Diffusion effects in optimal transport and mean-field planning models

Alessio Porretta
University of Rome Tor Vergata

Machine Learning and PDEs
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based on: [P. JFA '19], [Cardaliaguet-Munoz-P. JMPA '24], [Bocchi-P. Calc. Var. PDE '24]

Optimal transport $\leftrightarrow$ Machine learning

- OT used to match two given configurations (probabilities) $\rightsquigarrow$ computational optimal transport, Sinkhorn algorithm...[Cuturi '13], [Benamou,Carlier,Cuturi,Nenna.Peyré '15],[Cuturi-Peyré '16, '20...]...
- Use of Wasserstein distance as loss function in supervised learning [Courty- Flamary], [Frogner, Zhang + al], [Perrot+ al '16]...

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- regularization of Wasserstein distance
- geometric properties of transport

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In this talk, we discuss dynamical OT models, which:

(i) *regularize* Wasserstein geodesics

(ii) penalize congestion effects

(iii) enhance diffusivity (at different levels, Eulerian & Lagrangian)

$\rightsquigarrow$ link with quasilinear elliptic equations

$\rightsquigarrow$ finite Vs infinite speed of support propagation

Dynamical Optimal Transport pbs:

$$\begin{cases} \partial_t m - \text{ div } (vm) = 0 & \text{in } (0,1) \times \Omega, \\ m(0) = m_0 \, , m(1) = m_1 \end{cases}$$

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- Two main cases:

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- Here: suppose that Ω is a compact manifold without boundary

Motivations:

- congestion models in fluid dynamics, traffic flow, etc...

  $\rightsquigarrow$ variants of [Benamou-Brenier '00] formulation

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- Mean-Field Control & Mean-Field Game theory
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Particles are rational agents $\rightsquigarrow$ dyn. states $\{\xi_i(s)\}_s$

Value function of the generic agent: $u(t,x) := \inf_{\xi(t)=x} \int_t^1 \frac{|\xi'(s)|^2}{2} + f(\mu_s)$

where $\{\mu_t\}$ is the supposed distribution law of particles.

Nash equilibria $\rightarrow$ MFG system:
$$\begin{cases} -\partial_t u + \frac{1}{2}|Du|^2 = f(m)\,, \\ \partial_t m - \mathrm{div}(mDu) = 0\,, \end{cases}$$

Optimality system

- MFG system $\simeq$ optimality system of OT functional

$$\begin{cases} -\partial_t u + \frac{1}{2}|Du|^2 = f(m)\,, & (t,x) \in (0,1)\times\Omega \\ \partial_t m - \mathrm{div}(mDu) = 0\,, & (t,x) \in (0,1)\times\Omega \\ m(0) = m_0\,,\; m(1) = m_1\,, & x \in \Omega\,, \end{cases} \tag{1}$$

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If f is increasing, then (u, m) solves (1) $\Leftrightarrow$ (m, Du) is a minimum of

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Proof [Benamou-Brenier]: if $v \to w = mv$, then $\mathcal{E}$ is convex in (m, w)

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Rmk: Classical OT $\rightsquigarrow$ m is the geodesic, $u(0), u(1)$ are Kantorovich potentials

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where $\mathcal{D} := (\partial_t, D_x)$.

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$$\text{in divergence form} \quad \rightsquigarrow \quad \text{div}_{(t,x)}(\Phi(x, \mathcal{D}u)) = 0$$

where $\mathcal{D} := (\partial_t, D_x)$. Expanded in non divergence form as

$$-\mathrm{tr}\,(\mathcal{A}\,\mathcal{D}^2 u) = 0\,, \qquad \mathcal{A} := \mathcal{A}_0 + \mathcal{A}_1$$

$$\mathcal{A}_0 = \begin{pmatrix} 1 & -Du \\ -Du & Du \otimes Du \end{pmatrix}, \; \mathcal{A}_1 = \begin{pmatrix} 0 & 0 \\ 0 & (mf'(m))I_d \end{pmatrix}$$

in a cylindrical $d+1$ domain $(0,1)\times\Omega$.

