

Heterogeneous gradient flows

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Mar. 10, 2022

Heterogeneous phenomena; mixtures, multiple species

Outline

- 1 Classical gradient flows - from ODEs to curves in Hilbert and Polish spaces.
- 2 Gradient flows in Wasserstein topology and continuity equation.
- 3 Heterogeneous continuity equation and fibered Wasserstein space.
- 4 Main result - heterogeneous gradient flows and their applications.
- 5 Further discussion.

$$\dot{x}(t) = -\nabla\mathcal{E}(x(t))$$

- $[0, T) \ni t \mapsto x(t) \in \mathbb{R}^d$ – a curve,
- $\mathcal{E} : \mathbb{R}^d \rightarrow [-\infty, +\infty]$ – potential functional (usually required to satisfy some regularity or convexity assumptions).

Position x evolves along the vector field $-\nabla\mathcal{E}$ evaluated at x "in an attempt" to minimize $\mathcal{E}(x)$.

$$\dot{x}(t) \in -\partial^- \mathcal{E}(x(t))$$

- $[0, T) \ni t \mapsto x(t) \in H$ – a curve with values in a Hilbert space
- \mathcal{E} – λ -convex, *i.e.*

$$\mathcal{E}((1-t)x + ty) \leq (1-t)\mathcal{E}(x) + t\mathcal{E}(y) - \frac{\lambda}{2}t(1-t)|x - y|^2,$$

$$\partial^- \mathcal{E}(x) := \left\{ v \in H : \forall y \in H \right. \\ \left. \mathcal{E}(x) + \langle v, y - x \rangle + \frac{\lambda}{2}|x - y|^2 \leq \mathcal{E}(y) \right\}$$

Equivalently - Evolutionary Variational Inequality

$$\forall y \in H \quad \frac{1}{2} \frac{d}{dt} |x(t) - y|^2 + \mathcal{E}(x(t)) + \frac{\lambda}{2} |x(t) - y|^2 \leq \mathcal{E}(y)$$

Gradient flows in Polish spaces

$$\forall y \in X \quad \frac{1}{2} \frac{d}{dt} \text{dist}(x(t), y)^2 + \mathcal{E}(x(t)) + \frac{\lambda}{2} \text{dist}(x(t), y)^2 \leq \mathcal{E}(y)$$

If $\mathcal{E} : X \rightarrow (-\infty, +\infty]$ is proper, coercive, lsc and λ -(geodesically) convex then the above EVI has only one absolutely continuous solution. The solution is exponentially stable

$$\text{dist}(x_1(t), x_2(t)) \leq e^{-\lambda t} \text{dist}(x_1(0), x_2(0)).$$

Example: $X = \mathcal{P}_2(\mathbb{R}^d)$, $\text{dist}(\mu, \nu) = W_2(\mu, \nu)$, where

$$W_2^2(\mu, \nu) = \inf_{\gamma} \int_{\mathbb{R}^{2d}} |x - x'|^2 d\gamma(x, x'),$$

where γ are all probability measures with x -marginal μ and x' -marginal ν .

Wasserstein space (\mathcal{P}_2, W_2) has a weakly Riemannian structure (tangent space at $x \in \mathcal{P}_2$ is isomorphic to L_x^2). Thus, theory of gradient flows known for Hilbert spaces applies. We again have

$$\dot{x}(t) \in -\partial_{W_2} \mathcal{E}(x(t))$$

Writing $x = \mu$ and interpreting \dot{x} as local velocity \mathbf{u} of the transport of μ . Then absolutely continuous curves satisfying the EVI

$$\forall \sigma \in \mathcal{P}_2 \quad \frac{1}{2} \frac{d}{dt} W_2^2(\mu(t), \sigma) + \mathcal{E}(\mu(t)) + \frac{\lambda}{2} W_2^2(\mu(t), \sigma) \leq \mathcal{E}(\sigma)$$

are equivalent to distributional solutions to

$$\begin{aligned} \partial_t \mu + \operatorname{div}(\mathbf{u} \mu) &= 0, \\ \mathbf{u}(t) &\in \partial_{W_2} \mathcal{E}(\mu(t)). \end{aligned}$$

