

Hamilton-Jacobi PDE in space of Probability Measures

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Outline

1 Prelude

- Freidlin-Wentzell theory for singular diffusions
- Space of probability measures as a quotient space

2 Variational problems in space of probability measures

- Hamilton-Jacobi equations in $\mathcal{P}_2(\mathbb{R}^d)$
- Why are they interesting?

3 The LDP Problem (A simplified version):

- Optimal transport

4 The Mechanics problem

- H-J equation in $\mathcal{P}_2(\mathbb{R}^d)$ - inadequate choice of tangent space
- H-J equation in $\mathcal{P}_2(\mathbb{R}^d)$ – Geometric tangent cone

Small diffusions

- $dX_n(t) = b(X_n(s))ds + \frac{1}{\sqrt{n}}\sigma(X_n(s))dW(s).$
- $A_n f(x) = \frac{1}{2n} \sum_{ij} a_{ij}(x) \partial_{ij}^2 f(x) + b(x) \cdot \nabla f(x)$
- $H_n f(x) = \frac{1}{2n} \sum_{ij} a_{ij}(x) \partial_{ij}^2 f(x) + \frac{1}{2} |\sigma(x) \nabla f(x)|^2 + b(x) \cdot \nabla f(x),$
- $H_n f \rightarrow Hf$ with

$$Hf(x) = \frac{1}{2} |\sigma(x) \nabla f(x)|^2 + b(x) \cdot \nabla f(x) = H(x, \nabla f(x)).$$

- $L(x, q) = \sup_p \{pq - H(x, p)\}.$
- $\{X_n, n = 1, 2, \dots\}$ satisfies LDP with rate function

$$I(x(\cdot)) = \int_0^\infty L(x(s), \dot{x}(s)) ds.$$

Comparison Principle

$$f - \alpha Hf = h.$$

By available PDE theory, the comparison principle holds if,

- σ, b are Lipschitz, OR
- σ, b are bounded continuous and $\sigma(x)\sigma^T(x)$ is uniform nondegenerate.

Comparison Principle singular case

$$f - \alpha Hf = h.$$

where $E = \mathbb{R}_+$ and $\sigma(x) = \sqrt{x}$ and

$$Hf(x) = \frac{1}{2}x|\partial_x f|^2.$$

- The comparison principle is NOT known.
- Small time heat kernel estimate for $dX(t) = b(X(t))dt + \sigma(X(t))dW(t)$:

$$\lim_{\epsilon \rightarrow 0+} \lim_{n \rightarrow \infty} t \log P(X(n^{-1}t) \in B(y, \epsilon) | X(0) = x) = -\frac{d^2(x, y)}{t}.$$

- Rescaling: let $X_n(t) = X(n^{-1}t)$.

Comparison principle does hold for the singular case

- A geometrically invariant condition:

$$H_x \frac{d^2(x, y)}{\epsilon} - H_y \frac{-d^2(x, y)}{\epsilon} \leq \omega \left(\frac{d^2(x, y)}{\epsilon} + d^2(x, y) \right).$$

- Take $E := (\mathbb{R}_+, d)$ where

$$d^2(x, y) := \inf \left\{ \int_0^1 L(\dot{x}(s)) ds : x(0) = x, x(1) = y \right\} = |\sqrt{x} - \sqrt{y}|^2.$$

- A geometric identity

$$|\sqrt{x} \nabla_x d^2(x, y)|^2 = |\sqrt{y} \nabla_y (-d^2(x, y))|^2.$$

- $x \mapsto d^2(x, y)$ not smooth in classical sense.
- A deeper question: Right choice of test functions?
- Need for "viscosity extensions".