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- Note: the ellipticity degenerates when $m = 0$, unless $f'(m)m > 0$

PL Lions' approach:

$$(u,m) \text{ solve (classically)} \quad \begin{cases} -\partial_t u + \frac{1}{2}|Du|^2 = f(m) \\ \partial_t m - \mathrm{div}(mDu) = 0\,, \end{cases}$$

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- Entropy case: $f = \varepsilon \log m$ $\rightsquigarrow$ elliptic regularization in x

$$-\mathrm{tr}\left(\mathcal{A}_0\, \mathcal{D}^2 u\right) - \varepsilon \Delta u = 0$$

Rmk: $m = \exp(-\partial_t u + \frac{1}{2}|Du|^2)$ is bdd below $\leftrightarrow$ u is Lipschitz

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Rmk2: u is the minimum of $\int_0^1 \int e^{\frac{1}{2}|Du|^2 - \partial_t u} dxdt$

Lions'strategy $\rightsquigarrow$ Quasilinear elliptic equations $\rightsquigarrow$ gradient bounds
[Lions '10, Munoz '22, P. '22]

If u is a classical solution to

$$\begin{cases} -\mathrm{tr}\left(\mathcal{A}_0(x, \mathcal{D}u)\, \mathcal{D}^2 u\right) - f'(m)m\, \Delta u = 0 \\ + \text{OT boundary conditions (nonlinear Neumann)} \end{cases}$$

then

$$\|\mathcal{D}u\|_\infty \le K(1 + \|u\|_\infty)\,.$$

where K depends on: $\|f(m_0)\|_{W^{1,\infty}}, \|f(m_1)\|_{W^{1,\infty}}, \|V\|_{W^{2,\infty}}, \|m\|_\infty$ and lower bound of $f'(m)m$

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- Main application: provides smooth solutions for positive marginals and $f'(m)m$ bounded below
- Extends to noncompact domains by using the relative entropy w.r.t. $\varrho = e^{-V}dx$, with $D^2 V \geq \gamma_0\, I_d$, $\gamma_0 > 0$
$\rightsquigarrow$ Gaussian-like measures in $\mathbb{R}^d$ (m_0, m_1: $m_i e^V$ bdd below, above)

Uncovering diffusivity (Part II) $\rightsquigarrow$ displacement convexity

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$$\Rightarrow \quad \frac{d^2}{dt^2} \int_\Omega U(m(t)) \geq \int_\Omega U''(m) m\, f'(m) |Dm|^2$$

for any convex U: $U''(r)r - (1 - \frac{1}{d})[U'(r)r - U(r)] \geq 0$

(Ex: $U = r^p, r \log r$ etc...)

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- extends classical results [Mc Cann '97] known for Wasserstein geodesics

$\rightsquigarrow$ used to estimate L^p norms of $m(t)$

$\rightsquigarrow$ $L^1 \to L^\infty$ regularizing effect

$$\frac{d^2}{dt^2}\int_\Omega U(m(t)) \geq \int_\Omega U''(m)\underbrace{m\,f'(m)}_{\text{ellipticity}}|Dm|^2$$

Theorem (Lavenant-Santambrogio '18, P. '22)

Assume $f'(s)s \geq \lambda_0$ for s large. Then m satisfies

$$\|m(t)\|_\infty \leq K(t^{-\alpha} + (1-t)^{-\alpha})$$

for some $\alpha > 0$.

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$$\frac{d^2}{dt^2}\int_\Omega m(t)^p \geq \lambda_0 \int_\Omega m^{p-2}|Dm|^2 \geq c\left(\int_\Omega m^p\right)^{1+\frac{2}{d(p-1)}} - c\int_\Omega m^p$$

by Sobolev-Wirtinger inequality.

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by Sobolev-Wirtinger inequality. Then

$$\varphi(t) := \int_\Omega m(t)^p \quad \text{satisfies} \quad -\varphi'' + c\,\varphi^{1+\frac{2}{d(p-1)}} \leq C\,\varphi$$

$$\rightsquigarrow \varphi(t) \leq C(t \wedge (1-t))^{-d(p-1)}$$

Model problem: kinetic energy + entropy

$$\begin{cases} \partial_t m - \operatorname{div}(vm) = 0 & \text{in } Q := (0,1)\times\Omega, \\ m(0) = m_0\,, m(1) = m_1 \end{cases}$$

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Theorem (Bocchi - P. '24)

There exists a unique minimizer, which is the unique weak sol. $(m, \nabla u)$ of Opt. System, and we have:

(i) $m > 0$ *a.e. in* $(0,1)\times\Omega$.

(ii) $u, m \in L^\infty_{loc}((0,1)\times\Omega)$ *and* $u(0) \in L^1(dm_0)$, $u(1) \in L^1(dm_1)$.

(iii) *if* $m_0, m_1 \in W^{1,\infty}(\Omega)$ *with* $m_0, m_1 > 0$, *then* $V \in C^{k,\alpha}(M) \Rightarrow u \in C^{k+1,\alpha}, m \in C^{k,\alpha}$.

