Large deviations for the pure jump k-nary interacting particle systems

多元交互粒子系统中的大偏差

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例子：经典二元交互粒子系统

- Boltzmann 碰撞
- 聚合分裂反应 (Smoluchovski，Becker-Döring...)

经典例子：Boltzmann 二元碰撞粒子系统

- 封闭盒子中，N 个粒子的空间齐次理想气体模型
- 时刻 t 的状态为

$$\big(v_1(t), v_2(t), \ldots, v_N(t)\big),$$

其中 $v_i \in \mathbb{R}^d$ 为标号为 i 的粒子的速度。

- **二元碰撞**

状态为 x_1 的粒子和状态为 x_2 的粒子发生碰撞，状态变为 y_1 和 y_2

$$(x_1)+(x_2) \xrightarrow{B(x_1,x_2;\mathrm{d}y_1,\mathrm{d}y_2)} (y_1)+(y_2)$$

其中 $B(x_1, x_2; \mathrm{d}y_1, \mathrm{d}y_2)$ 为 collision kernel function，碰撞满足

动量 $E_1(v) = v$ 守恒: $\quad E_1(x_1) + E_1(x_2) = E_1(y_1) + E_1(y_2)$

动能 $E_2(v) = |v|^2$ 守恒: $\quad E_2(x_1) + E_2(x_2) = E_2(y_1) + E_2(y_2)$

经典例子: Boltzmann 二元碰撞粒子系统

- 经验测度

$$\mu_t^{1/N} := \frac{1}{N}\sum_{i=1}^{N} \delta_{v_i(t)} \quad \in \mathcal{P}(\mathbb{R}^d)$$

- 大数律 (Lanford 73', Sznitman 84'...) $\mu_t^{1/N} \Rightarrow$ **Boltzmann 方程**
- 中心极限定理 (Méléard 98')
- 大偏差**上界 (Léonard 95')**
- 大偏差**下界**

  Basile et al. 21', Heydecker 21' (分析方法)

  Sun 21' （概率方法）
- 长时间的相关性 – 累积量生成函数的极限
  Bodineau et al 20', Laure Saint-Raymond (2021 ICM)

经典例子: 二元聚合分裂模型

(1) **Smoluchovski's 二元聚合模型,**

$$(x)+(y) \xrightarrow{K(x,y)} (x+y)$$

其中 $x, y \in \mathbb{R}^+$ 为粒子质量, $K(x,y)$为聚合反应的核函数。

(2) **Becker-Döring 二元聚合分裂模型,**

$$\begin{cases} (1)+(k) & \xrightarrow{a_k} (k+1), \\ (k+1) & \xrightarrow{b_{k+1}} (1)+(k). \end{cases}$$

其中 $k \in \mathbb{N}$ 为粒子的质量, a_k为聚合核函数, b_k 为分裂核函数。

- 上述反应满足: 粒子总质量 $\equiv 1/h$ 守恒。
- 粒子数 $n^h(t)$ 不守恒。
- 系统状态 $(x_1(t), \ldots, x_{n^h(t)}(t))$
- 经验测度 $\mu^h := h \sum_{i=1}^{n^h(t)} \delta_{x_i(t)}$

（纯跳跃）多元交互粒子系统

- 微观马氏过程
- 宏观 PDE

Microscopic description – k-nary interacting particle

Dynamic of k-nary IPS (Kolokoltsov 2006)

Reaction occurs among any ℓ particles and "generating" m particles,

$$(x_1)+(x_2)+\dots(x_\ell) \longrightarrow (y_1)+(y_2)+\dots+(y_m)$$

at rate $P(x_1,\dots,x_\ell;\mathrm{d}y_1,\dots,\mathrm{d}y_m)$, where $x_\cdot, y_\cdot \in X$ **(Polish)**.
Assume $0 \le \ell, m \le k$.

Particle system $(x_1(t),\dots,x_{n^h(t)}(t))$.
Empirical measure Markov process

$$\mu_t^h = h\sum_{i=1}^{n^h(t)} \delta_{x_i(t)}$$

where h is some scaling parameter. (e.g. $h=$1/number of particles in Boltzmann; $h=$ 1/total mass in coag. & frag.)

