Large deviations and uncertainty relations in periodically driven Markov chains with applications to stochastic thermodynamics

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Dedicated to Anton for his 60th birthday.

Post-Doc position in Anton's group in Berlin from August 2002 to February 2005:

- A period of scientific growth in a scientifically vivid environment
- An occasion to learn from and interact with many brilliant persons (many of them are in this room)

Back to large deviations

Figure: A large deviation. Naple, 2004

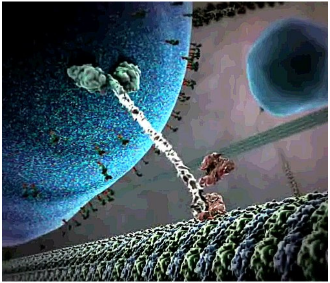
- L. Bertini, R. Chetrite, A. Faggionato, D. Gabrielli. *Level 2.5 large deviations for continuous time Markov chains with time periodic rates.* Annales Henri Poincaré. To appear.
- A. C. Barato, R. Chetrite, A. Faggionato, D. Gabrielli. *Bounds on current fluctuations in periodically driven systems.* arXiv:1806.07837v1
- A. C. Barato, R. Chetrite, A. Faggionato, D. Gabrielli. *Fluctuations bounds of additive functionals in periodically driven systems.* In preparation.

Statistical physics of small systems

- **(Biological) molecular motors:**
  - ▷ proteins, working as machines inside the cell. size 1nm=10^{-9} m
  - ▷ essential for cell division, cellular transport, muscle contraction, genetic transcription...
  - ▷ use chemical energies from ATP hydrolysis to produce mechanical work
  - ▷ rectification of motion (Parrondo's paradox: A combination of losing strategies becomes a winning strategy)

Statistical physics of small systems

- **(Biological) molecular motors**



Statistical physics of small systems

- **Artificial molecular motors:**
  Unlike their biological counterparts, artificial molecular machines are generally non-autonomous: they are manipulated by varying the external parameters or stimuli such as temperature, the chemical environment, or laser light.
- Often, the external parameters/stimuli vary in a **time-periodic** way.

Statistical physics of small systems

- The Nobel Prize in Chemistry 2016 has been assigned "for the design and synthesis of molecular machines";
- Stochastic thermodynamics
  - U. Seifert, *Stochastic thermodynamics, fluctuation theorems and molecular machines*. Rep. Prog. Phys. 75 (2012) 126001.
  - K. Sekimoto, *Stochastic energetics*. Lecture Notes in Physics 799, Springer Verlag, Berlin, 2010

Markov chains with time–periodic rates

- $(\xi_t)_{t\geq 0}$: continuous–time Markov chain
- V: finite state space
- $r_t(y,z)$: probability rate for a jump from y to z at time t

$$\mathbb{P}[\xi_{t+dt} = z \,|\, \xi_t = y] = r_t(y,z)dt$$

- $E := \{(y,z) \,:\, r_t(y,z) > 0 \text{ for some } t > 0\}$

Main assumptions

Recall: $E = \{(y,z) \,:\, r_t(y,z) > 0 \text{ for some } t > 0\}$

(A1) $t \mapsto r_t(y,z)$ is T_0–periodic;

(A2) $\exists C_1, C_2 > 0$

$$C_1 \le r_t(y,z) \le C_2 \qquad \forall t\,,\ \forall (y,z) \in E\,;$$

(A3) $t \mapsto r_t(y,z)$ is measurable and the set of discontinuity points has zero Lebesgue measure;

(A4) the directed graph (V,E) is strongly connected.

Oscillatory steady state

- $\mathbb{P}_\mu$: law of $(\xi_t)_{t\geq 0}$ starting with distribution μ
- $\left(\xi_{nT_0}\right)_{n\in\mathbb{N}}$: time–homogeneous discrete time Markov chain
- π_0: unique invariant distribution of $\left(\xi_{nT_0}\right)_{n\in\mathbb{N}}$
- π_0 is the unique distribution such that $\mathbb{P}_{\pi_0}$ is T_0–stationary
- π_t: marginal of $\mathbb{P}_{\pi_0}$ at time t. $\pi_t = \pi_{t+T_0}$