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- Needs to use weak solutions and relaxed formulations from MFG theory ([Cardaliaguet-Graber '15], [Orrieri-P.-Savare '19]..)

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  $\rightsquigarrow$ m^ε converges to the Wasserstein geodesic, u^ε converges uniformly to the Kantorovich potential

In search of diffusivity (Part III) $\rightsquigarrow$ slow diffusion & free boundary
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Rmk: the behavior is reminiscent of porous medium diffusion

(not surprising: porous medium equation is the associated gradient flow!)

Self-similar solutions

$$\begin{cases} -\partial_t u + \frac{1}{2}|Du|^2 = m^\theta \\ \partial_t m - \text{ div } (m\, Du) = 0 \end{cases}$$

$\rightsquigarrow$ $\exists$ self-similar solutions with compact support $m = t^{-\alpha}\phi(|x|/t^{-\alpha})$:

$$(d = 1) \qquad m = t^{-\alpha}\left(R - \frac{\alpha(1-\alpha)}{2}\left(\frac{|x|}{t^\alpha}\right)^2\right)_+^{1/\theta}, \qquad \alpha = \frac{2}{2+\theta}$$

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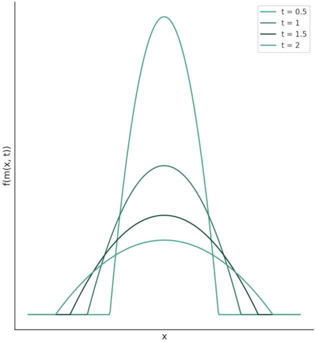
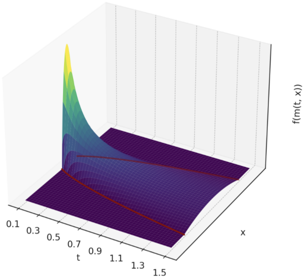
- m is very similar to the Barenblatt solution for porous media !!
- m connects a Dirac mass with a compactly supported bump function
- The support propagates with finite speed, m is only Hölder continuous
- the free boundary spreads outward with speed t^α





- Thanks to the self-similar solution, we can characterize the transport of Dirac masses: $(d = 1)$ There exists a unique solution of

$$\begin{cases} -u_t + \frac{1}{2}|u_x|^2 = m^\theta & \text{in } (0,T)\times\mathbb{R} \\ m_t - (mu_x)_x = 0 & \text{in } (0,T)\times\mathbb{R} \\ m(0) = \delta_0, \ m(T) = m_1 \end{cases}$$

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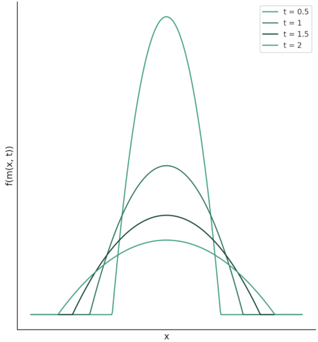

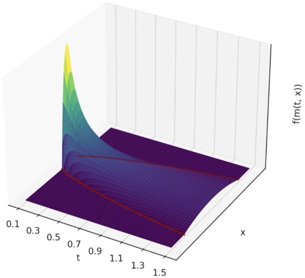

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- The self-similar solution gives the prototype behavior of the free-boundary evolution

Analysis of the free boundary (one-dimensional case)

- m_0, m_1 are bump-like functions

$$\{m_0 > 0\} = (a_0, b_0)\,, \qquad \{m_1 > 0\} = (a_1, b_1)$$

- m_0^θ is Lipschitz and semi-convex, and $m_0(x) \cong c_0\, \mathrm{dist}(x, \{a_0, b_0\})^\beta$ for some $\beta, c_0 > 0$ (+ similar conditions on m_1)

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Preliminary: under the above conditions, the system

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admits a (unique) solution (u, m) with m continuous and u Lipschitz.

$\rightsquigarrow$ Free boundary: $\partial\{m(t) > 0\}$

Flow of optimal trajectories (characteristics)

The function $\gamma : [a_0, b_0] \times [0, T] \to \mathbb{R}$ defined by

$$\begin{cases} \dot{\gamma}(\cdot) = -u_x(\gamma(\cdot), \cdot) \\ \gamma(0) = x \end{cases}$$

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- $\gamma(x, t)$ is well-defined, globally Lipschitz in $(a_0, b_0) \times [0, T]$, $\gamma_x > 0$

$$\{m > 0\} = \{(x, t) \in \mathbb{R} \times [0, T] : \gamma_L(t) < x < \gamma_R(t)\}$$