Gradient flows in \mathcal{P}_2 and continuity equation

If $\mathcal{E} : \mathcal{P}_2 \rightarrow (-\infty, +\infty]$ is proper, coercive, lsc and λ -convex (along generalized geodesics) then there exists a unique gradient flow $\mu \in AC(0, T; \mathcal{P}_2)$ issued at any $\mu_0 \in D(\mathcal{E})$. It satisfies continuity equation

$$\partial_t \mu + \operatorname{div}(\mathbf{u}\mu) = 0, \quad \mathbf{u}(t) \in -\partial_{W_2} \mathcal{E}(\mu(t))$$

in the sense of distributions.

We also get some more information for free e.g.

$$W_2(\mu_t^1, \mu_t^2) \lesssim e^{-\lambda t} W_2(\mu_0^1, \mu_0^2).$$

$$\partial_t \mu + \operatorname{div}(\mathbf{u}\mu) = 0, \quad u(t) \in -\partial_{W_2} \mathcal{E}(\mu(t)).$$

- Absolutely continuous measure $\mu = g\mathcal{L}_1$.
- Entropy functional $\mathcal{E}(g) = \log g$.
- Subdifferential $\partial\mathcal{E}(g) = \frac{\nabla g}{g} = -u$.
- Continuity equation becomes the heat equation

$$\partial_t g - \Delta g = 0$$

- We further can consider such models as: Fokker-Planck, Vlasov, Keller–Segel, and many models of first-order collective dynamics (interaction potentials).

To give credit where credit is due



Left: **David Poyato**

Right: **Javier Morales**

Heterogeneous continuity equation

Consider $(x, \omega) \in \mathbb{R}^{d_1+d_2}$ and the continuity equation for $\mu_t = \mu_t(x, \omega)$

$$\partial_t \mu + \operatorname{div}_x(\mathbf{u}\mu) = 0$$

We treat $\mu \in AC(0, T; \underbrace{(\mathcal{P}_{2,\nu}(\mathbb{R}^{d_1+d_2}), W_{2,\nu})}_{\mathcal{P}_{2,\nu}})$ as a curve

$t \in [0, T] \mapsto \mu_t \in \mathcal{P}_{2,\nu}$.

Equivalently

$$\partial_t \mu + \operatorname{div}_{(x,\omega)}(\mathbf{v}\mu) = 0, \quad \mathbf{v} = (\mathbf{u}, 0).$$

Fibered Wasserstein distance

Any probability measure $\mu = \mu(x, \omega)$ on $\mathbb{R}^{d_1+d_2}$ can be decomposed with respect to its marginal $\nu \in \mathcal{P}(\mathbb{R}^{d_2})$ as

$$\mu[\phi] = \int_{\mathbb{R}^{d_2}} \left(\int_{\mathbb{R}^{d_1}} \phi(x, \omega) d\mu^\omega(x) \right) d\nu(\omega)$$

for all Borel-measurable ϕ . We denote this representation as $\mu(x, \omega) = \mu^\omega(x) \otimes \nu(\omega)$

$$\mathcal{P}_{2,\nu} := \left\{ \mu \in \mathcal{P} : (\pi_\omega)_\# \mu = \nu, \int_{\mathbb{R}^{d_1+d_2}} |x|^2 d\mu(x, \omega) < \infty \right\}$$

$$W_{2,\nu}^2(\mu, \sigma) := \int_{\mathbb{R}^{d_2}} W_2^2(\mu^\omega, \sigma^\omega) d\nu(\omega)$$

Heterogeneous gradient flow in $\mathcal{P}_{2,\nu}$

- First we prove that the fibered Wasserstein space $(\mathcal{P}_{2,\nu}, W_{2,\nu})$ is a Polish space, and we get the EVI gradient flows for free.

