Optimal transport problems with interaction effects

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Mandatory slide on the history of OT

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An Extended Lagrangian Theory of Semi-Geostrophic Frontogenesis

M. J. P. CULLEN AND R. J. PURSER

Meteorological Office, Bracknell, Berkshire RG12 2SZ U.K.

(Manuscript received 9 August 1983, in final form 8 February 1984)

COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING 75 (1989) 325–332
NORTH-HOLLAND

A COMBINATORIAL ALGORITHM FOR THE EULER EQUATIONS OF INCOMPRESSIBLE FLOWS

Yann BRENIER

INRIA, Rocquencourt, 78153 Le Chesnay Cedex, France

Polar Factorization and Monotone Rearrangement of Vector-Valued Functions

YANN BRENIER

Université de Paris VI

Overview

Jean-David Benamou

Yann Brenier

Overview

Theorem (Benamou-Brenier)

$$d_2(\mu_0, \mu_1)^2 = \inf_{\rho, v} \int_0^1 \int_{\mathbb{R}^d} \tfrac{1}{2}|v(x,t|^2 \, d\rho_t(x) dt$$

The infimum being over all pairs (ρ, v) *such that*

$$\partial_t \rho + \mathrm{div}(\rho v) = 0, \ \rho_{|t=0} = \mu_0, \ \rho_{|t=1} = \mu_1$$

Overview

Question:
Modify Benamou-Brenier by adding an interaction energy term

$$\int_0^1 \int_{\mathbb{R}^d} \frac{1}{2}|v(x,t|^2 \, d\rho_t(x)dt + \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(x,y)d\rho_t(x)d\rho_t(y)dt$$

Then: is there a corresponding Monge-Kantorovich problem?

Overview
Main points

1. Introducing a "lifting" of the OT problem to the path space
2. Lifted problem naturally allows for interaction effects
3. Existence of minimizers, duality, and relation to standard OT
4. Problem formulation à la Benamou-Brenier

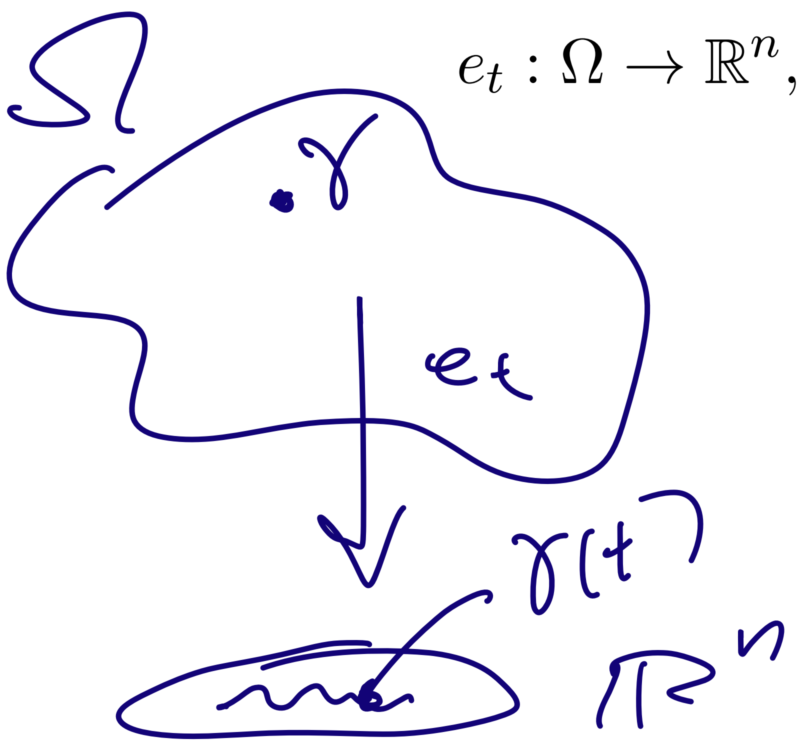
Optimal transport + paths

Setup (1/2)
We will be working with the space of all paths

$$\Omega := \{\gamma : I \to \mathbb{R}^n \mid \gamma \text{ is absolutely continuous } \}$$