Extended empirical measure $\mu^{(n)}$ and flow $Q^{(n)}$

- $\mathcal{S}_{T_0} := \mathbb{R}/T_0\mathbb{Z}$ circle. Circular time
- Path space $D(\mathbb{R}_+; V)$: càdlàg paths $X : \mathbb{R}_+ \to V$
- $n = 1, 2, \dots$
- $$D(\mathbb{R}_+; V) \ni X \;\mapsto\; \begin{cases} \mu^{(n)} \text{ measure on } V \times \mathcal{S}_{T_0}\,, \text{ mass } T_0\,, \\ Q^{(n)} \text{ measure on } E \times \mathcal{S}_{T_0}\,. \end{cases}$$

Extended empirical measure $\mu^{(n)}$ and flow $Q^{(n)}$

Extended empirical measure $\mu^{(n)} \in \mathcal{M}_{+,T_0}(V \times \mathcal{S}_{T_0})$

$$\mu^{(n)}(f) = \frac{1}{n} \int_0^{nT_0} f(X_t, t) dt \,, \quad f : V \times \mathcal{S}_{T_0} \to \mathbb{R}$$

Extended empirical flow $Q^{(n)} \in \mathcal{M}_+(E \times \mathcal{S}_{T_0})$

$$Q^{(n)}(g) = \frac{1}{n} \sum_{\substack{t \in [0, nT_0]: \\ X_{t-} \neq X_t}} g(X_{t-}, X_t, t) \,, \quad g : E \times \mathcal{S}_{T_0} \to \mathbb{R}$$

An example from molecular motors

- x state in V: $x = (a, b)$,
  $a=$ conformational state of the motor (protein),
  $b=$ detached/attached to the filament.
- For special states y, z:
  ATP hydrolysis takes place at any jump $y \curvearrowright z$,
  ATP synthesis takes place at any jump $z \curvearrowright y$.
-

$$\int_{\mathcal{S}_{T_0}} Q^{(n)}(y, z, dt) = \frac{1}{n} \sharp \text{ hydrolysed ATP's in } [0, nT_0]\,,$$
$$\int_{\mathcal{S}_{T_0}} Q^{(n)}(z, y, dt) = \frac{1}{n} \sharp \text{ synthesized ATP's in } [0, nT_0]\,.$$

LLN for $\mu^{(n)}$ and $Q^{(n)}$

Recall: π_t marginal distribution at time t in the oscillatory steady state $\mathbb{P}_{\pi_0}$

- $\mu^{(n)} \Rightarrow \pi_t dt$ in $\mathcal{M}_{+,T_0}(V \times \mathcal{S}_{T_0})$
- $Q^{(n)} \Rightarrow Q_t^\pi dt$ in $\mathcal{M}_+(E \times \mathcal{S}_{T_0})$, $Q_t^\pi(y,z) := \pi_t(y) r_t(y,z)$
- $\partial_t \pi_t + \operatorname{div} Q_t^\pi = 0$

$$\operatorname{div} Q_t^\pi(y) := \sum_{z:(y,z)\in E} Q_t^\pi(y,z) - \sum_{z:(z,y)\in E} Q_t^\pi(z,y)$$

$$= \text{ exiting flow } - \text{ entering flow}$$

What about the LDs of $\left(\mu^{(n)}, Q^{(n)}\right)$?

Why should we care of LDs?

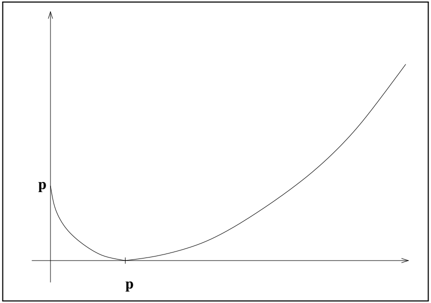
...
Thermodynamic potentials as free energy are given by exponential moments of additive functionals as work (cf. e.g. **Jarzynski relation**).

By Varadhan's lemma, the leading term of exponential moments is determined by means of the LD rate functional

Define $\Phi : \mathbb{R}_+ \times \mathbb{R}_+ \to [0, +\infty]$ as

$$\Phi(q,p) := \begin{cases} q \log \frac{q}{p} - q + p & \text{if } q, p \in (0, +\infty) \\ p & \text{if } q = 0,\ p \in (0, +\infty) \\ 0 & \text{if } q = p = 0 \\ +\infty & \text{if } p = 0 \text{ and } q \in (0, +\infty) \end{cases}$$

$\Phi(\cdot, p)$, $p > 0$, is LD rate function of Poisson process(p):



Joint LDP for the extended empirical measure and flow

$$\left(\mu^{(n)}, Q^{(n)}\right) \in \mathcal{M}_{+,T_0}(V \times \mathcal{S}_{T_0}) \times \mathcal{M}_{+}(E \times \mathcal{S}_{T_0}) =: \mathcal{M}$$

Definition

$(\mu, Q) \in \mathcal{M}$ is nice if

- $\mu = \mu_t dt$ with $\mu_t(V) = 1$;
- $Q = Q_t dt$;
- $\partial_t \mu_t + \mathrm{div} Q_t = 0$;
- for a.e. t: $\mu_t(y) = 0 \Longrightarrow Q_t(y,z) = 0$ for all $(y,z) \in E$.