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- Second, following OTTO approach, we prove that $(\mathcal{P}_{2,\nu}, W_{2,\nu})$ is a Riemannian manifold.
- We develop a fibered subdifferential calculus with

$$\begin{aligned} \partial_{W_{2,\nu}} \mathcal{E}(\mu) &= \left\{ \mathbf{u} \in L^2_\mu : \mathcal{E}[\sigma] - \mathcal{E}[\mu] \right. \\ &\geq \inf_{\gamma \in \Gamma_{\sigma,\nu}(\mu,\sigma)} \int_{\mathbb{R}^{4d}} \mathbf{u}(x, \omega) \cdot (x' - x) d\gamma(x, x', \omega, \omega') \\ &\quad \left. + o(W_{2,\nu}(\mu, \sigma)) \right\}. \end{aligned}$$

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- Second, following OTTO approach, we prove that $(\mathcal{P}_{2,\nu}, W_{2,\nu})$ is a Riemannian manifold.
- We develop a fibered subdifferential calculus.
- 'Assuming that $\mathcal{E} : \mathcal{P}_{2,\nu} \rightarrow (-\infty, +\infty]$ is proper, coercive, lsc and λ -convex (along fibered generalized geodesics) we prove that EVI is equivalent to the subdifferential notion of gradient flows

$$u_t \in -\partial_{W_{2,\nu}} \mathcal{E}(\mu_t)$$

where μ satisfies the parameterised continuity equation.

Main result

If $\mathcal{E} : \mathcal{P}_{2,\nu} \rightarrow (-\infty, +\infty]$ is proper, coercive, lsc and λ -convex (along fibered generalized geodesics), then there exists a unique gradient flow $\mu \in AC(0, T; \mathcal{P}_{2,\nu})$ issued at any $\mu_0 \in D(\mathcal{E})$. It satisfies continuity equation

$$\partial_t \mu + \operatorname{div}_x(\mathbf{u}\mu) = 0, \quad u_t \in -\partial_{W_{2,\nu}} \mathcal{E}(\mu_t)$$

in the sense of distributions.

We also get some more information for free e.g.

$$W_{2,\nu}(\mu_t^1, \mu_t^2) \lesssim e^{-\lambda t} W_{2,\nu}(\mu_0^1, \mu_0^2).$$

Applications

- Fokker Planck equations with various particles responding differently to the drag force and random motion.
- Vlasov equation for mixtures of different type of plasma.
- Multispecies first order collective dynamics.
- Kuramoto model of 1D synchronization.
- Lohe model of quantum coupled oscillators.
- Multispecies Keller-Segel model.

The fundamental example: Kuramoto-type equation

$$\mathcal{E}[\mu] = - \int_{\mathbb{R}^{2d}} \omega \cdot x d\mu + \int_{\mathbb{R}^{4d}} W(|x - x'|) d\mu d\mu',$$
$$W(|x - x'|) = \frac{1}{2 - \alpha} \frac{1}{1 - \alpha} |x - x'|^{2 - \alpha}, \quad \alpha \in (0, 1).$$

Then the fibered subdifferential is given by

$$\partial_{W_2, \nu} \mathcal{E}[\mu_t] = \nabla_x W * \mu - \omega$$

and the corresponding continuity equation reads

$$\partial_t \mu + \operatorname{div}_x [(\omega - \nabla_x W * \mu) \mu] = 0.$$

Two misconceptions



Ha! Aren't you just stacking a couple of (e.g. continuum) independent continuity equations one atop another? By disintegration:

$$\begin{aligned}\partial_t \mu^\omega(x) + \operatorname{div}_x(u^\omega(x)\mu^\omega(x)) &= 0, \\ u_t^\omega &\in -\partial_{W_2} \mathcal{E}^\omega(\mu_t^\omega)\end{aligned}$$

then just integrate with respect to ν .

Ax explained – **NO**. It is generally not true that u^ω depends only on μ^ω !

$$\partial_t \mu + \operatorname{div}_x[(\omega - \nabla_x W * \mu)\mu] = 0.$$

After disintegration we have $u_t^\omega(x) = \omega - \nabla W * \mu_t(x)$ and the velocity field clearly depends on the whole μ even with fixed ω .