Space of empirical measures:

- $x_i \in \mathbb{R}^d$, $i = 1, 2, \dots, n$.
- Ordered $\vec{x} := (x_1, \dots, x_n)$ v.s un-ordered $\{x_1, \dots, x_n\}$.
- Un-ordered n -points as a permutation invariant element in $(\mathbb{R}^d)^n / \sim$:

$$(x_1, \dots, x_n) \sim (x_{\pi(1)}, \dots, x_{\pi(n)}).$$

- Representing $(\mathbb{R}^d)^n / \sim$ as

$$E_n := \left\{ \rho(dx) := \frac{1}{n} \sum_{i=1}^n \delta_{x_i}(dx), x_i \in \mathbb{R}^d \right\}.$$

- Let $E := \mathcal{P}(\mathbb{R}^d)$ be a kind of limit of E_n s.
- Large deviation, limits and dynamics of HJ equations in E_n and in E .
- Very singular spaces (many "corners" and "edge") of metric geometry nature.
- Metric space analysis tools is natural – theory of mass transport.

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Lagrangian in space of probability measures

- $(X, d) := (\mathcal{P}_2(\mathbb{R}^d); W_2)$ Wasserstein order-2 metric space,

$$A_T[\rho(\cdot)] := \int_0^T L(\rho, \dot{\rho}) dt.$$

- A Large Deviation Problem: $S(\rho) := \int \rho \log \rho + \int \Psi d\rho - \log Z_\Psi$ and

$$L(\rho, \dot{\rho}) := \frac{1}{2} \|\dot{\rho} + \text{grad} S(\rho)\|_{-1, \rho}^2.$$

- A Mechanics Problem: ϕ, Φ smooth and bounded and

$$L(\rho, \dot{\rho}) := \frac{1}{2} \|\dot{\rho}\|_{-1, \rho}^2 - V(\rho), \quad V(\rho) := \int_{\mathbb{R}^d} \phi d\rho + \frac{1}{2} \langle \Phi * \rho, \rho \rangle.$$

Hamiltonian

All Hamiltonians are discontinuous and have a strong form of singularity

- The Large Deviation Problem:

$$H(\rho, \text{grad}_\rho f) = \langle -\text{grad} S, \text{grad} f \rangle_{-1, \rho} + \frac{1}{2} \|\text{grad} f\|_{-1, \rho}^2.$$

Feature: Controlled gradient flow in $\mathcal{P}_2(\mathbb{R}^d)$.

- The Mechanics Problem

$$H(\rho, \text{grad}_\rho f) = \frac{1}{2} \|\text{grad} f\|_{-1, \rho}^2 + V(\rho).$$

Feature: Condensation.

Hamilton-Jacobi equations

In the talk, we solve well-posedness for $f - \alpha H(\rho, \text{grad}_\rho f) = h$.

- The Large Deviation Problem: F. & Katsoulakis [ARMA 09], F. & Kurtz [AMS Book 06], F. & Nguyen [JMPA12].
- The Mechanics Problem: Ambrosio & F. [JDE 14]. Earlier: Hynd, Kim, Gangbo, Nguyen, Swiech, Tudorascu

Why are they interesting?

The Mechanics Problem:

- Variational formulation of compressible Euler equation

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho u) &= 0 \\ \partial_t(\rho u) + \operatorname{div}(\rho u \otimes u) &= -\rho \nabla(\phi + \Phi * \rho). \end{cases}$$

- Formally, Hamiltonian flow as time-dependent gradient flow:

$$\dot{\rho} \in \operatorname{grad}_{\rho} S(t, \rho)$$

- Understand certain behaviors of compressible Euler equation in \mathbb{R}^d by lifting it up to the level of Hamilton-Jacobi equation in $\mathcal{P}_2(\mathbb{R}^d)$.

Why are they interesting?

