} z_{k_3} z_{k_4} \\ \text{Initial cond } u_{\mathrm{in}} \simeq -1. \text{ Target } u_+ \equiv 1, \ \tau_+ = \inf\{t > 0 \colon \|u_t - u_+\|_\infty\} < \rho \\ \text{Transition state: } (\beta = 1 \text{ for Neumann b.c. } \beta = 2 \text{ for periodic b.c.}) \end{aligned}$$

$$u_{\rm ts}(x) = \begin{cases} u_0(x) \equiv 0 & \text{if } L \leq \beta \pi \\ u_1(x) \ \beta \text{-kink stationary sol.} & \text{if } L > \beta \pi \end{cases} \quad \text{with ev } \lambda_k = (\frac{\beta k \pi}{L})^2 - 1$$

[Faris & Jona-Lasinio 82]: LDP $\Rightarrow \mathbb{E}^{u_{in}}[\tau_+] \simeq e^{(V[u_{ts}] - V[u_-])/\varepsilon}$ [Maier & Stein 01]: formal computation; for Neumann b.c. $\Rightarrow \mathbb{E}^{u_{in}}[\tau_+] \simeq 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k}} e^{(V[u_{ts}] - V[u_-])/\varepsilon} \qquad (\nu_k = \text{ev at } u_-)$

Metastability in systems of coupled multistable SDEs

Theorem: [B & Gentz, Elec J Proba 2013]

Neumann b.c:

▷ If $L < \pi - c$, then

$$\mathbb{E}^{u_{\rm in}}[\tau_+] = 2\pi \sqrt{\frac{1}{|\lambda_0|\nu_0}} \prod_{k=1}^{\infty} \frac{\lambda_k}{\nu_k} \, \operatorname{e}^{(V[u_{\rm ts}] - V[u_-])/\varepsilon} \left[1 + \mathcal{O}(\varepsilon^{1/2} |\log \varepsilon|^{3/2})\right]$$

▷ If $L > \pi + c$, then same formula with extra factor $\frac{1}{2}$ (since 2 saddles)

Theorem: [B & Gentz, Elec J Proba 2013]

Neumann b.c:

▷ If $L < \pi - c$, then

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▷ If $L > \pi + c$, then same formula with extra factor $\frac{1}{2}$ (since 2 saddles) ▷ If $\pi - c \leq L \leq \pi$, then

$$\mathbb{E}^{u_{\rm in}}[\tau_+] = 2\pi \sqrt{\frac{\lambda_1 + \sqrt{3\varepsilon/2L}}{|\lambda_0|\nu_0\nu_1}} \prod_{k=2}^{\infty} \frac{\lambda_k}{\nu_k} \frac{{\rm e}^{(V[u_{\rm ts}] - V[u_-])/\varepsilon}}{\Psi_+(\lambda_1/\sqrt{3\varepsilon/2L})} [1 + R(\varepsilon)]$$

with Ψ_+ as before

 \triangleright If $\pi \leqslant L \leqslant \pi + c$, similar formula with Ψ_-

Periodic b.c: Similar expressions with different Ψ_{\pm} and extra factor $arepsilon^{1/2}$

Concluding remarks

Irreversible systems:

Cycling: ∂D periodic orbit, WKB doesn't work [Day '92, B & Gentz '14] Transition-path theory [Vanden-Eijnden & E '06, Lu & Nolen '15]

▷ SPDEs in higher space dim: Regularity structures [Hairer & Weber '14]

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