- $\langle 1, \mu_t^h\rangle$ can be time varying – **not a probability measure;**
- infinite many types of jumps – **State space X non-compact.**

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Assume $0 \le \ell, m \le k$.

Pure jump measure valued Markov process

$$\mu_t^h \to \mu_t^h + h\sum_{j=1}^{m}\delta_{y_j} - h\sum_{i=1}^{\ell}\delta_{x_i}$$

at rate

$$\approx h^{\ell-1}P(x_1,\dots,x_\ell;\mathrm{d}y_1,\dots\mathrm{d}y_m)\frac{1}{\ell!}\prod_{i=1}^{\ell}\mu_t^h(\mathrm{d}x_i).$$

- the jump rate "is" a **polynomial** of μ_t^h (non-Lipschitz);
- kernel $P(x_1,\dots,x_\ell;\mathrm{d}y_1,\dots\mathrm{d}y_m)$ unbounded.

Macroscopic description (weak form)

- k-nary kinetic evolution equation

$$\mathrm{d}\langle g, \sigma_t \rangle = \sum_{\ell} \sum_{m} \int \left(\sum_{j=1}^{m} g(y_j) - \sum_{i=1}^{\ell} g(x_i) \right) P(x_1, \ldots, x_\ell; \mathrm{d}y_1, \ldots \mathrm{d}y_m) \frac{1}{\ell!} \prod_{i=1}^{\ell} \sigma_t(\mathrm{d}x_i)\, \mathrm{d}t$$

- Example: Becker-Döring $(1) + (k) \underset{b_{k+1}}{\overset{a_k}{\rightleftharpoons}} (1+k)$

$$\mathrm{d}\langle g, \sigma_t \rangle = \sum_{k=1}^{\infty} \left(g(k+1) - g(k) - g(1)\right) \frac{a_k}{2} \sigma_t(\{k\}) \sigma_t(\{1\})\, \mathrm{d}t + \sum_{k=1}^{\infty} \left(g(k) + g(1) - g(k+1)\right) b_{k+1} \sigma_t(\{k+1\})\, \mathrm{d}t$$

From Microscopic to Macroscopic (Pathwise)

Let $\boldsymbol{E} : \boldsymbol{X} \mapsto \mathbb{R}^+$, assume the system is $\boldsymbol{E}$-non increasing, i.e., for all possible jumps,

$$\sum_{j=1}^{m} E(y_j) \leq \sum_{i=1}^{\ell} E(x_i).$$

For example, $E(v) = |v|^2$ energy in Boltzmann; $E(x) = x$ mass in coag./frag. Assume asymptotically, either

$$\int P(x_1, x_2, \ldots, x_\ell; \mathrm{d}y_1, \ldots, \mathrm{d}y_m) \lesssim o\left(\prod_{i=1}^{\ell}(1 + E(x_i))\right)$$

or

$$\int P(x_1, x_2, \ldots, x_\ell; \mathrm{d}y_1, \ldots, \mathrm{d}y_m) \lesssim \sum_{i=1}^{\ell}(1 + E(x_i)).$$

Law of large numbers

Assume the initial condition converges, then

$$(\mu_t^h, 0 \leq t \leq T) \Rightarrow (\sigma_t, 0 \leq t \leq T).$$

Literature

- Boltzmann collision:
  LLN (Lanford 73', Sznitman 84'), CLT (Méléard 98'), LDP (Léonard 95',Bodineau et al 20', Basile et al. 21', Heydecker 21', Sun 21')...

- Coagulation and fragmentation:
  LLN (Jeon 98', Norris 99', Fournier et al. 09'), CLT (Kolokoltsov 10', Sun 18'), LDP(Andreis et al. 19'), survey(Aldous 99')...