The Large Deviation Problem:

- Mean-field interacting diffusions (more general than the earlier model)

$$dX_i = K * \rho_n(t, X_i)dt + \sqrt{2\nu}dW_i(t), \quad \rho_n(t) := \frac{1}{n} \sum_i \delta_{X_i(t)}.$$

- LDP rate function as Boltzmann entropy in path space

$$\lim_{\epsilon \rightarrow 0} \lim_{n \rightarrow \infty} -\frac{1}{n} \log P(\rho_n(\cdot) \in B_\epsilon(\rho(\cdot))) = A_T(\rho(\cdot)).$$

- Feng&Kurtz [06] "Large Deviation for Stochastic Processes" :
 - 1 Hamiltonian for Markov process $\{\rho_n(\cdot)\}$: $H_n f(\rho) := \frac{1}{n} e^{-nf} A_n e^{nf}$;
 - 2 $H_n \rightarrow H$;
 - 3 Exp. tightness;
 - 4 Comparison principle for resolvent eqn of H .

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LDP for infinite particles

- LDP for $dX_i = \sqrt{2}dW_i - \nabla\Psi(X_i)dt$,

$$\rho_N(t, dx) = N^{-1} \sum_i \delta_{X_i(t)}(dx).$$

- For "polynomial" f s:

$$Hf(\rho) = \langle \Delta\rho + \operatorname{div}(\rho\nabla\Psi), \frac{\delta f}{\delta\rho} \rangle + \frac{1}{2} \int |\nabla \frac{\delta f}{\delta\rho}|^2 d\rho.$$

- The above is in fact,

$$Hf(\rho) = \langle -\operatorname{grad} S_\Psi(\rho), \operatorname{grad} f(\rho) \rangle_{-1,\rho} + \frac{1}{2} \|\operatorname{grad} f(\rho)\|_{-1,\rho}^2.$$

- What is the supporting notion of differential structure ?
- The answer: The Otto calculus, formalized by Ambrosio-Gigli-Savare.

The tangent space of $\mathcal{P}_2(\mathbb{R}^d)$

$$E := \mathcal{P}_2(\mathbb{R}^d).$$

- Identify $v \in T_\rho E$ in $\partial_t \rho + \operatorname{div}(\rho v) = 0$ with $\dot{\rho} = \partial_t \rho$. How?
- $\|m\|_{-1,\rho}^2 := \sup_{\varphi \in C_c^\infty(\mathbb{R}^d)} \{2\langle \varphi, m \rangle - \int_{\mathbb{R}^d} |\nabla \varphi|^2 d\rho\},$
- $\dot{\rho} \in H_{-1,\rho}(\mathbb{R}^d) := \{m \in \mathcal{D}'(\mathbb{R}^d) : \|m\|_{-1,\rho} < \infty\}$

$$\Leftrightarrow v \in T_\rho E.$$

A differential structure on $\mathcal{P}_2(\mathbb{R}^d)$

- Directional derivative along smooth direction $p \in C_c^\infty$

$$D^p f(\rho(0)) := \lim_{t \rightarrow 0+} \frac{f(\rho(t)) - f(\rho(0))}{t},$$

$$\partial_t \rho + \operatorname{div}(\rho \nabla p) = 0.$$

- Gradient

$$D^p f(\rho(0)) = \langle \operatorname{grad} f(\rho(0)), p \rangle.$$

- Why? A property

$$\langle m, -\nabla(\rho \nabla p) \rangle_{-1, \rho} = \langle m, p \rangle.$$

-

$$\operatorname{grad} f(\rho) = -\nabla(\rho \nabla \frac{\delta f}{\delta \rho}).$$

The Otto calculus on $\mathcal{P}_2(\mathbb{R}^d)$

- Let $S(\rho) = \int \rho \log \rho dx$, then

$$-\Delta \rho = -\nabla \cdot \left(\rho \frac{\nabla \rho}{\rho} \right) = \text{grad } S.$$

- Let

$$S_\Psi(\rho) = S(\rho) + \int \Psi d\rho + \log Z = \int \log \frac{d\rho}{d\mu^\Psi} d\rho,$$

$\mu^\Psi = Z^{-1} e^{-\Psi} dx$. Then

$$\text{grad } S_\Psi(\rho) = -\Delta \rho - \nabla(\rho \nabla \Psi).$$

- Fokker-Planck equation is $\dot{\rho} = -\text{grad } S_\Psi$.