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- γ is a classical solution in $(a_0, b_0) \times (0, T)$ of the elliptic equation

$$\gamma_{tt} + \frac{\theta m_0^\theta}{(\gamma_x)^{2+\theta}} \gamma_{xx} = \frac{(m_0^\theta)_x}{(\gamma_x)^{1+\theta}} \qquad x \in (a_0, b_0), t \in (0, T)$$

To get more regularity of the free boundary, we assume further:

$$(m_0^\theta)_{xx} \leq 0 \quad \text{for } x \text{ near } \partial[a, b]$$

Important: this condition implies $(m_0^\theta)_x(a_0) > 0$ and $(m_0^\theta)_x(b_0) < 0$

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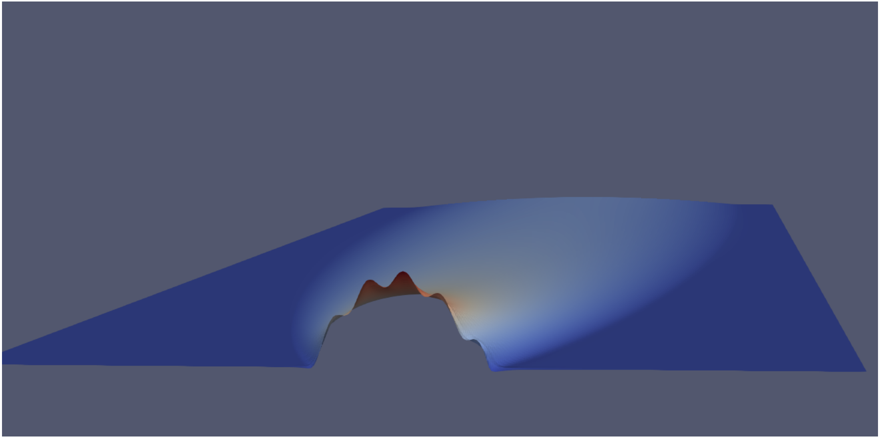
• Holder regularity is proved by intrinsic scaling methods.
Key-tool: look at the equation of m^θ along trajectories

$$v(t,x) := m^\theta(\gamma(x,t),t) \quad \text{satisfies} \quad -\left(\frac{v_x}{\gamma_x}\right)_x - \left(\frac{\gamma_x}{\theta v} v_t\right)_t = 0$$



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  - (i) embed Wasserstein geodesics into a larger family of more regular optimal curves
  - (ii) Have different geometric properties of transport, finite Vs infinite speed of propagation

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  - (ii) Have different geometric properties of transport, finite Vs infinite speed of propagation
  - (iii) The optimality system is an elliptic equation for u (but second order in time!) $\rightsquigarrow$ finite difference schemes, Newton's methods, etc...

- This is different from the entropic Optimal Transport:

  penalizing the Fisher information of m $\rightsquigarrow$ leads to fourth order equation in u

- Other congestion models in crowd dynamics of multiplicative type

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  Optimality system gives different quasilinear elliptic equations

  $$\begin{cases} -\partial_t u + \frac{1}{2}\frac{|Du|^2}{m^\alpha} = 0\,, \\ \partial_t m - \mathrm{div}(m\frac{Du}{m^\alpha}) = 0\,, \end{cases} \qquad m = \left(\frac{1}{2}\frac{|Du|^2}{\partial_t u}\right)^{\frac{1}{\alpha}} \rightsquigarrow \mathrm{tr}\left(A(\mathcal{D}u)\mathcal{D}^2 u\right) = 0$$

  Formally: the operator is elliptic iff $\alpha < 2$

  (cf. [Lions '10], [Achdou-P. '18]...)

...[more to come ?...]

- Other congestion models in crowd dynamics of multiplicative type

  $\rightsquigarrow$ cost of motion is proportional to the density of crowd

  Model cost: $L(m,q) = m^\alpha \frac{|q|^2}{2}$

  $\rightarrow$ lead to different distances between measures

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Thanks for the attention !

Key-point: the elliptic equation satisfied by γ

$$\gamma_{tt} + \frac{\theta m_0^\theta}{(\gamma_x)^{2+\theta}}\gamma_{xx} = \frac{(m_0^\theta)_x}{(\gamma_x)^{1+\theta}} \qquad x \in (a_0, b_0), t \in (0, T)$$

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Where does it come from ?

1. $\gamma(x, \cdot)$ is the minimizer of

$$\inf_{\alpha \in H^1,\ \alpha(t)=x} \int_t^T \frac{1}{2}|\dot{\alpha}|^2 + f(m(\alpha, s))\ ds + u(\alpha(T), T).$$

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