- ***k***-nary (Kolokoltsov 06', 10')

主要结论：轨道大偏差

I. 上界

Main results: Pathwise Large deviations

定理 (LDP Upper bound)

Let $\mathcal{M}^+(X)$ be the set of non-negative finite measures on X endowed with weak topology, then for any closed set $\mathcal{C}$ of $D_T(\mathcal{M}^+(X))$,

$$\limsup_{h\to 0} h \log \mathbb{P}\left((\mu_t^h, 0 \le t \le T) \in \mathcal{C}\right) \le - \inf_{\pi \in \mathcal{C}} \left\{ I_\nu(\pi_0) + \mathcal{R}^P_{\text{upper}}(\pi) \right\}$$

where $I_\nu(\pi_0)$ is the rate function related to the LDP of the initial condition (Chaos or Deterministic) and

$$\mathcal{R}^P_{\text{upper}}(\pi) := \sup_{g \in \mathcal{C}_b^{1,0}([0,T];X)} \left\{ \langle \pi_T, g_T \rangle - \langle \pi_0, g_0 \rangle - \int_0^T \langle \pi_s, \partial_s g_s \rangle \, \mathrm{d}s \right.$$
$$- \sum_{\ell} \sum_{m} \int_0^T \int \left(\exp\left(\sum_{j=1}^{m} g(y_j) - \sum_{i=1}^{\ell} g(x_i) \right) - 1 \right)$$
$$\left. P(x_1, \dots, x_\ell; \mathrm{d}y_1, \dots, \mathrm{d}y_m) \frac{1}{\ell!} \prod_{i=1}^{\ell} \pi_s(\mathrm{d}x_i) \, \mathrm{d}s \right\}.$$

Standard proof: perturbation by a regular function

Mimicking the proofs by Kipnis, Olla, and Varadhan (1989), for a regular function f on $[0, T] \times X$, let

$$\mathcal{M}_t^f[\mu] := \exp\Bigg\{ h^{-1} \left(\langle f_t, \mu_t \rangle - \langle f_0, \mu_0 \rangle - \int_0^t \langle \partial_s f_s, \mu_s \rangle \, \mathrm{d}s \right) - h^{-1} \sum_\ell \sum_m \int_0^t \int \left(\exp\left(\sum f_s(y_j) - \sum f_s(x_i) \right) - 1 \right) P(x_1, \dots, x_\ell; \mathrm{d}y_1, \dots, \mathrm{d}y_m) \frac{1}{\ell!} \prod_{i=1}^{\ell} \pi_s(\mathrm{d}x_i) \, \mathrm{d}s + o\left(h^{-1}\right) \Bigg\}$$

then $\mathbb{P}^f := \mathcal{M}_t^f \cdot \mathbb{P}$ is the unique solution to the martingale problem of a k-nary IPS with perturbed (time-inhomogeneous) jump kernel

$$\exp\left(\sum f_s(y_j) - \sum f_s(x_i) \right) P(x_1, \dots, x_\ell; \mathrm{d}y_1, \dots, \mathrm{d}y_m).$$

Thus, by changing the measure,

$$\mathbb{P}(\mu^h \in C) = \mathbb{E}^f \left((\mathcal{M}_t^f[\mu])^{-1} \mathbb{1}_{\{\mu \in C\}} \right) \lesssim \sup_{\mu \in C} (\mathcal{M}_t^f[\mu])^{-1},$$

then by a exp-tight result + Max-Min result, we have the LDP upper bound.

主要结论：轨道大偏差

II. Rate function

Explicit rate function

To study the rate function, we follow the idea of Léonard (1995). For all possible jumps $(x_1, \dots, x_\ell) \mapsto (y_1, \dots, y_m)$, denote

$$L[g](s, x_1, \dots, x_\ell; y_1, \dots, y_m) = \sum_{j=1}^{m} g_s(y_j) - \sum_{i=1}^{\ell} g_s(x_i),$$

then the rate function becomes

$$\mathcal{R}^{P}_{\text{upper}}(\pi) = \sup_{g \in \mathcal{C}_b^{1,0}([0,T];X)} \Big\{ \langle \pi_T, g_T \rangle - \langle \pi_0, g_0 \rangle - \int_0^T \langle \pi_s, \partial_s g_s \rangle \, \mathrm{d}s$$

