Optimal transport in an inhomogeneous media: convergence of gradient flows and the effective Wasserstein metric

Yuan Gao, Purdue University

Joint work with Aaron Yip (Purdue), arXiv 2312.01584

Outline

1. (I) Transport problem in an inhomogeneous media
   - The Wasserstein distance and the associated gradient flow
2. (II) Evolutionary Gamma-convergence of ε-gradient flows
   - The limiting gradient flow and the effective limiting Wasserstein distance
3. (III) The limiting Wasserstein distance in Gromov-Hausdorff convergence sence
   - It is smaller than the effective Wasserstein distance induced by limiting gradient flow

Transport problem in an inhomogeneous media

- ε-Wasserstein metric in the Kantorovich formulation

$$W_\varepsilon^2(\mu,\nu) := \inf\left\{\int\int d_\varepsilon^2(x,y)\,\mathrm{d}\pi(x,y);\quad \int_\Omega \pi(x,\mathrm{d}y) = \mu(x),\ \int_\Omega \pi(\mathrm{d}x,y) = \nu(y)\right\}.$$

d_ε is the ε-metric on $\Omega \subset \mathbb{R}^n$ defined via the least action (spatial inhomogeneity)

$$d_\varepsilon^2(x,y) := \inf\{\int_0^1 \langle B_\varepsilon(z_t)\dot{z}_t,\dot{z}_t\rangle\,\mathrm{d}t,\quad z_0 = x,\quad z_1 = y\}.$$

- The equivalent dynamic formulation in Benamou-Brenier form [Bernard-Buffoni '07]

$$W_\varepsilon^2(\rho_0,\rho_1) := \inf\left\{\int_0^1\int \rho_t(x)\langle B_\varepsilon(x)v_t(x),v_t(x)\rangle\,dx\,dt,\quad (\rho_t,v_t)\in CE(\rho_0,\rho_1)\right\}$$

where $B_\varepsilon(x)$ is positive definite matrix and

$$CE(\rho_0,\rho_1) := \left\{(\rho_t,v_t);\ \frac{\partial\rho_t}{\partial t} + \nabla\cdot(\rho_t v_t) = 0,\quad \rho(\cdot,0) = \rho_0,\quad \rho(\cdot,1) = \rho_1\right\}.$$

ε-Fokker-Planck with inhomogeneous noise and potential

- Take relative entropy with an oscillated invariant measure

$$E_\varepsilon(\rho) = \int_\Omega U_\varepsilon(x)\rho(x)\,\mathrm{d}x + \int_\Omega \rho(x)\log\rho(x)\,\mathrm{d}x = \int_\Omega \rho(x)\log\frac{\rho(x)}{\pi_\varepsilon(x)}\,\mathrm{d}x, \quad \pi_\varepsilon = e^{-U_\varepsilon}.$$

- Consider inhomogeneous Fokker-Planck equation

$$\boxed{\partial_t\rho_t^\varepsilon = \nabla\cdot\left(\rho_t^\varepsilon B_\varepsilon^{-1}\nabla\frac{\delta E_\varepsilon}{\delta\rho}(\rho_t^\varepsilon)\right) = \nabla\cdot\left(B_\varepsilon^{-1}\nabla\rho_t^\varepsilon + \rho_t^\varepsilon B_\varepsilon^{-1}\nabla U_\varepsilon\right) = \nabla\cdot\left(\rho_t^\varepsilon B_\varepsilon^{-1}\nabla(\log\rho_t^\varepsilon + U_\varepsilon)\right)}$$

- Drift-diffusion process with reversibility (w.r.t $\pi_\varepsilon = e^{-U_\varepsilon}$)

$$\mathrm{d}X_t = b(X_t)\,\mathrm{d}t + \sigma(X_t) * \mathrm{d}\mathscr{B}_t,$$

$$\text{with } b(x) = -B_\varepsilon^{-1}(x)\nabla U_\varepsilon(x), \quad \sigma(x) = \sqrt{2B_\varepsilon^{-1}(x)}.$$

where the multiplicative noise $\sigma(X_t) * \mathrm{d}\mathscr{B}_t$ is in the backward Ito integral sense

$$\int \sigma(X_t) * \mathrm{d}\mathscr{B}_t = \int \frac{1}{2}\nabla\cdot(\sigma\sigma^T)(X_t)\,\mathrm{d}t + \int \sigma(X_t)\,\mathrm{d}\mathscr{B}_t.$$

