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Stochastic Hamilton systems with singular potentials: quasi stationary distribution (QSD)

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based on recent joint work with A. Guillin, B. Nectoux

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1. Stochastic Hamilton's systems

We begin with the classic

1.1. Newton's equation for a system of celeste objects

Consider N suns of masses $m_1, \cdots, m_N$ (comparable) in the space $\mathbb{R}^3$. The Newton equation for their movement is

$$m_i x_i''(t) = \sum_{j \neq i} \frac{m_i m_j e(x_j - x_i)}{|x_i(t) - x_j(t)|^2}, \ \ i = 1, \cdots, N,$$

where $e(x) = \frac{x}{|x|}$,

$$x(t) = (x_1(t), \cdots, x_N(t)), \ v(t) = x'(t) = (x_1'(t), \cdots, x_N'(t))$$

are the position and velocity of the system (the couple $(x(t), v(t))$ is called configuration).

For $N = 2$, according to the initial condition on $(x(0), v(0))$, the system of two suns has three behaviors:

1. the two suns colllapse;
2. moving one around the other;
3. they go away.

For $N = 3$ problem, Poincaré proved that the system is chaotic (sensitive w.r.t. the initial position-velocity condition $(x(0), v(0))$: topologicaly recurrent) by introducing the notions of topology.

For simplicity let $m_i = 1$. Then Newton's equation can be written in the form of Hamilton system

$$\begin{cases} dx(t) = v(t)dt \\ dv(t) = -\nabla V(x(t))dt \end{cases}$$

where

$$V(x_1, \cdots, x_N) = -\sum_{i \neq j} \frac{1}{|x_i - x_j|}$$

$-1/|x|$ being the Newtonian potential.

1.2. Stochastic damped Hamilton systems for microscopic objects

Consider a stochastic damped Hamilton system of N particles (equal masses) moving in $\mathbb{R}^d$: whose configuration $(x(t) = (x_1(t), \cdots, x_N(t)), v(t) = (x'_1(t), \cdots, x'_N(t)))$ satisfies

$$\begin{cases} dx(t) &= v(t)dt \\ dv(t) &= \sigma(x(t), v(t))dB_t - c(x(t), v(t))v(t)dt - \nabla V(x(t))dt \end{cases} \tag{1}$$

where

- $\sigma\sigma^T(x, v) > 0$, C^1-smooth (depending on the media);
- $c(x, v)$ damping coefficient but may be negative;

- the potential V is of form

$$V(x_1, \cdots, x_N) = \sum_{i=1}^{n} U(x_i) + \sum_{1 \le i < j \le N} V_I(x_i - x_j) \tag{2}$$

$U : \mathbb{R}^d \to \mathbb{R}$ is the confinement potential, C^1-smooth, but the interaction potential $V_I : \mathbb{R}^d \backslash \to \{0\} \to \mathbb{R}$ has a singularity at the origin 0.

For example,

1. V_I is the coulomb potential

$$V_I(x) = \frac{\beta}{|x|}, \text{ if } d = 3$$

where $\beta > 0$ is a physical constant. It is the negative Newtonian potential.

2. V_I is the generalized Lennard-Jones potential

$$V_I(x) = \frac{b}{|x|^\alpha} + \Phi_I(x),\ x \in \mathbb{R}^d \backslash \{0\}$$

where $b > 0$, $\alpha > 0$. Lennard-Jones potential corresponds to $\alpha = 12$ and

$$V_I(x) = \frac{a}{|x|^{12}} - \frac{b}{|x|^6},\ (a, b > 0).$$

3. $b > 0$ and

$$V_I(x) = \begin{cases} -b \log |x|, & \text{(log-potential) if } d = 2 \\ \frac{b}{|x|^{d-2}}, & \text{if } d \geq 3 \end{cases}.$$

(called often as Newtonian potential in mathematics, it is a particular case of Riesz potential if $d \geq 3$).

1.3. Few known results

Problem 1. *Whether the stochastic Hamilton equation has a unique solution ?*

Key: find a method and sufficient condition for no-collapse.