can be seen as a continuous linear functional on $L[g]$

$$- \sum_{\ell} \sum_{m} \int_0^T \int (\exp(L[g]) - 1)(s, x_1, \dots, x_\ell; y_1, \dots, y_m)$$

$$P(x_1, \dots, x_\ell; \mathrm{d}y_1, \dots, \mathrm{d}y_m) \frac{1}{\ell!} \prod_{i=1}^{\ell} \pi_s(\mathrm{d}x_i) \, \mathrm{d}s \Big\}$$

can be seen as a convex functional on $L[g]$

Explicit rate function

In short, for any path π fixed

$$\mathcal{R}^P_{\text{upper}}(\pi) = \sup_{L[g]} \{\text{Linear}(L[g]) - \text{Convex}(L[g])\}$$

where $\{L[g]\}$ is a subspace of L^∞. By some convex analysis,

$$\mathcal{R}^P_{\text{upper}}(\pi) = \inf_{\eta} \{\text{Convex}^*(\eta)\}$$

where the **inf** running over all $\eta \in L^1$ and $\text{Linear}(L[g]) = \langle \eta, L[g] \rangle$.

定理 (Rate function)

For any path μ such that $\sup_{t \le T} \langle 1 + E, \mu_t \rangle < \infty$,

$$\mathcal{R}^P_{\text{upper}}(\pi) = \inf_{\eta} \sum_{\ell} \sum_{m} \int_0^T \int (\eta \log(\eta) - \eta + 1)(s, x_1, \ldots, x_\ell; y_1, \ldots, y_m) \, P(x_1, \ldots, x_\ell; \mathrm{d}y_1, \ldots, \mathrm{d}y_m) \frac{1}{\ell!} \prod_{i=1}^{\ell} \pi_s(\mathrm{d}x_i) \, \mathrm{d}s$$

Domain of the Upper Bound Rate function

定理 (Rate function (continue))

... where $\eta \geq 0$ *and* (η, π) *satisfying*

$d\langle g, \pi_t \rangle = \sum_{\ell,m} \int L[g]\eta P(s, x_1, \ldots, x_\ell; dy_1, \ldots, dy_m) \frac{1}{\ell!} \prod_{i=1}^{\ell} \pi_t(dx_i)\, dt$

Therefore, $\mathcal{R}^P_{\text{upper}}(\pi) < \infty$ iff $\exists$ at least one (η, π) above, such that

$$\int (\eta \log(\eta) - \eta + 1)\, d\left(P \prod \pi_t\right) < \infty$$

this domain is the "Cameron-Martin" space in the sense of Fleischmann, Gärtner & Kaj (1996).

- In most cases of $1-$nary interation:

  η is unique, $f-$perturbated paths are **dense** in CM space.

- In most cases of $k-$nary interation:

  η is **not unique** (can be infinite many);

  the **existence** of the path in the domain is questionable.

The Kipnis, Olla and Varadhan approach is not working!

主要结论：轨道大偏差

III. 下界

Lower bound (KOV's f-perturbed "good" path)

- It is enough to prove the lower bound around the "good" path $\pi \in$ Domain of the upper bound, i.e.

$$\mathbb{P}(\mu^h \in \mathcal{B}_\varepsilon(\pi)) \gtrsim \ ?$$

- Recall the particle system perturbed by a regular function f, one has law of large number $\mathbb{P}^f \Rightarrow \delta_{\sigma^f}$ where σ^f solves

$$\mathrm{d}\langle g, \sigma^f\rangle = \int L[g]\,\mathrm{d}\left(\mathbf{e}^{\mathbf{L}[\mathbf{f}]}\mathbf{P}\prod \sigma^f\right)\mathrm{d}t \qquad \forall g.$$