ε-Fokker-Planck with interactions

- Take relative entropy with an oscillated invariant measure

$$E_\varepsilon(\rho) = \int_\Omega U_\varepsilon(x)\rho(x)\,\mathrm{d}x + \int_\Omega \rho(x)\log\rho(x)\,\mathrm{d}x + \frac{1}{2}\iint W(x,y)\rho(y)\,\mathrm{d}y\rho(x)\,\mathrm{d}x.$$

- Assume $W(x,y) = W(y,x)$, no oscillation, $(W*\rho)(x) := \int W(x,y)\rho(y)\,\mathrm{d}y$.
- Consider inhomogeneous Fokker-Planck equation

$$\boxed{\partial_t\rho_t^\varepsilon = \nabla\cdot\left(\rho_t^\varepsilon B_\varepsilon^{-1}\nabla\frac{\delta E_\varepsilon}{\delta\rho}(\rho_t^\varepsilon)\right) = \nabla\cdot\left(\rho_t^\varepsilon B_\varepsilon^{-1}\nabla(\log\rho_t^\varepsilon + U_\varepsilon + W*\rho_t^\varepsilon)\right)}$$

- Interacting particle process

$$\mathrm{d}X_t^i = b^i(X_t)\,\mathrm{d}t + \sigma(X_t^i)*\mathrm{d}\mathscr{B}_t^i,$$

$$\text{with } b^i(x) = -B_\varepsilon^{-1}(x^i)\left(\nabla U_\varepsilon(x^i) + \frac{1}{N}\sum_j \nabla_x W(x^i,x^j)\right), \quad \sigma(x) = \sqrt{2B_\varepsilon^{-1}(x)}.$$

Oscillatory invariant measure and dissipation

- Dissipation coefficient on fast variable $y = \frac{x}{\varepsilon}$: $B_\varepsilon(x) = B\left(\frac{x}{\varepsilon}\right)$, B is 1-periodic.
- Oscillatory invariant measure with separation of scales:

$$\pi_\varepsilon(x) = \pi\left(x, \frac{x}{\varepsilon}\right)$$

  * Note highly wiggled potential is allowed for bounded domain. $\pi_\varepsilon \rightharpoonup \bar{\pi}$.
  * For $\mathbb{R}^n$, we need π_ε satisfies Log-Sobolev inequality.

- eg: $\pi_\varepsilon = \pi_0(x) + \varepsilon\pi_1(x, \frac{x}{\varepsilon})$, or $\pi_\varepsilon = \pi_0(x) + \pi_1(x, \frac{x}{\varepsilon})$

Asymptotic expansion gives a homogenized FP

- Convert to divergence (symmetric) form in terms of $f_t^\varepsilon := \frac{\rho_t^\varepsilon}{\pi_\varepsilon}$

$$\text{linear:} \quad \partial_t f_t^\varepsilon = \frac{1}{\pi_\varepsilon} \nabla \cdot \left(\pi_\varepsilon B_\varepsilon^{-1} \nabla f_t^\varepsilon \right) =: L_\varepsilon(f_t^\varepsilon)$$

$$\text{nonlinear:} \quad \partial_t f_t^\varepsilon = \frac{1}{\pi_\varepsilon} \nabla \cdot \left(\pi_\varepsilon B_\varepsilon^{-1} \nabla f_t^\varepsilon + f_t^\varepsilon \pi_\varepsilon B_\varepsilon^{-1} \nabla_x W * (f_t^\varepsilon \pi_\varepsilon) \right) =: N_\varepsilon(f_t^\varepsilon)$$

- Asymptotic expansion for ε-Fokker Planck

$$\text{linear:} \quad \partial_t \rho_t = \nabla \cdot \left(\rho_t \bar{B}^{-1} \nabla \log \frac{\rho_t}{\bar{\pi}} \right), \quad \bar{B}^{-1} := \frac{1}{\bar{\pi}} \bar{D},$$

$$\text{nonlinear:} \quad \partial_t \rho_t = \nabla \cdot \left(\rho_t \bar{B}^{-1} \nabla (\log \frac{\rho_t}{\bar{\pi}} + W * \rho_t) \right)$$

where $\bar{D} := \int \pi(x,y) B^{-1}(y) \left(\delta_{ij} + \nabla_{y_i} w_j(x,y) \right) \mathrm{d}y$;
Cell problem $\quad \nabla_y \cdot (A(x,y) \nabla_y w_i(y)) + \nabla_y \cdot (A(x,y) \vec{e}_i) = 0$;