Problem 2. *If Yes for problem 1, what is the behavior of the Hamilton system for large time ? Is there exponential convergence to its unique stationary measure ?*

At first we see what means no collapse:

$$\tau_c := \sup_{\varepsilon>0} \inf\{t > 0 : \min_{i\neq j} |x_i(t) - x_j(t)| < \varepsilon\} = +\infty,$$

with probability 1.

1. If $d = 1$, let

$$\mathcal{O} = \{x = (x_1, \cdots, x_N) \in \mathbb{R}^N;\ x_1 < x_2 < \cdots < x_N\}$$

no collapse means that if $x(0) \in \mathcal{O}$, then $x(t) \in \mathcal{O}$ for all time $t > 0$.

2. If $d \geq 2$, let

$$\mathcal{O} = \{x = (x_1, \cdots, x_N) \in (\mathbb{R}^d)^N;\ |x_i - x_j| \neq 0\}.$$

no collapse means that if $x(0) \in \mathcal{O}$, then $x(t) \in \mathcal{O}$ for all time $t > 0$.

If no collapse, the stochastic Hamilton system lies in the state space

$$S = \mathcal{O} \times (\mathbb{R}^d)^N.$$

Mathematical difficulties:

1. the generator of the stochastic Hamilton system

$$\mathcal{L}f(x,v) = v\partial_x f + \frac{1}{2}\sum_{i,j}(\sigma\sigma^T)_{i,j}\partial_v f - (c(x,v)v + \nabla V)\partial_v f,$$

   $((x,v) \in \mathcal{O} \times (\mathbb{R}^d)^N)$ is hypoelliptic.

   The distribution μ_t of $X_t = (x(t), v(t))$ satisfies the kinetic Fokker-Planck equation in PDE's theory. Equally difficult in PDEs.

2. Hormander's hypoellipcility theory fails in the presence of singularity

3. Villani's hypocoercivity theory fails too in the presence of singularity.

Answer:

Y. Lu and J.C. Mattingly. Geometric ergodicity of Langevin dynamics with Coulomb interactions. *Nonlinearity*, 33(2):675, 2019.

Method: via Lyapunov function. Work if coulomb potential and

$$\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{v}) = \boldsymbol{\sigma} \boldsymbol{I}_d(\text{constant}),\ \boldsymbol{c}(\boldsymbol{x},\boldsymbol{v}) = \boldsymbol{c} > \boldsymbol{0}(\text{constant}).$$

But in the elliptic case, many results are known today, see

Feng-Yu Wang, Xi-Chen Zhang

Jabin-Wang (McKean-Vlasov's equation)

etc.

2. Quasi Stationary Distribution (QSD):

background and motivations

Let

- the state space S is Polish (metric, complete, separable) with Borel σ-field $\mathcal{B}$

- $D \subset S$ a non-empty open domain

- $(X_t)_{t\geq 0}$ be a strong Markov process with càdlàg trajectories, defined on $(\Omega, \mathcal{F}_t, (\mathbb{P}_x)_{x\in S})$.

- $(P_t(x, dy))_{t\geq 0}$ the transition probability semigroup of (X_t),

$$P_t f(x) = \mathbb{E}_x f(X_t).$$

- $\mathcal{L}$ the generator of $\mathcal{L}$: $f \in \mathbb{D}_e(\mathcal{L})$ if

$$M_t(f) := f(X_t) - f(X_0) - \int_0^t \mathcal{L} f(X_s) ds$$

is a local martingale under $\mathbb{P}_x$ for every starting point x in S.

Then $u(t,x) := P_t f(x)$ satisfies the Kolmogorov backward equation

$$\partial_t u(t,x) = \mathcal{L} u(t,x),\ u(0,x) = f(x)$$

and for any initial distribution ν, the distribution $\nu_t = \nu P_t$ of X_t at time t satisfies the Kolmogorov forward equation

$$\partial_t \nu_t = \mathcal{L}^* \nu_t,\ \nu_0 = \nu.$$

Both are parabolic PDEs, when

$$\mathcal{L} f = \frac{1}{2} \sum_{i,j} a_{ij}(x) \partial_{ij}^2 f + \sum_i b_i(x) \partial_i f.$$

Definition 1 *A probability measure μ is said to be a stationary distribution of X_t, if*

$$\mu(A) = (\mu P_t)(A) := \int_S P_t(x,A) d\mu(x),\ \forall A \in \mathcal{B}.$$

In statistical mechanics or biology, μ is called often equilibrium state.