In fact, σ^f is a "good" path, and

$$\mathbb{P}(\mu^h \in \mathcal{B}_\varepsilon(\sigma^f)) = \mathbb{E}^f \frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\mathbb{P}^f}[\mu^h]\mathbb{1}_{\{\mu^h \in \mathcal{B}_\varepsilon(\sigma^f)\}}$$
$$\gtrsim (\mathcal{M}_T^f[\sigma^f])^{-1} e^{-O(\varepsilon)}\mathbb{P}^f(\mu^h \in \mathcal{B}_\varepsilon(\sigma^f)),$$

by a straightforward calculation,

$$h\log(\mathcal{M}_T^f[\sigma^f]) \to \mathcal{R}^P_{\text{upper}}(\sigma^f).$$

Thus $\mathcal{R}^P_{\text{lower}}(\sigma^f) = \mathcal{R}^P_{\text{upper}}(\sigma^f)$.

Lower bound (η-perturbed "good" path)

- For a bounded function $\eta(t,\cdot)$ defined on all possible jumps

$$\eta(t, x_1, \ldots, x_\ell; y_1, \ldots, y_m)$$

consider a particle system with rate function ηP, i.e. the jump

$$(x_1)+(x_2)+\ldots(x_\ell) \longrightarrow (y_1)+(y_2)+\ldots+(y_m)$$

occurs at rate $\eta P(t, x_1, \ldots, x_\ell; \mathrm{d}y_1, \ldots \mathrm{d}y_m)$.
Then by law of large number $\mathbb{P}^\eta \Rightarrow \delta_{\sigma^\eta}$ where σ^η solves

$$\mathrm{d}\langle g, \sigma^\eta\rangle = \int L[g]\,\mathrm{d}\left(\eta P \prod \sigma^\eta\right)\mathrm{d}t \qquad \forall g.$$

Formally, we could expect

$$\mathbb{P}(\mu^h \in \mathcal{B}_\varepsilon(\sigma^\eta)) \gtrsim \left(\frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\mathbb{P}^\eta}[\sigma^\eta]\right)^{-1} e^{-O(\varepsilon)}\mathbb{P}^\eta(\mu^h \in \mathcal{B}_\varepsilon(\sigma^\eta)),$$

then

$$\lim h \log \frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\mathbb{P}^\eta}[\sigma^\eta]$$

should give a LDP lower bound.

"SDE" representation of measure-valued Markov

- The lower bound problem reduces to calculate the Radon-Nikodym derivative

$$\frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\mathbb{P}^{\eta}}[\mu]$$

on $\mathcal{D}([0,T];\mathcal{M}^{+}(X))$.

- Same type of jumps, absolutely continuous kernels, $\eta P \ll P$.
- Define a counting measure

$$\mathcal{N}[h^{-1}\mu](\mathrm{d}t,\mathrm{d}x_1,\dots,\mathrm{d}x_\ell,\mathrm{d}y_1,\dots,\mathrm{d}y_m) := \text{number of jumps of type } (x)\to(y) \text{ of path } \mu \text{ around time } t$$

the measure valued process μ^h can be seen as a solution to the SDE

$$\mathrm{d}\mu^h_t = h\int\left(\sum_{j=1}^{m}\delta_{y_j}-\sum_{i=1}^{\ell}\delta_{x_i}\right)\mathcal{N}[h^{-1}\mu^h](\mathrm{d}t,\mathrm{d}x_1,\dots,\mathrm{d}x_\ell,\mathrm{d}y_1,\dots,\mathrm{d}y_m)$$

Martingale measures (in the sense of Walsh 1986)

- under $\mathbb{P}$, the process
$$\mathrm{d}\mathcal{N}[h^{-1}\mu] - h^{-1}\,\mathrm{d}\left(P\prod\mu\right)$$
is an orthogonal martingale measure on $[0, T] \times \{\text{all type of jumps}\}$.
- by Girsanov's Theorem, let
$$\mathcal{M}_t^{\eta}[\mu] := \exp\left\{\int_0^t\int \log(\eta)\,\mathcal{N}[h^{-1}\mu] - h^{-1}\int_0^t\int\left(\mathrm{d}\left(\eta P\prod\mu\right) - \mathrm{d}\left(P\prod\mu\right)\right)\right\},$$
then the process
$$\mathrm{d}\mathcal{N}[h^{-1}\mu] - h^{-1}\,\mathrm{d}\left(\eta P\prod\mu\right)$$
is an orthogonal martingale measure under $\mathcal{M}^{\eta}\mathbb{P}$