W_ε-gradient flows

- Using the Riemannian metric $\langle \cdot,\cdot\rangle_{T_\mathscr{P},T_\mathscr{P}}$ on the tangent plane $T_\mathscr{P}$ of $(\mathscr{P}(\Omega), W_\varepsilon)$,

$$\langle s_1, s_2\rangle_{T_\mathscr{P},T_\mathscr{P}} := \int \rho(x)\langle B_\varepsilon(x)\nabla\phi_1(x), \nabla\phi_2(x)\rangle\, dx, \quad \text{where } s_1 = -\nabla\cdot(\rho\nabla\phi_1),\ s_2 = -\nabla\cdot(\rho\nabla\phi_2)$$

- one can express the gradient of E_ε in $(\mathscr{P}(\Omega), W_\varepsilon)$

$$\boxed{\partial_t \rho_t^\varepsilon = -\nabla^{W_\varepsilon} E_\varepsilon(\rho) = \nabla\cdot\left(\rho B_\varepsilon^{-1}\nabla\frac{\delta E_\varepsilon}{\delta\rho}\right)}$$

- ε-dissipation on the tangent plane (metric speed) and co-tangent plane (metric slope)

$$\psi_\varepsilon(\rho, s) := \frac{1}{2}\int_\Omega \langle\nabla u, B_\varepsilon^{-1}\nabla u\rangle\rho\,\mathrm{d}x, \quad \text{with } s = -\nabla\cdot\left(\rho B_\varepsilon^{-1}\nabla u\right); \quad \psi_\varepsilon^*(\rho,\xi) := \frac{1}{2}\int_\Omega \langle\nabla\xi, B_\varepsilon^{-1}\nabla\xi\rangle\rho\,\mathrm{d}x.$$

- Fenchel-Young inequality

$$\langle\xi, s\rangle \le \psi_\varepsilon^*(\rho,\xi) + \psi_\varepsilon(\rho,s), \quad \text{for all} \quad \xi\in T_\rho^*, \text{ and } s\in T_\rho$$

with equality holds iff $s \in \partial_\xi \psi_\varepsilon^*(\rho,\xi) = -\nabla\cdot(\rho B_\varepsilon^{-1}\nabla\xi)$

W_ε-gradient flows in EDI form

- Energy dissipation inequality (EDI) equivalent formulation

$$E_\varepsilon(\rho_t^\varepsilon) + \int_0^t \left[\psi_\varepsilon(\rho_\tau^\varepsilon, \partial_\tau \rho_\tau^\varepsilon) + \psi_\varepsilon^*(\rho_\tau^\varepsilon, -\frac{\delta E_\varepsilon}{\delta \rho}(\rho_\tau^\varepsilon))\right] \mathrm{d}\tau \leq E_\varepsilon(\rho_0^\varepsilon).$$

- more geometric information than PDE
- Whether the gradient flow structure converges? [Serfaty, Mielke, Peletier ...]
- Homogenized W*-gradient flow?

Pass limit for ε-gradient flow in EDI form

- Assumptions:
  - Domain Ω is periodic; $\pi_\varepsilon(x) = \pi(x, \frac{x}{\varepsilon})$ is bounded from above and below away zero
  - Initial data is well prepared with $\bar{E}(\rho_0) = \int \rho_0 \log \frac{\rho_0}{\bar{\pi}} < +\infty$ and

$$E_\varepsilon(\rho_0^\varepsilon) \to \bar{E}(\rho_0), \quad \text{as } \varepsilon \to 0.$$

- Then there exists a subsequence (still denoted as) ρ^ε and $\rho \in C([0,T]; L^2 \cap \mathscr{P}(\Omega))$ s.t.

$$W_2^2(\rho_t^\varepsilon, \rho_t) \to 0, \quad \text{uniformly in } t \in [0,T]$$

  - lower bound for free energy holds

$$\liminf_{\varepsilon \to 0} E_\varepsilon(\rho_t^\varepsilon) \geq \bar{E}(\rho_t);$$

  - lower bound for the dissipation on the cotangent plane holds

$$\liminf_{\varepsilon \to 0} \int_0^t \psi_\varepsilon^*(\rho_\tau^\varepsilon, -\frac{\delta E_\varepsilon}{\delta \rho}(\rho_\tau^\varepsilon))\, \mathrm{d}\tau \geq \int_0^t \psi^*(\rho_\tau, -\frac{\delta \bar{E}}{\delta \rho}(\rho_\tau))\, \mathrm{d}\tau;$$

  - lower bound for the dissipation on the tangent plane holds

$$\liminf_{\varepsilon \to 0} \int_0^t \psi_\varepsilon(\rho_\tau^\varepsilon, \partial_\tau \rho_\tau^\varepsilon)\, \mathrm{d}\tau \geq \int_0^t \psi(\rho_\tau, \partial_\tau \rho_\tau)\, \mathrm{d}\tau.$$