A fundamental question in the ergodicity is

(1) Does the stationary distribution μ exist ? unique ?

If Yes,

(2) How fast ν_t converges to μ ?

Methods :

Lyapunov functions : books by Khasminski, Meyn-Tweedie

Functional inequalities : books by D. Bakry, M.F. Chen, M. Ledoux, Saloff-Coste, F.Y. Wang,

Coupling : M.F. Chen's book.

Now consider the process $(X_t)_{t<\sigma_D}$ killed outside D, where

$$\sigma_D := \inf\{t \geq 0; X_t \notin D\}$$

is the first exit time. Its transition semigroup is given by

$$P_t^D f(x) = \mathbb{E}_x \mathbf{1}_{t<\sigma_D} f(X_t).$$

For a physical system described by Langevin equations in low temperature, though the system will converge to its equilibrium state μ at "infinite" time, in reality it stays in an attraction domain D for long time!

The mathematical notion to describe this meta-stable state is

Definition 2 *A quasi-stationary distribution (QSD in short) of the Markov process* (X_t) *in the domain* D *is a probability measure on* D *such that for all* $t > 0, A \subset D, A \in \mathcal{B}$,

$$\mu_D(A) = \mathbb{P}_{\mu_D}(X_t \in A | t < \sigma_D) = \frac{\mathbb{P}_{\mu_D}(X_t \in A, t < \sigma_D)}{\mathbb{P}_{\mu_D}(t < \sigma_D)} \tag{3}$$

A fundamental question in the study of QSD is

(1) Does the QSD μ_D exist ? unique ?

If Yes,

(2) How fast $\nu_t^D := \mathbb{P}_\nu(X_t \in \cdot | t < \sigma_D)$ converges to μ_D ?

Remark 1 From the definition (3), μ_D is a QSD if and only if

$$\mu_D P_t^D = \lambda(t)\mu_D, \ \lambda(t) = \mathbb{P}_{\mu_D}(t < \sigma_D)$$

in other words, μ_D must be a common positive left-eigenvector of P_t^D.

Motivations :

For the QSD of population processes or more generally of models derived from biological systems, see

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Accelerated algorithms: Fleming-Viot processes

Proposed by

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A.F. Voter. Parallel replica method for dynamics of infrequent events. Physical Review B, 57(22):R13 985, 1998.

Applications:

X. Bai, A. F. Voter, R. G. Hoagland, M. Nastasi, and B. P. Uberuaga. Efficient annealing of radiation damage near grain boundaries via interstitial emission. Science, 327(5973):1631-1634, 2010.

F. Montalenti, M. R. Sorensen, and A. F. Voter. Closing the gap between experiment and theory: Crystal growth by temperature accelerated dynamics. Physical Review Letters, 87:126101, Aug 2001.

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Mathematical justifications.

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3. General framework and tools

We first present a general framework on (X_t).

(C1) **(strong Feller property)** There is some $t_0 > 0$ such that for each $t \geq t_0$, P_t is strong Feller, i.e. $P_t f$ is continuous for all $f \in b\mathcal{B}$.

(C2) **(trajectory Feller property)** For every $T > 0$, $x \to \mathbb{P}_x(x_{[0,T]} \in \cdot)$ is continuous from S to the space $\mathcal{M}_1(\mathbb{D}([0,T],E))$ of probability measures on $\mathbb{D}([0,T],S)$ equipped with the weak convergence topology.