Change of measure

In conclusion

$$\frac{\mathrm{d}\mathbb{P}^{\eta}}{\mathrm{d}\mathbb{P}} = \mathcal{M}^{\eta},$$

then

$$\begin{aligned}
h \log \frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\mathbb{P}^{\eta}}[\mu] &= -h \int_0^T \int \log(\eta) \mathcal{N}[h^{-1}\mu] \\
&\quad + \int_0^T \int \left(\mathrm{d}\left(\eta P \prod \mu\right) - \mathrm{d}\left(P \prod \mu\right)\right) \\
&= -h \int_0^T \int \log(\eta) \left(\mathrm{d}\mathcal{N}[h^{-1}\mu] - h^{-1}\, \mathrm{d}\left(\eta P \prod \mu\right)\right) \\
&\quad - \int_0^T \int (\log(\eta)\, \eta - \eta + 1)\, \mathrm{d}\left(P \prod \mu\right)
\end{aligned}$$

the blue term is a vanishing martingale under $\mathbb{P}^{\eta}$ by calculating its increasing process.

Main Result: LDP Lower bound

定理

for any open neighborhood of σ^η, *where* η *is non-negative and bounded,*

$$\liminf_{h\to 0} h \log \mathbb{P}(\mathcal{B}_\varepsilon(\sigma^\eta)) \geq -\left\{ I_\nu(\sigma_0^\eta) + \mathcal{R}^P_{\text{lower}}(\sigma^\eta) \right\},$$

where

$$\mathcal{R}^P_{\text{lower}}(\sigma^\eta) = \inf_{\eta'} \sum_\ell \sum_m \int_0^T \int \left(\eta' \log(\eta') - \eta' + 1\right)(s, x_1, \dots, x_\ell; y_1, \dots, y_m)$$
$$P(x_1, \dots, x_\ell; \mathrm{d}y_1, \dots, \mathrm{d}y_m) \frac{1}{\ell!} \prod_{i=1}^{\ell} \sigma_s^\eta(\mathrm{d}x_i)\, \mathrm{d}s$$

where **inf** *running over all* **bounded** $\eta' \geq 0$, *such that for all test function* g,

$$\mathrm{d}\langle g, \sigma_t^\eta \rangle = \sum_{\ell,m} \int L[g]\eta' P(s, x_1, \dots, x_\ell; \mathrm{d}y_1, \dots, \mathrm{d}y_m) \frac{1}{\ell!} \prod_{i=1}^{\ell} \sigma_t^\eta(\mathrm{d}x_i)\, \mathrm{d}t$$

问题 & 讨论

上界 ＝下界？

Discussion

- $\mathcal{R}^P_{\text{upper}} = \inf_{\eta \geq 0, \eta \in \mathcal{L}^1} \cdots$
- $\mathcal{R}^P_{\text{lower}} = \inf_{\eta \geq 0, \eta \in \mathcal{L}^\infty} \cdots$
- **Does $\mathcal{R}^P_{\text{upper}} = \mathcal{R}^P_{\text{lower}}$ holds?**

- In some cases, yes. (Most of $\mathbf{1}-$nary interations)

  for $\boldsymbol{k}-$nary interations, if the state space is **finite (/compact)**, then the jump rates are naturally bounded (/can be approximated by cut-off rates). (See Dupuis, Ramanan, and Wu 2016 for the finite case)

- In the **non-compact case**, this problem is related to the existence of the kinetic equation with growing kernels.

- Ongoing work

- pathwise and fixed times LDPs in the Smoluchovski's coagulation with gelling kernels (Sun 23'+);
- LDP, condensation and long time correlations in the equilibrium of the stochastic Becker-Döring model (Sun 23'+)

Thank you!