

Thermodynamics of Piecewise Deterministic Markov Processes

Alessandra Faggionato

University La Sapienza - Rome

D. Gabrielli, M. Ribezzi Crivellari

Motivations

- **Biophysics**: modeling of molecular motors
- **Statistical physics**: the continuous variable in PDMPs follows a non-Markovian stochastic dynamics, on which to test **Macroscopic Fluctuation Theory**.

Macroscopic Fluctuation Theory: developed by Bertini, De Sole, Gabrielli, Jona-Lasinio, Landim; Bodineau, Derrida et al. It concerns large deviations in (Markov) stochastic systems and establishes relations of physical relevance for large deviations (as fluctuation–dissipation relations, Gallavotti-Cohen typed symmetries, generalized Onsager–Machlup symmetry)

Some targets

- characterize **stationary distribution**
 - investigate **time-reversed process** under stationarity
 - derive **averaging principle**, **static** and **dynamical large deviations**
 - restricting to the continuous variable, check the validity of the **fluctuation-dissipation relation**, **Gallavotti-Cohen typed symmetry**
- ① (FGR) *Non-equilibrium thermodynamics of piecewise deterministic Markov process*. J. Stat. Phys. (2009)
 - ② (FGR) *Averaging and Large Deviation Principles for fully-coupled PDMPs ...* MPRF (2010)
 - ③ (FG) *A representation formula for the Freidlin-Wentzell quasipotential on the one dimensional torus*. AIHP (2012)

PDMPs (random switching fields)

State $(\mathbf{x}, \sigma) \in \Omega \times \Gamma$,

$\Omega \subset \mathbb{R}^d$ or $\Omega = \mathbb{T}^d$, $|\Gamma| < +\infty$

Molecular motor: x **mechanical state**, σ **chemical state**

$\lambda > 0$ parameter

Markov generator:

$$\begin{aligned} \mathbf{L}f(\mathbf{x}, \sigma) &= \mathbf{F}_\sigma(\mathbf{x}) \cdot \nabla f(\mathbf{x}, \sigma) + \lambda \sum_{\sigma' \in \Gamma} r(\sigma, \sigma' | \mathbf{x}) (f(\mathbf{x}, \sigma') - f(\mathbf{x}, \sigma)) \\ &= \mathbf{F}_\sigma(\mathbf{x}) \cdot \nabla f(\mathbf{x}, \sigma) + \lambda \mathbf{L}_c[\mathbf{x}]f(\mathbf{x}, \sigma). \end{aligned}$$

$F_\sigma(x)$ = vector fields, $r(\sigma, \sigma' | x)$ = rates of jumps.

Assumptions: (i) mechanical confinement, (ii) no explosion,
(iii) $\mathbf{L}_c[\mathbf{x}]$ is irreducible

High jump frequency limit: averaging principle

$\mu(\sigma|\mathbf{x})$: invariant distribution for $L_c[x]$, quasi-stationary measure

$\bar{\mathbf{F}}(\mathbf{x}) = \sum_{\sigma} \mu(\sigma|\mathbf{x}) \mathbf{F}_{\sigma}(\mathbf{x})$, averaged vector field

$\mathbb{P}_{\mathbf{x}_0, \sigma_0}^{\lambda}$ law of PDMP starting at (x_0, σ_0)

Theorem

Given $x_0 \in \Omega$ let

$$\dot{x}_{\infty}(t) = \bar{F}(x_{\infty}(t)), \quad x_{\infty}(0) = x_0.$$

Then, as $\lambda \rightarrow \infty$, in $\mathbb{P}_{x_0, \sigma_0}^{\lambda}$ probability it holds:

$$\begin{cases} x(t) \rightarrow x_{\infty}(t) \text{ in } C([0, T]; \Omega), \|\cdot\|_{\infty} \\ \mathbf{1}(\sigma(t) = \sigma) dt \rightarrow \mu(\sigma|x_{\infty}(t)) dt \text{ weakly, for all } \sigma \in \Gamma. \end{cases}$$

High jump frequency limit: LDP

Given $\sigma \in \Gamma$, $\{\sigma(\mathbf{t})\}_{\mathbf{t} \in [0, \mathbf{T}]} \rightsquigarrow \mathbb{1}(\sigma(t) = \sigma) dt$

Space: $\mathbf{C}([0, \mathbf{T}]; \Omega) \times \mathcal{M}([0, \mathbf{T}])^\Gamma$

Process concentrated on compact subspace $\mathcal{Y}_{\mathbf{x}_0}$:

$\mathbf{x}(\cdot) \in \mathbf{C}([0, \mathbf{T}]; \Omega)$, $(\nu_\sigma)_{\sigma \in \Gamma} \in \mathcal{M}([0, \mathbf{T}])^\Gamma$

such that

- 1 $\nu_\sigma = \chi_\sigma(\mathbf{t}) d\mathbf{t}$
- 2 $\sum_{\sigma \in \Gamma} \chi_\sigma(\mathbf{t}) = \mathbf{1}$ a.e.
- 3 $\mathbf{x}(\mathbf{t}) = \mathbf{x}_0 + \int_0^{\mathbf{t}} \sum_{\sigma \in \Gamma} \chi_\sigma(\mathbf{s}) \mathbf{F}_\sigma(\mathbf{x}(\mathbf{s})) d\mathbf{s}$

From now on we restrict to $\mathcal{Y}_{\mathbf{x}_0}$; $\chi(\mathbf{t}) = (\chi_\sigma(\mathbf{t}))_{\sigma \in \Gamma}$

Theorem

As $\lambda \rightarrow \infty$,

$$\begin{aligned} \mathbb{P}_{\mathbf{x}_0, \sigma_0}^\lambda \left(\left\{ \mathbf{x}(t), \mathbb{1}(\sigma(t) = \sigma) dt \right\}_{t \in [0, T], \sigma \in \Gamma} \right) \\ \approx \left\{ \hat{\mathbf{x}}(t), \hat{\chi}(t) dt \right\}_{t \in [0, T]} \\ \sim e^{-\lambda \mathbf{J}_{[0, T]} \left(\left\{ \hat{\mathbf{x}}(t), \hat{\chi}(t) dt \right\}_{t \in [0, T]} \right)} \end{aligned}$$

$\mathbf{J}_{[0, T]}$ lower semi-continuous, $\neq \infty$, compact level set.

For each \mathcal{A} open, \mathcal{C} close:

$$\liminf_{\lambda \uparrow \infty} \frac{1}{\lambda} \ln \mathbf{P}_{\mathbf{x}_0, \sigma_0}^\lambda \left(\left\{ \mathbf{x}(t), \mathbb{1}(\sigma(t) = \sigma) dt \right\}_{t \in [0, T], \sigma \in \Gamma} \in \mathcal{A} \right) \geq - \inf_{\mathcal{A}} \mathbf{J}$$

$$\limsup_{\lambda \uparrow \infty} \frac{1}{\lambda} \ln \mathbf{P}_{\mathbf{x}_0, \sigma_0}^\lambda \left(\left\{ \mathbf{x}(t), \mathbb{1}(\sigma(t) = \sigma) dt \right\}_{t \in [0, T], \sigma \in \Gamma} \in \mathcal{C} \right) \leq - \inf_{\mathcal{C}} \mathbf{J}$$

Rate function

Integral representation:

$$\mathbf{J}_{[0, \mathbf{T}]}(\{\mathbf{x}(\mathbf{t}), \chi(\mathbf{t})\}_{\mathbf{t} \in [0, \mathbf{T}]}) := \int_0^{\mathbf{T}} \mathbf{j}(\mathbf{x}(\mathbf{t}), \chi(\mathbf{t})) \mathbf{d}\mathbf{t}. \quad (1)$$

$\mathbf{j}(\mathbf{x}, \cdot)$ is the Donsker–Varadhan LD rate functional for the empirical measure, time–homogeneous Markov chain (Z_t) on Γ with generator $L_c[x]$ (x frozen variable)

Recall: empirical measure $\pi_{\mathbf{T}} \in \mathcal{P}(\Gamma)$,

$$\pi_{\mathbf{T}}(\sigma) = \frac{1}{\mathbf{T}} \int_0^{\mathbf{T}} \mathbb{1}(Z_t = \sigma) \mathbf{d}\mathbf{t}$$

LDP mechanical trajectory

By contraction principle, LDP for mechanical trajectory $\mathbf{x}(\cdot)$.

Rate function: $\mathbf{J}_{[0, \mathbf{T}]}^m : \mathbf{C}([0, \mathbf{T}]; \Omega) \rightarrow [0, \infty]$

$$\mathbf{J}_{[0, \mathbf{T}]}^m (\{\mathbf{x}(t)\}_{t \in [0, \mathbf{T}]}) = \int_0^{\mathbf{T}} \mathbf{j}_m(\mathbf{x}(t), \dot{\mathbf{x}}(t)) dt$$

$$\mathbf{j}_m(\mathbf{x}, \dot{\mathbf{x}}) = \inf \left\{ \mathbf{j}(\mathbf{x}, \chi) : \chi \in \mathcal{P}(\Gamma) \text{ with } \dot{\mathbf{x}} = \sum_{\sigma} \chi_{\sigma} \mathbf{F}_{\sigma}(\mathbf{x}) \right\}.$$

Time-reversed process (very briefly)

Suppose $\exists!$ regular stationary measure ρ_λ , consider time-reversed stationary process.