Comparison principle holds

$$(I - \alpha H)f = h$$

- $Hf(\rho) = \langle -\text{grad } S_\Psi, \text{grad } f \rangle_{-1,\rho} + \frac{1}{2} \|\text{grad } f(\rho)\|_{-1,\rho}^2$.
- Optimal controlled gradient flow

$$\dot{\rho} = -\text{grad } S_\Psi(\rho) + m, \quad L(\rho, m) = \frac{1}{2} \|m\|_{-1,\rho}^2.$$

- F.&Kurtz and F.&Katsoulakis : This HJ equation is well-posed, in particular, the comparison holds.

Choice of test functions, useful for comparison

- Choice of test functions:

$$f_0(\rho) = \alpha d^2(\rho, \gamma) + \epsilon S(\rho),$$

$$f_1(\gamma) = -\alpha d^2(\rho, \gamma) - \epsilon S(\gamma).$$

- Lyapunov functional: (I is Fisher information)

$$H\epsilon S(\rho) = -\epsilon(1 - \frac{1}{2}\epsilon)I(\rho).$$

- Wasserstein metric

$$d^2(\rho, \gamma) := \inf \left\{ \int_0^1 \|\dot{\rho}\|_{-1, \rho(r)}^2 dr : \rho(0) = \rho, \rho(1) = \gamma \right\}.$$

- Brenier, Otto, Ambrosio-Gigli-Savare, Villani....

$$\|\text{grad}_\rho \frac{1}{2} d^2(\rho, \gamma)\|_{-1, \rho}^2 = d^2(\rho, \gamma) = \|\text{grad}_\gamma \frac{1}{2} d^2(\rho, \gamma)\|_{-1, \gamma}^2.$$

Estimate

- HWI inequality:

$$S_{\Psi}(\rho) - S_{\Psi}(\gamma) \leq C_{\Psi}(d(\rho, \gamma)\sqrt{I(\gamma)} + d^2(\rho, \gamma)).$$

- Fisher information

$$I(\rho) = \|\text{grad } S_{\Psi}\|_{-1, \rho}^2 = \int \frac{|\nabla \rho|^2}{\rho} dx + \int (|\nabla \Psi|^2 - 2\Delta \Psi) d\rho.$$

- The strong regularization of I helps (mass transport HWI inequalities...)

$$Hf_0(\rho) - Hf_1(\gamma) \leq \omega(\alpha d^2(\rho, \gamma)).$$

Explained using Euclidean space analogy:

$$Hf(x) := -\nabla S(x)\nabla f(x) + \frac{1}{2}|\nabla f(x)|^2.$$

- Mass transport version of: $|\nabla_x|x - y|^2| = |\nabla_y(-|x - y|^2)|$.
- Contraction of flows by $-\nabla S$, with respect to $d(x, y) := |x - y|$

$$-\nabla S(x)\nabla_x d^2(x, y) - \nabla S(y)\nabla_y d^2(x, y) \leq Cd^2(x, y).$$

The case of $E := \mathcal{P}(\mathbb{R}^d)$

- If ρ has Lebesgue density, by Brenier's theory on mass transport

$$\text{grad}_\rho \frac{d^2(\rho, \gamma)}{2} = \nabla p, \quad p(x) := \frac{|x|^2}{2} - \varphi(x),$$

where $\varphi := \varphi^{\rho, \gamma}$ is the convex optimal potential in the Monge formulation of d such that $(\nabla \varphi)_\# \rho = \gamma$. In the above,

$$\|\text{grad}_\rho \frac{d^2(\rho, \gamma)}{2}\|_\rho^2 = \int |\nabla p|^2 d\rho = \int_{\mathbb{R}^d} |x - \nabla \varphi(x)|^2 \rho(dx) = d^2(\rho, \gamma).$$