For each $t \in [0,1]$ we have the evaluation map e_t,

$$e_t : \Omega \to \mathbb{R}^n,\ e_t(\gamma) := \gamma(t),\ t \in [0,1].$$



Optimal transport + paths

Setup (2/2)
We will also fix an energy / cost functional

$$c : \Omega \to \mathbb{R}$$

$$c(\gamma) = \frac{1}{2}\int_0^1 |\dot{\gamma}(t)|^2 dt \,,$$

$$c(\gamma) = \int_0^1 \frac{1}{2}|\dot{\gamma}(t)|^2 - V(\gamma(t)) dt$$

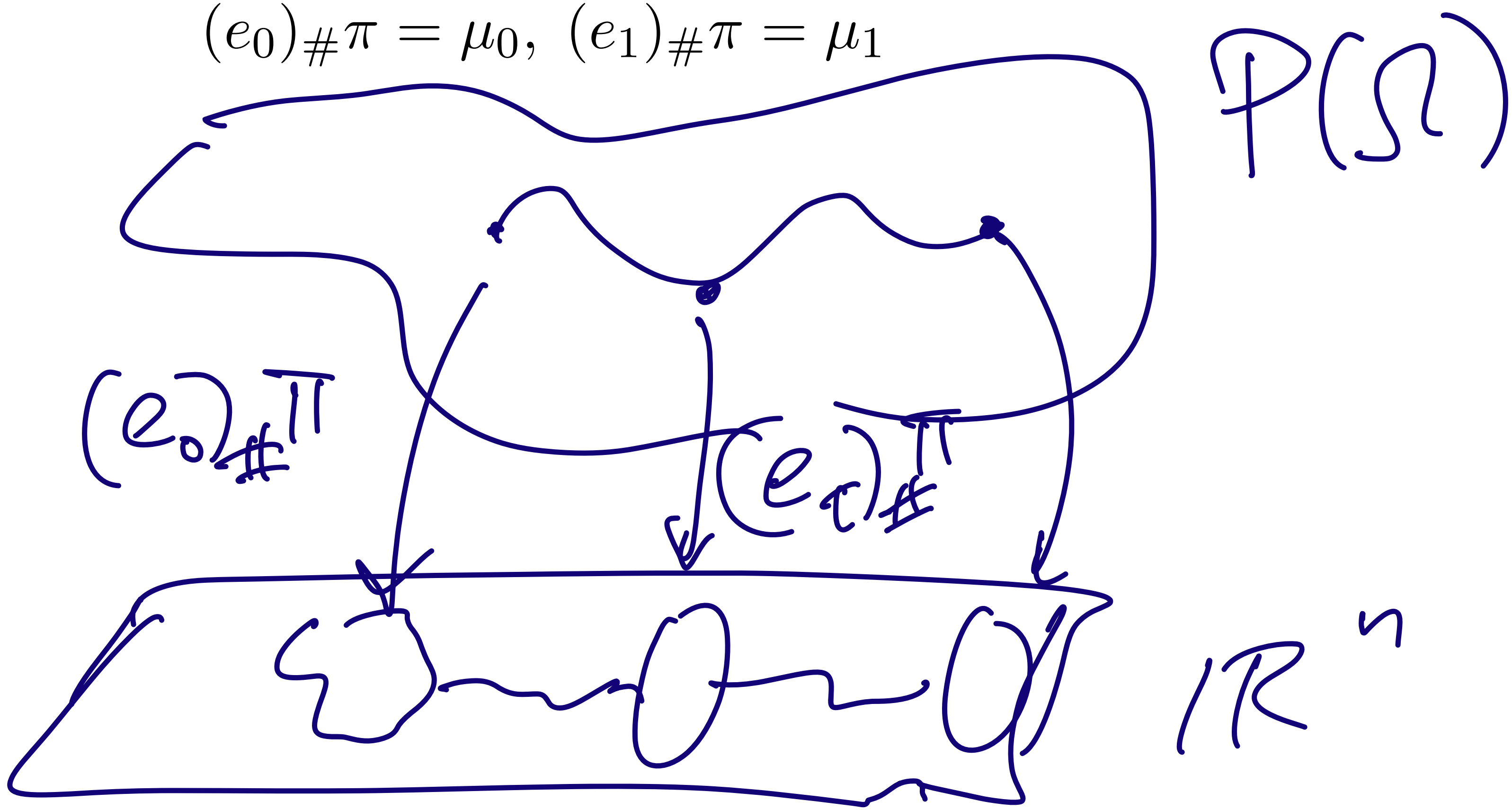
Optimal transport + paths

Dynamic transport plans

Consider: μ_0, μ_1 = prob. measures in $\mathbb{R}^n$ + finite second moment

A dynamic transport plan is a measure $\pi \in \mathcal{P}(\Omega)$ such that

$$(e_0)_{\#}\pi = \mu_0, \ (e_1)_{\#}\pi = \mu_1$$

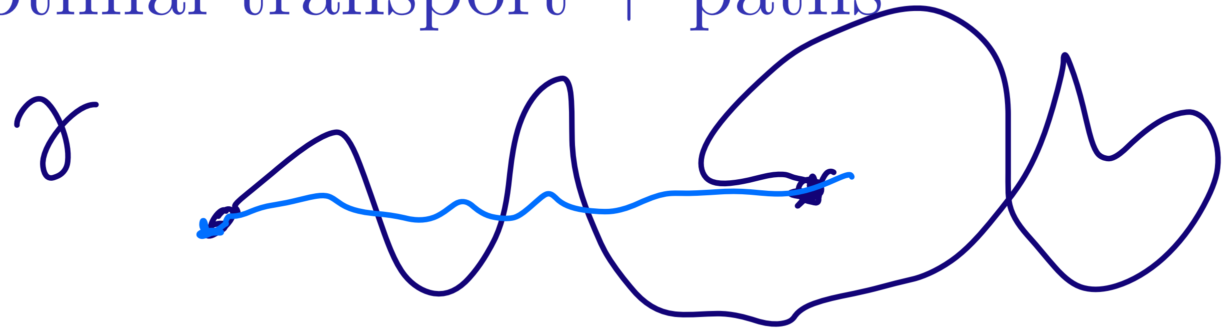


Optimal transport + paths

The OT+paths problem

$$
\begin{aligned}
\text{Minimize } \pi &\mapsto \int_\Omega c(\gamma)\, d\pi(\gamma) \\
\text{subject to: } &\pi \geq 0 \\
&(e_0)_\# \pi = \mu_0 \\
&(e_1)_\# \pi = \mu_1
\end{aligned}
$$

Optimal transport + paths



If γ appears in an optimal plan γ, then one would expect that

$$c(\gamma) = c_e(\gamma(0), \gamma(1))$$

Here c_e denotes what we shall call "the end-point cost"

$$c_e(x, y) := \inf\{c(\gamma) \mid \gamma(0) = x,\ \gamma(1) = y\}$$

Such paths will be said to be c-minimal.

Optimal transport + paths

Theorem

If π solves the OT+paths problem, then

(1) π is supported in the set of c-minimal paths
(2) The joint probability measure

$$(e_0, e_1)_{\#}\pi \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$$

solves the Kantorovich Problem for μ_0, μ_1 and cost c_e.

(A proof of this theorem can be found in Cabrera's thesis)

Optimal transport + paths + interactions

Consider an interaction kernel (even and positive definite)