It is again PDMP but λ -dependence not necessarily linear:

$$\mathbf{F}_\sigma^+(\mathbf{x}) = -\mathbf{F}_\sigma(\mathbf{x})$$

$$\mathbf{r}^+(\sigma, \sigma' | \mathbf{x}) := \mathbf{r}(\sigma', \sigma | \mathbf{x}) \frac{\rho_\lambda(\mathbf{x}, \sigma')}{\rho_\lambda(\mathbf{x}, \sigma)}$$

Rates can depend on λ .

Hence, previous LD results **cannot** be applied.

Time-reversed process (very briefly)

Isolated a class of exactly solvable PDMP with stationary distribution

$$\rho_\lambda = \mathbf{c}(\lambda) e^{-\lambda \mathbf{S}(\mathbf{x})} \rho(\mathbf{x}, \sigma) d\mathbf{x} d\sigma$$

Rates of reversed process are λ -independent. Hence, previous LD results **can** be applied.

Comparison of LD of direct and reversed process gives deep insight into irreversibility (Onsager–Machlup symmetries, fluctuation–dissipation relation)

Fluctuation–dissipation relation

$$\mathbf{j}_m(\mathbf{x}, \dot{\mathbf{x}}) = \nabla \mathbf{S}(\mathbf{x}) \cdot \dot{\mathbf{x}} + \mathbf{j}_m^+(\mathbf{x}, -\dot{\mathbf{x}}) \quad \mathbf{x} \in \Omega, \dot{\mathbf{x}} \in \mathbb{R}^d$$

$$\bar{\mathbf{F}}^+(\mathbf{x}) = \sum_{\sigma} \mu^+(\sigma|\mathbf{x}) \mathbf{F}_{\sigma}^+(\mathbf{x}) = - \sum_{\sigma} \mu^+(\sigma|\mathbf{x}) \mathbf{F}_{\sigma}(\mathbf{x}).$$

Start from equilibrium. For large T, λ , if $x(t) = x$, then with high probability

$$\left(\mathbf{x}(t) \right)_{t \in [0, T]} \sim \mathbf{x}_{\infty}^+(\mathbf{T} - \cdot)$$

where

$$\begin{cases} \dot{\mathbf{x}}_{\infty}^+(t) = \bar{\mathbf{F}}^+(\mathbf{x}_{\infty}^+(t)) \\ \mathbf{x}_{\infty}^+(0) = \mathbf{x} \end{cases}$$

Typically, $\mathbf{x}_{\infty}^+(\cdot)$ is not time-reversed of $\mathbf{x}_{\infty}(\cdot)$

PDMP on 1D torus

- state (\mathbf{x}, σ) , $x \in \mathbb{T}$, $\sigma \in \{0, 1\}$
- $\mathbf{F}_0, \mathbf{F}_1 : \mathbb{T} \rightarrow \mathbb{R}$ Lipschitz
- $\mathbf{r}(0, 1|\cdot), \mathbf{r}(1, 0|\cdot)$ positive continuous jump rates on \mathbb{T} .
- $\lambda > 0$ parameter

Formal generator:

$$\begin{aligned}\mathbb{L}f(\mathbf{x}, \sigma) &= \mathbf{F}_\sigma(\mathbf{x}) \cdot \nabla f(\mathbf{x}, \sigma) + \lambda(\sigma, \mathbf{1} - \sigma|\mathbf{x}) (f(\mathbf{x}, \mathbf{1} - \sigma) - f(\mathbf{x}, \sigma)) \\ &= \mathbf{F}_\sigma(\mathbf{x}) \cdot \nabla f(\mathbf{x}, \sigma) + \lambda \mathbf{L}_c[\mathbf{x}]f(\mathbf{x}, \sigma)\end{aligned}$$

Invariant distribution

Theorem

Assume (i) nonvanishing fields F_0, F_1 ,
(ii) positive rates $r(0, 1|x), r(1, 0|x)$.