- Log-Sobolev type/HWI inequality

$$\langle \text{grad}_\rho d^2, \text{grad}_\rho(-S) \rangle_\rho + \langle \text{grad}_\gamma d^2, \text{grad}_\gamma(-S) \rangle_\gamma \leq Cd^2$$

- The strong regularization of I helps to give

$$Hf_0(\rho) - Hf_1(\gamma) \leq \omega(\alpha d^2(\rho, \gamma) + d(\rho, \gamma)).$$

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H-J equation for compressible Euler equations

The continuum mechanics problem

$$Hf(\rho) := \frac{1}{2} \|\text{grad} f(\rho)\|_{-1,\rho}^2 + V(\rho).$$

- Earlier attempts by Gangbo, Nguyen, Tadorascu, Swiech, Hydn, Kim, ... on equivalent re-formulation

$$L(\rho, v) := \frac{1}{2} \int_{\mathcal{O}} |v|^2 d\rho - V(\rho), \quad H(x, \xi) := \frac{1}{2} \int_{\mathcal{O}} |\xi|^2 d\rho + V(\rho)$$

where $\mathcal{O} := \mathbb{T}^d, \mathbb{R}^1, \mathbb{R}^d$.

- Using sub- super-gradients in Wasserstein space.
- Open Problem: No uniqueness theory (i.e. comparison principle).

It should **not** be expected to work, metric nature of $\mathcal{P}_2(\mathbb{R}^d)$

- Kantorovich formulation of

$$d^2(\rho, \gamma) := \inf_{\pi_{\#}^1 m = \rho, \pi_{\#}^2 m = \gamma} \int_{\mathbb{R}^d \times \mathbb{R}^d} |x - y|^2 m(dx, dy)$$

$\Gamma(\rho, \gamma) :=$ those optimal m in the inf problem.

- For every $m \in \Gamma(\rho, \gamma)$, let

$$m(dx, dy) := m(dy|x)\rho(dx), \quad u(x) := \int_{\mathbb{R}^d} (x - y)m(dy|x).$$

Then $\text{grad}_{\rho} \frac{d^2(\rho, \gamma)}{2} = u$ (equivalent class). (By A.G.S.05)

- By Jensen, equality holds if and only if $\gamma = T_{\#} \rho$ (map v.s. plan)

$$\|\text{grad}_{\rho} \frac{d^2(\rho, \gamma)}{2}\|_{\rho}^2 = \int_{\mathbb{R}^d} |u|^2 d\rho \leq \int \int |x - y|^2 m(dy|x)\rho(dx) = d^2(\rho, \gamma)$$

What happened

- The T_ρ did not generate enough velocity fields.
- There is a metric analysis (hence taking care of singularity of space) based re-formulation by Ambrosio- Feng 15.
- When ρ is singular (i.e. "corned"), certain "direction" in the metric formulation cannot be modelled by the tangent space here – think of a Polyhedron.

Geometric tangent cone

Idea: relaxed formulation of tangent $\mathbf{m}(dx, d\xi) := \delta_{u(x)}(d\xi)\rho(dx)$.

- $G(\rho) := \{\mathbf{m} \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d) : (\pi^1, \pi^1 + \epsilon\pi^2)_\# \mathbf{m} \in \Gamma_o(\rho, \gamma), \exists \gamma \in X, \epsilon > 0\}$
- $D_\rho(\mathbf{m}_1, \mathbf{m}_2) := \inf\{\int_{(\mathbb{R}^d)^3} |\xi - \eta|^2 M(dx; d\xi, d\eta) : M \in \mathcal{P}_2((\mathbb{R}^d)^3), \pi_\#^{1,2} M = \mathbf{m}_1, \pi_\#^{1,3} M = \mathbf{m}_2\}$
- $\langle m_1, m_2 \rangle_\rho := \max\{\int_{(\mathbb{R}^d)^3} \xi\eta M(dx; d\xi, d\eta) : M \in \mathcal{P}_2((\mathbb{R}^d)^3), \pi_\#^{1,2} M = \mathbf{m}_1, \pi_\#^{1,3} M = \mathbf{m}_2\}$
- $\|\mathbf{m}\|_\rho^2 := \langle \mathbf{m}, \mathbf{m} \rangle_\rho$