$$K : \mathbb{R}^d \to \mathbb{R}$$

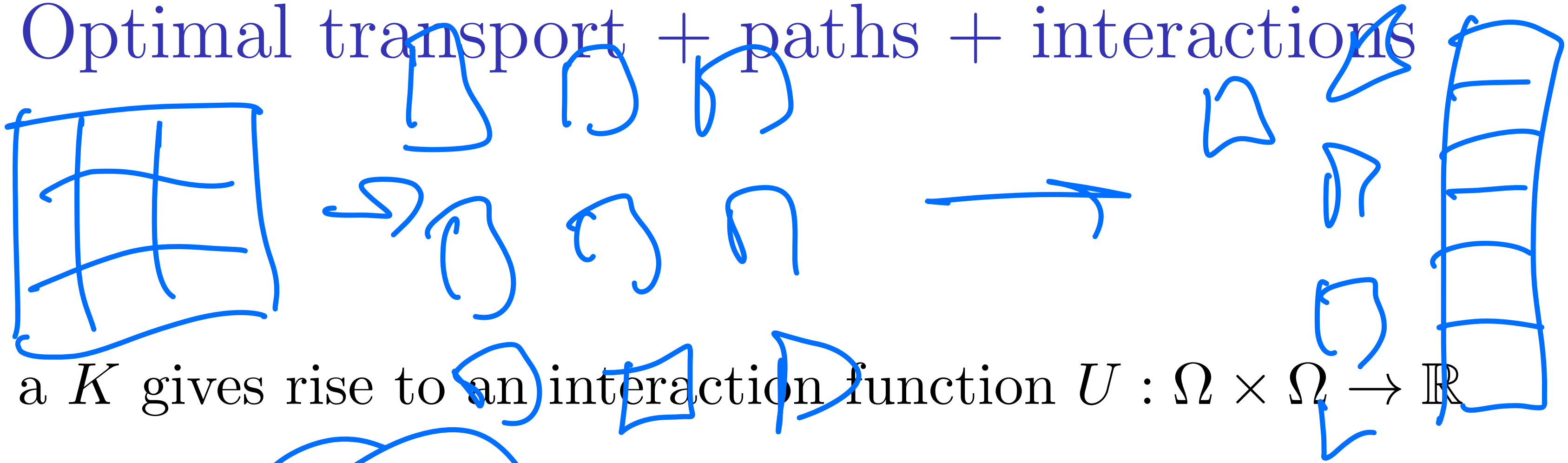
This includes the Gaussian

$$K_G(z) = \lambda e^{-\beta|z|^2}, \;\; \lambda, \beta > 0$$

and the Coulomb potential

$$K_C(z) = \lambda |z|^{2-d}, \;\; \lambda > 0, \; d \geq 3$$

Optimal transport + paths + interactions



Such a K gives rise to an interaction function $U : \Omega \times \Omega \to \mathbb{R}$

$$U(\gamma_1, \gamma_2) = \int_0^1 K(\gamma_1(t) - \gamma_2(t))\, dt$$

As K is positive definite, this gives rise to a convex functional

$$\pi \mapsto \int_\Omega \int_\Omega U(\gamma_1, \gamma_2)\, d\pi(\gamma_1) d\pi(\gamma_2)$$

Optimal transport + paths + interactions

The OT+interaction problem

$$\text{Minimize } \pi \mapsto \int_\Omega c(\gamma)\, d\pi(\gamma)$$

$$\begin{aligned} \text{subject to: } & \pi \geq 0 \\ & (e_0)_\# \pi = \mu_0 \\ & (e_1)_\# \pi = \mu_1 \end{aligned}$$

Optimal transport + paths + interactions

$$\left(K(x_i - x_j) \right)_{i,j=1}^{N}$$

The OT+interaction problem

$$\text{Minimize } \pi \mapsto \int_\Omega c(\gamma)\, d\pi(\gamma) + \int_\Omega \int_\Omega U(\gamma_1, \gamma_2)\, d\pi(\gamma_1) d\pi(\gamma_2)$$

$$\text{subject to: } \pi \geq 0$$

$$(e_0)_\# \pi = \mu_0$$

$$(e_1)_\# \pi = \mu_1$$

Optimal transport + paths + interactions

(In what follows, $c(\gamma) = \int_0^1 \frac{1}{2}|\dot{\gamma}|^2 - V(\gamma(t))\,dt$ for a fixed V, the measures μ_0, μ_1 have compact support)

Theorem (Cabrera 2021)

The OT+path problem has at least one minimizer π_0.

Optimal transport + paths + interactions

Characterization of minimizers

Lemma (Cabrera 2021)

The measure π_0 *is a minimizer for the OT+interaction problem*

$$\Leftrightarrow$$

$$\exists\ \phi, \psi : \mathbb{R}^d \to \mathbb{R} \text{ such that:}$$

$$\phi(\gamma(0)) + \psi(\gamma(1)) \leq c(\gamma) + \int U(\gamma, \sigma)\, d\pi_0(\sigma) \quad \forall\, \gamma \in \Omega$$

$$\phi(\gamma(0)) + \psi(\gamma(1)) = c(\gamma) + \int U(\gamma, \sigma)\, d\pi_0(\sigma) \quad \text{for } \pi_0\text{-a.e.}\gamma$$

Optimal transport + paths + interactions

Characterization of minimizers

[Sketch of the proof]

$$
\begin{aligned}
\Lambda(\pi, \phi, \psi, \lambda) := \int_\Omega c(\gamma)\, d\pi(\gamma) &+ \int_\Omega \int_\Omega U(\gamma, \sigma) d\pi(\gamma) d\pi(\sigma) \\
&+ \int_{\mathbb{R}^d} \phi(x)\, d\mu_0(x) - \int_\Omega \phi(\gamma(0))\, d\pi(\gamma) \\
&+ \int_{\mathbb{R}^d} \psi(y)\, d\mu_0(y) - \int_\Omega \psi(\gamma(1))\, d\pi(\gamma) \\
&+ \int_\Omega \lambda(\gamma)\, d\pi(\gamma)
\end{aligned}
$$