(C3) There are some continuous function function $W : S \to [1,+\infty[$, belonging to the generalized domain $\mathbb{D}(\mathcal{L})$, two sequences of positive constants (r_n) and (b_n) where $r_n \to +\infty$, and an increasing sequence of compact subsets (K_n) of S, such that

$$-\mathcal{L}W(x) \geq r_n W(x) - b_n 1_{K_n}(x),\ q.e.$$

Definition 3 *Two functions g_1, g_2 are said to be equal q.e., if $g_1 = g_2$ almost everywhere in the (resolvent) measure*

$$R_1(x, \cdot) = \int_0^{+\infty} e^{-t} P_t(x, \cdot) dt$$

for **every** $x \in S$.

Suppose that the killed process $(X_t)_{t<\sigma_D}$ satisfies

(C4) $P_t^D, t \geq 0$ are Feller on $C_b(D)$;

(C5) there exists $t_0 > 0$ such that for all $t \geq t_0$, for all $x \in D$ and non-empty open subsets O of D,

$$P_t^D(x, O) > 0$$

and there is some $x_0 \in D$ such that $\mathbb{P}_{x_0}(\sigma_D < +\infty) > 0$.

Our talk is based on our following general result obtained in (Guillin, Nectoux and Wu 2020, submitted to JEMS).

Theorem 1 *Assume* **(C1), (C2), (C3), (C4), (C5)**. *Then*

(a) *there is only one QSD* μ_D *satisfying*

$$\mu_D(W^{1/p}) := \int_D W^{1/p}(x)\mu_D(dx) < +\infty$$

for some $p \in]1, +\infty[$.

(b) *In particular if* W *is bounded, the QSD inside* D *is unique.*

(c) *the spectral radius of* P_t^D *on* $b_{\mathsf{W}^{1/p}}\mathcal{B}(\mathcal{D})$ *equals to* $e^{-\lambda_D t}$ *for all* $t \geq 0$ *where* $0 < \lambda_D < +\infty$ *(which is often called least Dirichlet eigenvalue of the killed Markov process), and there is a unique continuous function* φ *bounded by* $c\mathsf{W}^{1/p}$ *and positive everywhere on* $\mathcal{D}$ *such that* $\mu_D(\varphi) = 1$ *and*

$$\mu_D P_t^D = e^{-\lambda_D t}\mu_D,\ P_t^D\varphi = e^{-\lambda_D t}\varphi \text{ on } D, \forall t \geq 0. \quad (4)$$

Here $b_{\mathsf{W}^{1/p}}\mathcal{B}(\mathcal{D})$ *is the Banach space of all* $\mathcal{B}(\mathcal{D})$*-measurable functions on* $\mathcal{D}$ *so that its norm*

$$\|f\|_{b_{\mathsf{W}^{1/p}}\mathcal{B}(\mathcal{D})} := \sup_{\mathsf{x}\in\mathcal{D}} \frac{|f(\mathsf{x})|}{\mathsf{W}^{1/p}(\mathsf{x})} < +\infty.$$

(d) *for any* $p \in]1, +\infty[$ *fixed, there are some constants* $\delta > 0$ *and* $C \geq 1$ *such that for any initial distribution* ν *on* D *with* $\nu(W^{1/p}) < +\infty$*, for all* $A \in \mathcal{B}_D, t > 0$*,*

$$|\mathbb{P}_\nu(X_t \in A | t < \sigma_D) - \mu_D(A)| \leq C e^{-\delta t} \frac{\nu(W^{1/p})}{\nu(\varphi)}. \qquad (5)$$

(e) $\lambda_D > 0$*,* $\mathbb{P}_x(\sigma_D < +\infty) = 1$ *for every* $x \in D$*,* X_{σ_D} *and* σ_D *are* $\mathbb{P}_{\mu_D}$*-independent and*

$$\mathbb{P}_{\mu_D}(t < \sigma_D) = e^{-\lambda_D t}.$$

4. Main results

The stochastic Hamilton system lies in the state space $\boldsymbol{S} = \boldsymbol{\mathcal{O}} \times (\mathbb{R}^d)^N$.

Consider a domain

$$\boldsymbol{D} = \boldsymbol{O} \times (\mathbb{R}^d)^N$$

where $\boldsymbol{O}$ is a non-empty connected open domain with $\boldsymbol{C^2}$-boundary outside the singularity set $\partial\boldsymbol{\mathcal{O}}$, i.e. $\partial\boldsymbol{O}\backslash\partial\boldsymbol{\mathcal{O}}$ is $\boldsymbol{C^2}$.