The limiting gradient flow in EDI form

- Limiting dissipation functionals: convex conjugate, bilinear

  for speed $\psi(\rho, s) := \frac{1}{2}\int_\Omega \langle \nabla u, \bar{B}^{-1}\nabla u\rangle \rho \, \mathrm{d}x,$ with $s = -\nabla\cdot\left(\rho \bar{B}^{-1}\nabla u\right);$

  for slope $\psi^*(\rho, \xi) := \frac{1}{2}\int_\Omega \langle \nabla\xi, \bar{B}^{-1}\nabla\xi\rangle \rho \, \mathrm{d}x.$

  Recall $\bar{B}$ is the effective coefficients in $\partial_t\rho_t = \nabla\cdot\left(\rho_t \bar{B}^{-1}\nabla \frac{\delta \bar{E}}{\delta\rho}\right)$

- Consequence (1): limiting gradient flow in EDI form

$$\bar{E}(\rho_t) + \int_0^t \left[\psi(\rho_\tau, \partial_\tau\rho_\tau) + \psi^*(\rho_\tau, -\frac{\delta\bar{E}}{\delta\rho}(\rho_\tau))\right] \mathrm{d}\tau \le \bar{E}(\rho_0).$$

- Consequence (2): limiting dissipation for speed induces Benamou-Brenier action functional

$$\psi(\rho_\tau, \partial_\tau\rho_\tau) = \frac{1}{2}|\dot{\rho}_\tau|^2_{W_*}, \quad W_*^2(\rho_0, \rho_1) := \inf\left\{\int_0^1\int \rho_t(x)\langle \bar{B}v_t(x), v_t(x)\rangle\, dx\, dt, \quad (\rho_t, v_t) \in V(\rho_0, \rho_1)\right\}$$

  The effective equation is a gradient flow $\partial_t\rho_t = -\nabla^{W_*}\bar{E}(\rho_t)$ w.r.t. the induced metric W_*

Key ingredients in proof

- Lower bound for $\int_0^t \psi_\varepsilon^*(\rho_\tau^\varepsilon, -\frac{\delta E_\varepsilon}{\delta \rho}(\rho_\tau^\varepsilon))\,\mathrm{d}\tau$
  - Fisher information $\langle \nabla \log \frac{\rho}{\pi_\varepsilon}, B_\varepsilon^{-1} \nabla \log \frac{\rho}{\pi_\varepsilon} \rho \rangle = 4 \langle \nabla \sqrt{\frac{\rho}{\pi_\varepsilon}}, B_\varepsilon^{-1} \pi_\varepsilon \nabla \sqrt{\frac{\rho}{\pi_\varepsilon}} \rangle$
  - $H^1(L^2) \cap L^\infty(H^1)$ a priori estimate for $f_\varepsilon = \frac{\rho}{\pi_\varepsilon}$ which solves $\partial_t f = \frac{1}{\pi_\varepsilon} \nabla \cdot \left(\pi_\varepsilon B_\varepsilon^{-1} \nabla f \right)$
  - Generalized Fatou lemma (time-space) [Stefanelli '08] for weak limit $\sqrt{f_\varepsilon}$ in $L^2(H^1)$
- Lowe bound for $\int_0^t \psi_\varepsilon(\rho_\tau^\varepsilon, \partial_\tau \rho_\tau^\varepsilon)$
  - use Γ-convergence of $\psi_\varepsilon^*(\rho, \xi)$ to construct recovery sequence $\xi^\varepsilon \rightharpoonup \xi^*$ in H^1

$$\lim_{\varepsilon \to 0} \frac{1}{2} \int_\Omega \langle \nabla \xi^\varepsilon, B_\varepsilon^{-1} \nabla \xi^\varepsilon \rangle \rho_\varepsilon \,\mathrm{d}x = \lim_{\varepsilon \to 0} \frac{1}{2} \int_\Omega \langle \nabla \xi^\varepsilon, B_\varepsilon^{-1} \pi_\varepsilon \nabla \xi^\varepsilon \rangle f^\varepsilon \,\mathrm{d}x = \frac{1}{2} \int_\Omega \langle \nabla \xi^*, \bar{B}^{-1} \nabla \xi^* \rangle \rho^* \,\mathrm{d}x$$