Optimal transport + paths + interactions

Characterization of minimizers

[Sketch of the proof]

$$\Lambda(\pi, \phi, \psi, \lambda) = \int_\Omega c(\gamma)\, d\pi(\gamma) + \int_\Omega \int_\Omega U(\gamma, \sigma) d\pi(\gamma) d\pi(\sigma)$$
$$+ \int_\Omega \lambda(\gamma) - \phi(\gamma(0)) - \psi(\gamma(1))\, d\pi(\gamma)$$
$$+ \int_{\mathbb{R}^d} \phi(x)\, d\mu_0(x) + \int_{\mathbb{R}^d} \psi(y)\, d\mu_0(y)$$

Optimal transport + paths + interactions

Characterization of minimizers

[Sketch of the proof]

$$\frac{d}{ds}_{|s=0}\Lambda(\pi(s),\phi,\psi,\lambda) = \int_\Omega c(\gamma)\,d\dot{\pi}(\gamma) + 2\int_\Omega\int_\Omega U(\gamma,\sigma)d\pi_0(\sigma)d\dot{\pi}(\gamma) + \int_\Omega \lambda(\gamma) - \phi(\gamma(0)) - \psi(\gamma(1))\,d\dot{\pi}(\gamma)$$

Minimality means there must be ϕ,ψ,λ ($\lambda \geq 0$) such that

$$c(\gamma) + 2\int_\Omega U(\gamma,\sigma)d\pi_0(\sigma) + \lambda(\gamma) - \phi(\gamma(0)) - \psi(\gamma(1)) = 0$$

moreover, $\lambda \equiv 0$ in the support of π.

Optimal transport + paths + interactions

Characterization of minimizers

If π_0 is a minimizer, define the effective cost

$$c_{\pi_0}(\gamma) = c(\gamma) + \int_\Omega U(\gamma, \sigma) d\pi(\sigma)$$

and the corresponding endpoint cost

$$c_{e,\pi_0}(x, y) := \inf\{c_{\pi_0}(\gamma) \mid \gamma(0) = x,\ \gamma(1) = y\}$$

Optimal transport + paths + interactions

Characterization of minimizers

Theorem (Cabrera, 2021)

If π_0 solves the OT+interaction roblem, then

(1) π_0 is supported in the set of c_{π_0}-minimal paths

(2) The joint probability measure

$$(e_0, e_1)_{\#}\pi_0$$

solves the Kantorovich problem for μ_0, μ_1 and cost $c_{e,\pi_0}(x, y)$.

This theorem opens the door to using the rich OT theory to understand minimizers of the problem with interaction.

Benamou-Brenier with interaction effects

Theorem (with Cabrera and Homerosky, 2023)

The min value for the OT+interaction problem = the infimum of

$$\int_0^1 \int_{\mathbb{R}^d} \frac{1}{2}|v(x,t)|^2 \, d\rho_t(x)dt + \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(x-y) \, d\rho_t(x)d\rho_t(y)dt$$

here the infimum is taken over all pairs (ρ, v) *such that*

$$\partial_t \rho + \mathrm{div}(\rho v) = 0, \ \rho_0 = \mu_0, \ \rho_1 = \mu_1$$

Benamou-Brenier with interaction effects

Basics of the proof

As done since Benamou-Brenier, one can do a change variables

$$(\rho, v) \to (\rho, E) \text{ where } E = v\rho$$

and obtain a convex functional in (ρ, E)

$$\int_0^1 \int_{\mathbb{R}^d} \frac{|E|^2}{\rho_t(x)} dxdt + \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(x-y)\rho_t(x)\rho_t(y)dxdydy$$

This convexity of the functional allows us to work with smooth approximations.