Joint LDP for the extended empirical measure and flow

$\left(\mu^{(n)}, Q^{(n)}\right) \in \mathcal{M}$

Theorem (AHP 2018, online)

Under $\mathbb{P}_x$ *a joint LDP for* $\left(\mu^{(n)}, Q^{(n)}\right)$ *holds with speed* n *and good, convex and explicit rate functional* $I(\mu, Q)$,

$$I(\mu, Q) := \begin{cases} +\infty & \text{if } (\mu, Q) \text{ is not nice;} \\ \int_0^{T_0} I_t(\mu_t, Q_t)dt & \text{if } (\mu, Q) \text{ if nice;} \end{cases}$$

and

$$I_t(\mu_t, Q_t) = \sum_{(y,z)\in E} \Phi\left(Q_t(y,z)\,,\, \mu_t(y) r_t(y,z)\right).$$

Comments

- $\mathbb{P}_x \big(\, (\mu^{(n)}, Q^{(n)}) \approx (\mu, Q) \, \big) \sim e^{-nI(\mu,Q)}$
- $I(\mu, Q) = 0 \Leftrightarrow \mu = \pi_t dt,\ Q = Q^{\pi}$
- $I(\mu, Q)$ is explicit

Comments

- Level 2.5 LDP.
  Level 1= Cramér's Theorem, Level 2=Sanov's Theorem, Level 3=LDP of empirical process
- Level 2.5 LDPs for time–homogeneous Markov chains with countable state space:

▷ Bertini, Faggionato, Gabrielli. *Large deviations of the empirical flow for continuous time Markov chains.* AIHP 2015

▷ Bertini, Faggionato, Gabrielli. *Flows, currents, and cycles for Markov Chains: large deviation asymptotics.* SPA 2015

Cascades of LDPs by contraction

- Joint LDP for empirical measure $\tilde{\mu}_T \in \mathcal{P}(V)$ and empirical flow $\tilde{Q}_T \in \mathcal{M}_+(E)$ for $T \to \infty$:

$$\tilde{\mu}_T(x) = \frac{1}{T}\int_0^T \mathbb{1}(X_s = x)ds\,, \tag{1}$$

$$\tilde{Q}_T(y,z) = \frac{1}{T}\sum_{\substack{s\in[0,T]:\\ X_{s-}\neq X_s}} \mathbb{1}\big((X_{s-},X_s)=(y,z)\big) \tag{2}$$

- Join LDP for $\big(\mu^{(n)}, J^{(n)}\big)$, $J^{(n)}$ extended empirical current

$$J^{(n)}(y,z,dt) = Q^{(n)}(y,z,dt) - Q^{(n)}(z,y,dt)$$

In this case: Explicit rate functional !!!

- ...

Gallavotti–Cohen duality relation

Entropy flow

- $\mathbb{P}^*_{\pi_0}$: law of Markov chain (ξ^*_t) with initial distribution π_0 and rates
$$r^*(y,z;t) := r(y,z;T_0 - t)\,.$$
- $R_{[0,nT_0]}$ time–reversal on $[0, nT_0]$
- Entropy flow:

$$\sigma_{nT_0}[X] = -\log \frac{d\mathbb{P}^*_{\pi_0} \circ R_{[0,nT_0]}\big|_{[0,nT_0]}}{d\mathbb{P}_{\pi_0}\big|_{[0,nT_0]}}\big((X_s)_{s\in[0,nT_0]}\big)\,,$$

Fact

$$\frac{1}{n}\sigma_{nT_0} = O(1/n) + \sum_{(y,z)\in E}\int_0^{T_0} Q^{(n)}(y,z,ds)\log\frac{r(y,z;s)}{r(z,y;s)}$$

Gallavotti–Cohen duality relation

- **Stochastic entropy flow**

$$\sigma_{nT_0}[X] = -\log \frac{d\mathbb{P}^*_{\pi_0}\big|_{[0,nT_0]}}{d\mathbb{P}_{\pi_0}\big|_{[0,nT_0]}}\big((X_s)_{s\in[0,nT_0]}\big)\,, \qquad (3)$$

Contraction principle: LDP for $\frac{1}{n}\sigma_{nT_0}$.
Call $\mathcal{I}$ LD rate function of $\frac{1}{n}\sigma_{nT_0}$, $\mathcal{I}(\cdot;r)$ to stress choice of rates

Theorem (GC duality relation)

$$\mathcal{I}(s;r) = \mathcal{I}(-s;r^*) - s\,.$$

- Several other GC–duality relations, also with $\mathbb{P}^*$ defined by other jump rates.