Definition

$$\text{Tan}_\rho := \overline{G(\rho)}^{D_\rho(\cdot, \cdot)}, \quad \text{Tan} := \cup_\rho \text{Tan}_\rho.$$

Geometric tangent cone continued

Lemma

$T_\rho \hookrightarrow \text{Tan}_\rho$. When $\rho(dx) = \rho(x)dx$, the embedding is isometric and $1 - 1$, generally the inclusion is strict.

sub-, super-differential calculus

- ① Fréchet super-differentials for $f : X \mapsto \bar{\mathbb{R}}$. $\mathbf{n} \in \partial_\rho^+ f$ if there exists a modulus $\omega_{\mathbf{n}}$ such that, for every $\rho_1 \in X$ and every $\mathbf{M} \in \mathcal{P}_2((\mathbb{R}^d)^3)$ with $(\pi^1, \pi^1 + \pi^2)_\# \mathbf{M} \in \Gamma_o(\rho, \rho_1)$ and $\pi_\#^{1,3} = n$, we have

$$f(\rho_1) - f(\rho) \leq \int_{(\mathbb{R}^d)^3} (\xi \cdot \eta) \mathbf{M}(dx; d\xi, d\eta) + d(\rho, \rho_1) \omega_{\mathbf{n}}(d(\rho, \rho_1)) \quad (1)$$

- ② Similarly define (sub-) derivative. $\mathbf{n} \in \partial_\rho^- f$.
- ③ $\partial f := \partial^+ f \cap \partial^- f$.
- ④ $\mathbf{n} \oplus \mathbf{m} := \{\mathbf{n} := (\pi^1, \pi^2 + \pi^3)_\# \mathbf{N}, \pi_\#^{1,2} \mathbf{N} = \mathbf{n}, \pi_\#^{1,3} \mathbf{N} = \mathbf{m}\}$.

Lemma

$$\partial^i \partial \varphi_1 \oplus \partial^i \partial \varphi_2 \subset \partial^i (\varphi_1 + \varphi_2)$$

Geometric Hamiltonian

① $f - \mathbf{H}_0 f \leq h$ and $f - \mathbf{H}_1 f \geq h$.

Lagrangian and Hamiltonian geometric tangent cone

$\mathcal{P}_2(\mathbb{R}^d)$ is a quotient space.

- ① $\mathbf{m}(dx, dv) := \mathbf{m}(dv|x)\rho(dx)$ in stead of $(\rho(dx), v(x))$.
- ② $\mathbf{L}(\mathbf{m}) := \frac{1}{2}\|\mathbf{m}\|_\rho^2 - V(\rho)$ and $\mathbf{H}(\mathbf{n}) := \frac{1}{2}\|\mathbf{n}\|^2 + V(\rho)$;
- ③ $\mathbf{H}_0 f(\rho) := \inf\{\mathbf{H}(\mathbf{n}) : \mathbf{n} \in \partial_\rho^+ f \cap \text{Tan}_\rho\}$;
- ④ $\mathbf{H}_1 f(\gamma) := \sup\{\mathbf{H}(\mathbf{n}) : \mathbf{n} \in \partial_\gamma^- f \cap \text{Tan}_\gamma\}$.

Theorem

(Ambrosio-Feng15.) *The HJ equation in the geometric tangent cone formulation is well posed. In particular, comparison principle holds.*