Benamou-Brenier with interaction effects

Basics of the proof

In terms of the variables (ρ, E) we can regularize via convolutions

$$\rho^{(\varepsilon)} := \rho * \eta_\varepsilon,\ E^{(\varepsilon)} := E * \eta_\varepsilon,\ v^{(\varepsilon)} := \frac{E_\varepsilon}{\rho^\varepsilon}$$

and obtain smooth approximations to $(\rho, v)/(\rho, E)$ that still solve the transport equation

$$\partial_t \rho^{(\varepsilon)} + \mathrm{div}(\rho^{(\varepsilon)} v^{(\varepsilon)}) = 0$$

Benamou-Brenier with interaction effects

Basics of the proof

Take a smooth vector field $v(x,t)$.
The flow of v, $\Gamma : \mathbb{R}^n \times [0,1] \to \mathbb{R}^n$ is characterized by

$$\partial_t \Gamma_t(x) = v(\Gamma_t(x), t), \;\; \Gamma_0(x) = x \; \forall \, x.$$

Equivalently, the flow defines a map $\Gamma : \mathbb{R}^n \to \Omega$.

$x \to \gamma(t) = \Gamma_t(x)$

Benamou-Brenier with interaction effects

Basics of the proof

With Γ and μ_0, we can create measures

$$\pi := \Gamma_{\#}\mu_0, \;\; \rho_t := (e_t)_{\#}\pi$$

Then, observe

$$\begin{aligned}
\int_\Omega c(\gamma)\, d\pi(\gamma) &= \int_\Omega \int_0^1 \frac{1}{2}|\dot{\gamma}(t)|^2 \, dt d\pi(\gamma) \\
&= \frac{1}{2}\int_{\mathbb{R}^n}\int_0^1 |\partial_t \Gamma_t(x)|^2 dt d\rho_0(x) \\
&= \frac{1}{2}\int_0^1 \int_{\mathbb{R}^n} |v(\Gamma_t(x), t)|^2 d\rho_0(x) dt \\
&= \frac{1}{2}\int_0^1 \int_{\mathbb{R}^n} |v(y,t)|^2 d\rho_t(y) dt
\end{aligned}$$

$$\mu_0 = (e_0)_{\#}\pi$$

$$\mu_1 = (e_1)_{\#}\pi$$

$$\delta_0$$

$$\pi = (\Gamma)_{\#}\mu_0$$

$$y = \Gamma_t(x)$$

Benamou-Brenier with interaction effects

Basics of the proof

On the other hand,

$$\int_\Omega \int_\Omega U(\gamma_1, \gamma_2)\, d\pi(\gamma_1) d\pi(\gamma_2)$$

$$= \int_\Omega \int_\Omega \int_0^1 K(\gamma_1(t) - \gamma_2(t))\, dt d\pi(\gamma_1) d\pi(\gamma_2)$$

$$= \int_0^1 \int_\Omega \int_\Omega K(\gamma_1(t) - \gamma_2(t))\, d\pi(\gamma_1) d\pi(\gamma_2) dt$$

$$= \int_0^1 \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} K(x - y)\, d\rho_t(x) d\rho_t(y) dt$$

Benamou-Brenier with interaction effects

Basics of the proof

Therefore, for $\pi = \Gamma_{\#}\mu_0$ and $\rho_t = (e_t)_{\#}\pi$,

$$\int_\Omega c(\gamma)\, d\pi + \int_\Omega \int_\Omega U(\gamma,\sigma) d\pi(\gamma) d\pi(\sigma)$$

$$= \frac{1}{2}\int_0^2 \int |v(x,t)|^2 \rho_t(dx) dt + \int_0^1 \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(x-y)\, d\rho_t(x) d\rho_t(y) dt$$