Define

$$S(x) = \int_0^x \left(\frac{r(0, 1|y)}{F_0(y)} + \frac{r(1, 0|y)}{F_1(y)} \right) dy \quad x \in \mathbb{R}.$$

Then:

- $\exists!$ invariant distribution,

$$\rho_\lambda = \rho_\lambda(x, 0) dx \delta_0 + \rho_\lambda(x, 1) dx \delta_1$$

$$\begin{cases} \rho_\lambda(x, 0) := \frac{k}{F_0(x)} \int_x^{x+1} \left[\frac{r(1, 0|y)}{F_1(y)} e^{\lambda(S(y)-S(x))} \right] dy, \\ \rho_\lambda(x, 1) := \frac{k}{F_1(x)} \int_x^{x+1} \left[\frac{r(0, 1|y)}{F_0(y)} e^{\lambda(S(y)-S(x))} \right] dy. \end{cases}$$

Theorem

...

- If $\mathbf{S}(\mathbf{x}) = \int_0^{\mathbf{x}} \left(\frac{r(\mathbf{0},1|y)}{F_0(y)} + \frac{r(\mathbf{1},0|y)}{F_1(y)} \right) d\mathbf{y}$ is **periodic** with period 1 ($S(1) = 0$) then exactly solvable PDMP:

$$\begin{cases} \rho_\lambda(x, 0) = \frac{c(\lambda)}{F_0(x)} e^{-\lambda S(x)}, \\ \rho_\lambda(x, 1) = \frac{c(\lambda)}{F_1(x)} e^{-\lambda S(x)}. \end{cases} \quad (2)$$

- Setting $\mu_\lambda(\mathbf{x}) := \rho_\lambda(\mathbf{x}, \mathbf{0}) + \rho_\lambda(\mathbf{x}, \mathbf{1})$, it holds

$$\lim_{\lambda \uparrow \infty} -\frac{1}{\lambda} \mu_\lambda(\mathbf{x}) =$$

$$\min_{\mathbf{y} \in [\mathbf{x}, \mathbf{x}+1]} (\mathbf{S}(\mathbf{x}) - \mathbf{S}(\mathbf{y})) - \min_{x' \in [0,1]} \min_{y' \in [x', x'+1]} (S(x') - S(y')).$$

Diffusion $(\mathbf{X}_t^\epsilon)_{t \geq 0}$ on \mathbb{T}

- Diffusion $\dot{\mathbf{X}}_t^\epsilon = \mathbf{b}(\mathbf{X}_t^\epsilon) + \epsilon \dot{\mathbf{w}}_t$
- $b : \mathbb{T} \rightarrow \mathbb{R}$ Lipschitz, w_t Wiener process, $\epsilon > 0$

Theorem (Freidlin–Wentzell)

Assume $\{x \in \mathbb{T} : b(x) = 0\}$ has finite number of connected components.

Then $\exists!$ invariant distribution $\mu_\epsilon(\mathbf{x})d\mathbf{x}$ and

$$\lim_{\epsilon \downarrow 0} -\epsilon^2 \log \mu^\epsilon(\mathbf{x}) = \mathbf{W}(\mathbf{x}) - \min_{\mathbf{y} \in \mathbb{T}} \mathbf{W}(\mathbf{y}), \quad \mathbf{x} \in \mathbb{T},$$

W solving graph optimization problem.

Theorem

Define $\mathbf{S}(\mathbf{x}) = -2 \int_0^{\mathbf{x}} \mathbf{b}(s) ds$. Then,

$$\mu_\epsilon(\mathbf{x}) = \frac{1}{c(\epsilon)} \int_{\mathbf{x}}^{\mathbf{x}+1} e^{\epsilon^{-2}(\mathbf{S}(y) - \mathbf{S}(\mathbf{x}))} dy ,$$

In particular, it holds

$$\lim_{\epsilon \downarrow 0} -\epsilon^2 \log \mu_\epsilon(\mathbf{x}) =$$

$$\min_{\mathbf{y} \in [\mathbf{x}, \mathbf{x}+1]} (\mathbf{S}(\mathbf{x}) - \mathbf{S}(\mathbf{y})) - \min_{\mathbf{x}' \in [0, 1]} \min_{\mathbf{y}' \in [\mathbf{x}', \mathbf{x}'+1]} (\mathbf{S}(\mathbf{x}') - \mathbf{S}(\mathbf{y}')) .$$

Maxwell-like construction

Theorem

Take $F : \mathbb{T} \rightarrow \mathbb{R}$ continuous

$$\text{Define for } x \in \mathbb{R} \begin{cases} S(x) = \int_0^x F(s) ds, \\ \Phi(x) = \min_{y \in [x, x+1]} (S(x) - S(y)). \end{cases}$$

Then

- Φ Lipschitz and periodic of period 1
- Sunset at Alps (wait next slide)
- Suppose $\{\mathbf{x} \in \mathbb{T} : \mathbf{F}(\mathbf{x}) = \mathbf{0}\}$ has finite number of connected components. Then,

$$\Phi(\mathbf{x}) - \min_{\mathbf{x}' \in [0,1]} \Phi(\mathbf{x}') = \mathbf{W}(\mathbf{x}) - \min_{y \in \mathbb{T}} \mathbf{W}(y),$$

W the function defined by $[FW]$ with $b(x) := -F(x)/2$.