Time–homogeneous Markov chains

- Conjectured by A.C. Barato and U. Seifert in Phys. Rev. Lett. 114, 158101 (2015)
- Derived by Gingrich et al. in Phys. Rev. Lett. 116, 120601 (2016) using the explicit formula of level 2.5 rate function for empirical measure and current obtained in
  - Bertini, Faggionato, Gabrielli. *Flows, currents, and cycles for Markov Chains: large deviation asymptotics*. SPA 2015

Uncertainty relations

Time–homogeneous Markov chains

- $E = \{(x, y) : r(x, y) > 0\}$.
  Assumption: $(x, y) \in E$ iff $(y, z) \in E$
- $\alpha = (\, \alpha(x, y)\,)_{x,y \in V}$ antisymmetric

$$J_T^\alpha := \frac{1}{T} \sum_{\substack{s \in [0,T]: \\ X_{s-} \neq X_s}} \alpha(X_{s-}, X_s)$$

- LLN: $J_T^\alpha \to j_\alpha = \sum_{x,y} \alpha(x, y)\pi(x)r(x, y)$
- asymptotic edge current

$$j(x, y) := \pi(x)r(x, y) - \pi(y)r(y, x)$$

- $j_\alpha = \frac{1}{2} \sum_{(x,y) \in E} \alpha(x, y) j(x, y)$

Uncertainty relations

Time–homogeneous Markov chains

J_T^α satisfies an LDP with rate function I_α
Suppose $j_\alpha \neq 0$

- Global parabolic bound:

$$I_\alpha(x) \leq \frac{\sigma}{4j_\alpha^2}(x - j_\alpha)^2,$$

σ average rate of entropy production

$$\sigma = \frac{1}{2} \sum_{(x,y)\in E} j(x,y) \ln \frac{\pi(x)r(x,y)}{\pi(y)r(y,x)}\,.$$

Uncertainty relations

Time–homogeneous Markov chains

J_T^α satisfies an LDP with rate function I_α

Suppose $j_\alpha \neq 0$

- D_α: asymptotic diffusion coefficient of TJ_T^α,
  $D_\alpha = I''_\alpha(j_\alpha)$
- Trade–off relation between precision and speed:

$$D_\alpha \geq \frac{j_\alpha^2}{2\sigma}$$

Additive functionals: $\alpha(x,y)$ generic.

J.P. Garrahan. Phys. Rev. E 95, 032134 (2017)

Uncertainty relations in periodically driven Markov chains

A.C. Barato, U. Seifert, Phys. Rev. X 6 041053, 2016

The previous global/local bounds are violated if σ is the average rate of entropy production

$$\sigma = \frac{1}{2T_0} \int_0^{T_0} \sum_{(x,y)\in E} j_t(x,y) \ln \frac{\pi_t(x) r_t(x,y)}{\pi_t(y) r_t(y,x)} \, .$$

Uncertainty relations in periodically driven Markov chains

- Global parabolic bound:

$$I_\alpha(x) \leq \frac{\sigma^*}{4j_\alpha^2}(x - j_\alpha)^2.$$

- Trade–off relation between precision and speed:

$$D_\alpha \geq \frac{j_\alpha^2}{2\sigma^*}$$

Uncertainty relations in periodically driven Markov chains

$$\sigma = \frac{1}{2T_0} \int_0^{T_0} \sum_{(x,y)\in E} j_t(x,y) \ln \frac{\pi_t(x) r_t(x,y)}{\pi_t(y) r_t(y,x)} \,,$$

$$\sigma^* = \frac{1}{2T_0} \int_0^{T_0} \sum_{(x,y)\in E} \frac{\bar{j}(x,y)^2}{j_t(x,y)} \ln \frac{\pi_t(x) r_t(x,y)}{\pi_t(y) r_t(y,x)} \,,$$

$$\bar{j}(x,y) = \frac{1}{T_0} \int_0^{T_0} j_t(x,y) dt$$

Further results for $\alpha(x,y)$ generic

Happy birthday, Anton!