Two misconceptions



Anyway... aren't all of the proofs you need following the same idea? Step 1: disintegrate the energy \mathcal{E} . Step 2: solve the problem on each fiber using classical theory. Step 3: Integrate with respect to ν .

- Works 50 % of the time.
- In particular classical approach usually involves narrow topology, which fails in fibered problems.
- Again, reversing the disintegration theorem usually requires some thought such as using Kuratowski–Ryll–Nardzewski measurable selection theorem.

Stability of optimality (classical)

Let $\mu_n^1 \rightarrow \mu^1$ and $\mu_n^2 \rightarrow \mu^2$ narrowly. Then any sequence of optimal plans $\gamma_n \in \Gamma_{opt}(\mu_n^1, \mu_n^2)$ is narrowly relatively compact and any of its limit plans belongs to $\Gamma_{opt}(\mu^1, \mu^2)$.

Sketch of the proof.

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 - 1 finitely valued costs (Ambrosio, Pratelli 2003)
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- Our cost function is neither finitely valued nor continuous. Back to the drawing board.

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Sketch of the proof.

- Narrow convergence of μ_n^1 and μ_n^2 imply that for ν -a.a. ω we have $\mu_n^{1\omega} \rightarrow \mu^{1\omega}$ and $\mu_n^{2\omega} \rightarrow \mu^{2\omega}$.

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- Thus for ν -a.a. ω , by Prokhorov, γ_n^ω is narrowly compact.
- Then we would like to use classical optimal stability for γ_n^ω . Done?
- No. The problem is we have a convergent subsequence fixed to match each ω (and there is continuum of ω).

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Let $\mu_n^1 \rightarrow \mu^1$ and $\mu_n^2 \rightarrow \mu^2$ narrowly. Then any sequence of optimal plans $\gamma_n \in \Gamma_{opt}(\mu_n^1, \mu_n^2)$ is narrowly relatively compact and any of its limit plans belongs to $\Gamma_{opt}(\mu^1, \mu^2)$.

Sketch of the proof.

Stability of optimality (fibered – attempt 3)

Let $\mu_n^1 \rightarrow \mu^1$ and $\mu_n^2 \rightarrow \mu^2$ ν -random narrowly. Then any sequence of optimal plans $\gamma_n \in \Gamma_{opt,\nu}(\mu_n^1, \mu_n^2)$ is ν -random narrowly relatively compact and any of its limit plans belongs to $\Gamma_{opt,\nu}(\mu^1, \mu^2)$.

Sketch of the proof.

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Sketch of the proof.

- The ν -random narrow convergence is tested with ν -random continuous functions ϕ :
 - 1 For all x the function $\omega \mapsto \phi(x, \omega)$ is Borel-measurable.
 - 2 For all ω the function $x \mapsto \phi(x, \omega)$ is bounded and continuous.
 - 3 We have

$$\int_{\mathbb{R}^{d_2}} |\phi(\cdot, \omega)|_\infty d\nu(\omega) < \infty.$$

Stability of optimality (fibered – attempt 3)

Let $\mu_n^1 \rightarrow \mu^1$ and $\mu_n^2 \rightarrow \mu^2$ ν -random narrowly. Then any sequence of optimal plans $\gamma_n \in \Gamma_{opt,\nu}(\mu_n^1, \mu_n^2)$ is ν -random narrowly relatively compact and any of its limit plans belongs to $\Gamma_{opt,\nu}(\mu^1, \mu^2)$.

Sketch of the proof.

- The ν -random narrow convergence is tested with ν -random continuous functions ϕ :
 - 1 For all x the function $\omega \mapsto \phi(x, \omega)$ is Borel-measurable.
 - 2 For all ω the function $x \mapsto \phi(x, \omega)$ is bounded and continuous.
 - 3 We have

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- Then the idea of attempt 2 works...?
- One still needs to prove a variant of "points in $\text{supp}\gamma$ are limits of points in $\text{supp}\gamma_n$ " that works for the so called ν -random sets. Which we did.