  - lower bound for time-independent case (relaxation+recovering)

$$\begin{aligned} \psi(\rho^*, s^*) &= \lim_{\varepsilon \to 0} \left\{ \int_\Omega \xi^\varepsilon s^\varepsilon \,\mathrm{d}x - \frac{1}{2} \int_\Omega \langle \nabla \xi^\varepsilon, B_\varepsilon^{-1} \nabla \xi^\varepsilon \rangle \rho^\varepsilon \,\mathrm{d}x \right\} \\ &\le \liminf_{\varepsilon \to 0} \sup_\xi \left\{ \int_\Omega \xi s^\varepsilon \,\mathrm{d}x - \frac{1}{2} \int_\Omega \langle \nabla \xi, B_\varepsilon^{-1} \nabla \xi \rangle \rho^\varepsilon \,\mathrm{d}x \right\} \le \liminf_{\varepsilon \to 0} \psi(\rho^\varepsilon, s^\varepsilon). \end{aligned}$$

  - Generalized Fatou lemma (time-space) for weak limit $\partial_t \rho_t^\varepsilon$ in $L^2(L^2)$

Direct limit of W_ε in the Gromov-Hausdroff sense

The explicit 1D example for $W_{GH} < W_*$: (n D example can also be constructed)

- Pointwise convergence

$$d_\varepsilon^2(x,y) := \inf_{z_0=x,\quad z_1=y} \{ \int_0^1 \langle B_\varepsilon(z_t)\dot{z}_t, \dot{z}_t \rangle \, \mathrm{d}t \} = (\int_x^y \sqrt{B_\varepsilon(z)} \, \mathrm{d}z)^2$$

$$\Longrightarrow |x-y|^2 (\int_0^1 \sqrt{B(s)} \, \mathrm{d}s)^2 =: d_{GH}^2(x,y)$$

implies $(\Omega, d_\varepsilon) \to (\Omega, d_{GH})$ in the Gromov-Hausdorff convergence.

$$D_{GH}(\mathscr{X}, \mathscr{Y}) = \frac{1}{2} \inf_{\mathscr{R}} \sup_{(x,y),(x',y') \in \mathscr{R}} \left| d_{\mathscr{X}}(x,x') - d_{\mathscr{Y}}(y,y') \right|$$

where $\mathscr{R} \subset \mathscr{X} \times \mathscr{Y}$ is a correspondence or relation between $\mathscr{X}$ and $\mathscr{Y}$.

- Implies the Gromov-Hausdroff convergence of the Wasserstein space $(\mathscr{P}(\Omega), W_\varepsilon)$

- Wasserstein distance W_ε converges to the limiting Wasserstein distance W_{GH}

$$W_{GH}^2(\mu,\nu) := \inf\left\{\int\int d_{GH}^2(x,y)\,\mathrm{d}\pi(x,y); \quad \int_\Omega \pi(x,\mathrm{d}y) = \mu(x),\ \int_\Omega \pi(\mathrm{d}x,y) = \nu(y)\right\}.$$

- The equivalent Benamou-Brenier formulation

$$W_{GH}^2(\rho_0,\rho_1) := \inf\left\{\int_0^1\int \rho_t(x)\langle \bar{c}v_t(x), v_t(x)\rangle\, dx\, dt, \quad (\rho_t,v_t)\in CE(\rho_0,\rho_1).\right\}$$

- $\bar{c} = (\int_0^1 \sqrt{B(s)}\,\mathrm{d}s)^2 < \bar{B} = \bar{\pi}\int \frac{B(y)}{\pi(x,y)}\,\mathrm{d}y.$ Thus $W_{GH} < W^*$.
  Here in one dimension, we can solve the cell problem explicitly

$$\partial_y\big(A(x,y)\partial_y w(x,y)\big) = -\partial_y\left(A(x,y)\right), \quad \partial_y w(x,y) = -1 + \frac{C(x)}{A(x,y)}, \quad \text{with } C(x) = \left(\int \frac{1}{A(x,y)}\,\mathrm{d}y\right)^{-1}.$$

$$\bar{B}^{-1} := \frac{1}{\bar{\pi}}\bar{D} = \frac{1}{\bar{\pi}}\int \pi(x,y)B^{-1}(y)\big(\delta_{ij} + \nabla_{y_i} w_j(x,y)\big)\,\mathrm{d}y$$

- $n-D$ example can be constructed using bulk-boundary difference.

Conclusion

- The Wasserstein distance W_ε (OT) and gradient flows in inhomogeneous media
- Evolutionary Gamma-convergence of ε-gradient flows
- The limiting gradient flow preserves EDI structure
- The effective limiting Wasserstein distance W_* and induced Riemannian metric
- The limiting Wasserstein distance W_{GH} in Gromov-Hausdorff convergence sence
  $<$ the effective Wasserstein distance W_* induced by limiting gradient flow

Thank you!