Benamou-Brenier with interaction effects

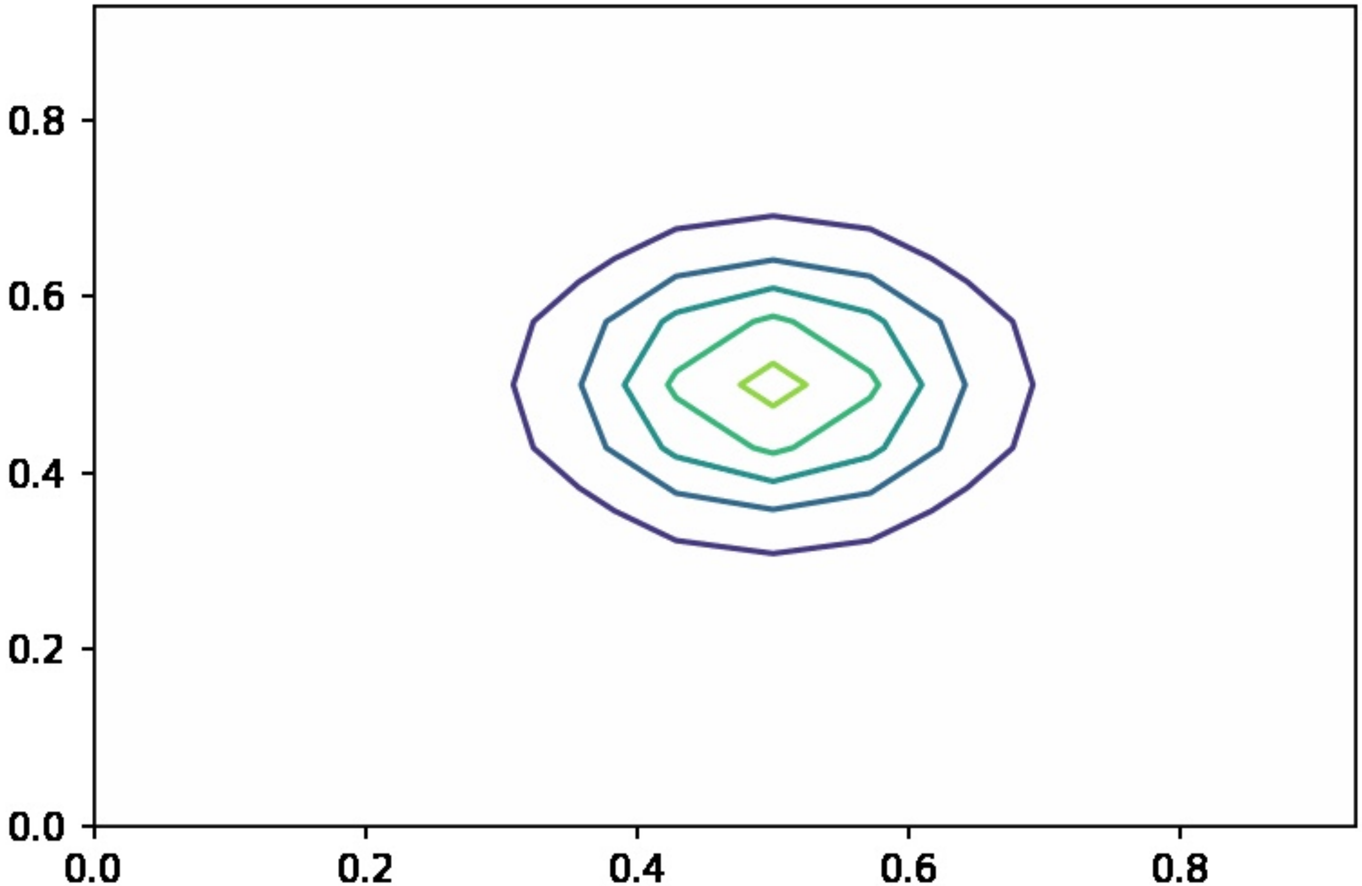
Hamilton-Jacobi equation

As in the interaction-free case, the minimizer ρ, v yields a solution to a HJ equation, in fact:

There is a $\phi(x,t)$ such that $v = -\nabla\phi$, and (ρ,ϕ) solves

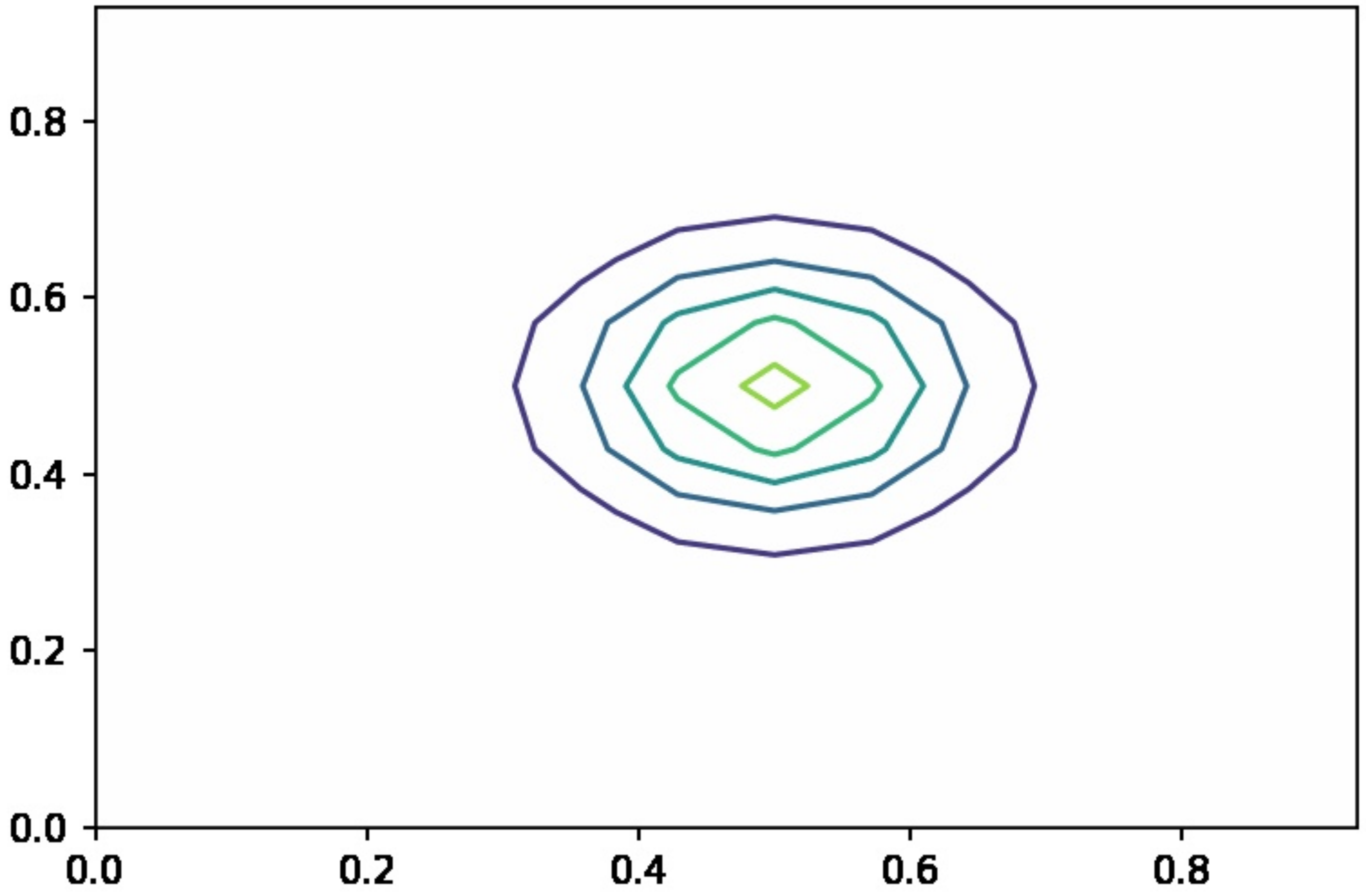
$$\partial_t \rho = \mathrm{div}(\rho\nabla\phi)$$
$$\partial_t \phi = \tfrac{1}{2}|\nabla\phi|^2 - K * \rho$$

A numerical experiment



~~A numerical experiment~~

An artistic rendering !



A two-phase problem

We have begun studying the problem of minimizing

$$
\begin{aligned}
&E(\rho^{(1)}, \rho^{(2)}, v^{(1)}, v^{(2)}) \\
&:= \frac{1}{2}\int_0^1 \int_{\mathbb{R}^d} |v^{(1)}(x,t)| d\rho_t^{(1)}(x) dt \\
&\quad + \frac{1}{2}\int_0^1 \int_{\mathbb{R}^d} |v^{(2)}(x,t)| d\rho_t^{(2)}(x) dt \\
&\quad + \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(x-y)\ d\rho_t^{(1)}(x) d\rho_t^{(2)}(y) dt
\end{aligned}
$$

constrained to initial/final time constraints and

$$\partial_t \rho^{(i)} + \mathrm{div}(\rho^{(i)} v^{(i)}) = 0 \text{ for } i = 0, 1.$$

Problems

1. Build a dedicated solver (we used CVXPY)
2. How smooth is the Brenier map?
3. Kinetic version $\Rightarrow$ build solutions to Vlasov-Poisson?
4. Are there interesting extensions to other functions

   $$\mathcal{U} : \mathcal{P}(\Omega) \to \mathbb{R}$$

   which are "lifted" from functions $\mathcal{P}(\mathbb{R}^n) \to \mathbb{R}$?
5. (serious question!) What else is this hammer good for?

$$\ddot{x} = -\nabla \int_{\mathbb{R}^n} K(x - z)\, d\rho_t(z)$$

Thank you!

Questions / Comments / Suggestions:

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