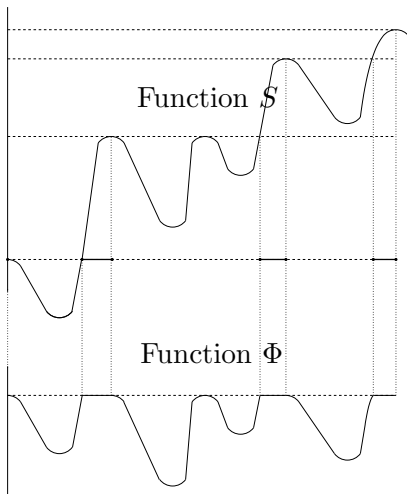
Sunset at Alps

Graph of S : **mountain profile**

Sunset: light comes from the left

$$\begin{cases} x \text{ is in shadow} \Rightarrow \nabla\Phi = \nabla S \\ x \text{ is lightened} \Rightarrow \nabla\Phi = 0 \end{cases}$$

Note: $S(x+1) - S(x)$ constant



Hamilton–Jacobi equations and universality

$$\left\{ \begin{array}{l} F : \mathbb{T} \rightarrow \mathbb{R} \text{ continuous} \\ S(x) = \int_0^x F(s) ds, \\ \Phi(x) = \min_{y \in [x, x+1]} (S(x) - S(y)). \end{array} \right.$$

Theorem

Let $H(x, p)$, with $(x, p) \in \mathbb{T} \times \mathbb{R}$, such that

(A) $H(x, \cdot)$ is a convex function for any $x \in \mathbb{T}$,

(B) $H(x, 0) = H(x, F(x)) = 0$ for any $x \in \mathbb{T}$.

Then $\Phi(x)$ as above is a **viscosity solution of the Hamilton-Jacobi equation**

$$H(x, \nabla \Phi(x)) = 0, \quad x \in \mathbb{T}.$$

Viscosity solution

φ is a viscosity solution for HJ equation $H(x, \nabla\varphi(x)) = 0$ iff $\varphi \in C(\mathbb{T})$ and

$$\begin{aligned} \mathbf{H}(\mathbf{x}, \mathbf{p}) &\leq 0 & \forall \mathbf{x} \in \mathbb{T}, \mathbf{p} \in \mathbf{D}^+\varphi(\mathbf{x}), \\ \mathbf{H}(\mathbf{x}, \mathbf{p}) &\geq 0 & \forall \mathbf{x} \in \mathbb{T}, \mathbf{p} \in \mathbf{D}^-\varphi(\mathbf{x}). \end{aligned}$$

Superdifferential $D^+\varphi(x)$, subdifferential $D^-\varphi(x)$ defined as

$$\begin{aligned} \mathbf{D}^+\varphi(\mathbf{x}) &= \left\{ \mathbf{p} \in \mathbb{R} : \limsup_{\mathbf{y} \rightarrow \mathbf{x}} \frac{\varphi(\mathbf{y}) - \varphi(\mathbf{x}) - \mathbf{p}(\mathbf{y} - \mathbf{x})}{|\mathbf{y} - \mathbf{x}|} \leq 0 \right\}, \\ \mathbf{D}^-\varphi(\mathbf{x}) &= \left\{ \mathbf{p} \in \mathbb{R} : \liminf_{\mathbf{y} \rightarrow \mathbf{x}} \frac{\varphi(\mathbf{y}) - \varphi(\mathbf{x}) - \mathbf{p}(\mathbf{y} - \mathbf{x})}{|\mathbf{y} - \mathbf{x}|} \geq 0 \right\}. \end{aligned}$$

Hamiltonian and Quasipotential

Quasipotential theory gives Hamiltonians fulfilling main assumption.

$$\mathbf{H}(\mathbf{x}, \mathbf{p}) = \sup_{\mathbf{y}} [\mathbf{p}\mathbf{y} - \mathbf{j}_m(\mathbf{x}, \mathbf{y})]$$

$\mathbf{j}_m(\mathbf{x}, \mathbf{y})$ density of the dynamical LDP (Lagrangian)

- Diffusion: $\mathbf{H}(\mathbf{x}, \mathbf{p}) = \mathbf{p}(\mathbf{p} - \mathbf{F}(\mathbf{x}))$
- PDMP: much more complex expression (see [FGR][JSP 2010])