Problem 3. *Whether* $\boldsymbol{X_t} = (\boldsymbol{x}(\boldsymbol{t}), \boldsymbol{v}(\boldsymbol{t}))$ *has a unique QSD* $\boldsymbol{\mu_D}$ *?*

Problem 4. *Whether* $\mathbb{P}_{\boldsymbol{\nu}}(\boldsymbol{X_t} \in \cdot|\boldsymbol{\sigma_D} > \boldsymbol{t}) \to \boldsymbol{\mu_D}$ *with an exponential rate ?*

Hypotheses in the generalized Lennard-Jones potential

The interaction V_I is of form

$$V_I(x) = \frac{b}{|x|^\alpha} + \Phi_I(x),\ x \in \mathbb{R}^d \backslash \{0\} \tag{6}$$

where $b > 0$, $\alpha > 0$.

1. The confinement potential $U : \mathbb{R}^d \to \mathbb{R}$ satisfies:
   for some $A > 0, \gamma > 1$

   $$U(x) = A|x|^\gamma + \Psi(x),\ x \in \mathbb{R}^d$$

   where

   $$\lim_{|x|\to+\infty} \frac{|\Psi(x)|}{|x|^\gamma} = \lim_{|x|\to+\infty} \frac{|\nabla\Psi(x)|}{|x|^{\gamma-1}} = \lim_{|x|\to+\infty} \frac{|\mathrm{Hess}\Psi(x)|}{|x|^{\gamma-2}} = 0$$

2. $\Phi_I(x)$ in (6) defined on $(0,+\infty)$ if $d=1$ and $\mathbb{R}^d\backslash\{0\}$ if $d\geq 2$, satisfies

$$\lim_{x\to 0}|x|^{\alpha}\Phi_I(x)=\lim_{x\to 0}|x|^{\alpha+1}|\nabla\Phi_I(x)|$$
$$=\lim_{x\to 0}|x|^{\alpha+2}|\nabla\Phi_I(x)|=0$$

and $\Phi_I,\nabla\Phi_I,\nabla^2\Phi_I$ are bounded and continuous for $|x|>R$ (for some $R>0$).

The set of the above hypotheses is named as **(H-LJ)**.

Hypotheses on the damping coefficient and the diffusion matrix

(Ac) $c(x,v) : (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N \to M_{Nd}(\mathbb{R})$ is C^1 and bounded, and $\exists c_0 > 0, R > 0$ such that if $|(x,v)| > R$

$$c(x,v)c(x,v)^T > c_0 I.$$

(Aσ) $\sigma(x,v)$ is C^∞ and there are $0 < a < b$ such that

$$aI \leq \sigma\sigma^T(x,v) \leq bI$$

in the sense of definite positive matrices.

Theorem 2 *Assume* **(H-JS), (Ac), (Aσ)**. *Then*

1. (X_t) *does not explode, has no collapse (essentially due to Lu and Mattingly 19).*

2. *Let*

$$D = O \times (\mathbb{R}^d)^N$$

where O *is a connected open domain in* $\mathcal{O}$ *such that* $\mathcal{O}\backslash\bar{O}$ *is non-empty and* $\partial O\backslash\mathcal{O}$ *is* C^2.

3. *There are some constant* $\eta \in (0, 1]$ *and a Lypunov function*

$$W(x, v) \leq e^{mH(x,v)^\eta},\ H(x, v) = \frac{1}{2}|v|^2 + V(x) \text{ is the Hamiltonian}$$

such that all five conclusions in Theorem 1 for this Lyapunov function.

Remark 2 *This theorem covers the Riesz potential* $V_I(x) = \frac{1}{|x|^{d-\alpha}}$ *for* $\alpha \in (0, d)$*, including the Coulomb potential.*

4.2. Log-potential

For the log-potential (if $d = 1, 2$, $V_I(x) = -b \log |x|$), the same results in Theorem 2 still hold true with a different Lyapunov function W.

Thanks !