Optimal transport problems with interaction effects

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An Extended Lagrangian Theory of Semi-Geostrophic Frontogenesis

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

A COMBINATORIAL ALGORITHM FOR THE EULER EQUATIONS OF INCOMPRESSIBLE FLOWS

Yann Brenier
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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)

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

The infimum being over all pairs \((\rho, v)\) such that

\[ \partial_t \rho + \text{div}(\rho v) = 0, \quad \rho|_{t=0} = \mu_0, \quad \rho|_{t=1} = \mu_1 \]
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 \( e_t \),

\[ e_t : \Omega \to \mathbb{R}^n, \quad e_t(\gamma) := \gamma(t), \quad t \in [0, 1]. \]
Setup (2/2)
We will also fix an energy / cost functional

\[ c : \Omega \to \mathbb{R} \]

\[ c(\gamma) = \frac{1}{2} \int_0^1 |\gamma'(t)|^2 \, dt \]

\[ c(\gamma) = \int_0^1 \frac{1}{2} |\check{\gamma}'(t)|^2 - \sqrt{\check{\gamma}(t)} \, dt \]
Consider: \( \mu_0, \mu_1 = \text{prob. measures in } \mathbb{R}^n + \text{finite second moment} \)

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

\[
(e_0)\#\pi = \mu_0, \quad (e_1)\#\pi = \mu_1
\]
Optimal transport + paths

The OT+paths problem

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

subject to: $\pi \geq 0$

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

$(e_1) \# \pi = \mu_1$
If $\gamma$ appears in an optimal plan $\gamma$, 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.
Theorem

If $\pi$ solves the OT+paths problem, then

1. $\pi$ 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 $\mu_0, \mu_1$ 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)

\[ K : \mathbb{R}^d \rightarrow \mathbb{R} \]

This includes the Gaussian

\[ K_G(z) = \lambda e^{-\beta|z|^2}, \quad \lambda, \beta > 0 \]

and the Coulomb potential

\[ K_C(z) = \lambda |z|^{2-d}, \quad \lambda > 0, \quad d \geq 3 \]
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

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

subject to: $\pi \geq 0$

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

$(e_1) \# \pi = \mu_1$
Optimal transport + paths + interactions

The OT+interaction problem

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

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 $\mu_0, \mu_1$ have compact support)

**Theorem (Cabrera 2021)**

The $OT+$ path problem has at least one minimizer $\pi_0$. 
The measure $\pi_0$ is a minimizer for the $OT+interaction$ problem

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

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

\[ \phi(\gamma(0)) + \psi(\gamma(1)) = c(\gamma) + \int U(\gamma, \sigma) \ d\pi_0(\sigma) \quad \text{for } \pi_0\text{-a.e.} \gamma \]
Optimal transport + paths + interactions

Characterization of minimizers

[Sketch of the proof]

\[ \Lambda(\pi, \phi, \psi, \lambda) := \int_\Omega c(\gamma) \, d\pi(\gamma) + \int_\Omega \int_\Omega U(\gamma, \sigma) \, d\pi(\gamma) \, d\pi(\sigma) \]

\[ + \int_{\mathbb{R}^d} \phi(x) \, d\mu_0(x) - \int_\Omega \phi(\gamma(0)) \, d\pi(\gamma) \]

\[ + \int_{\mathbb{R}^d} \psi(y) \, d\mu_0(y) - \int_\Omega \psi(\gamma(1)) \, d\pi(\gamma) \]

\[ + \int_\Omega \lambda(\gamma) \, d\pi(\gamma) \]
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 \( \phi, \psi, \lambda \ (\lambda \geq 0) \) 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 \( \pi \).
If $\pi_0$ 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

$$c_{e,\pi_0}(x, y) := \inf\{c_{\pi_0}(\gamma) \mid \gamma(0) = x, \gamma(1) = y\}$$
Theorem (Cabrera, 2021)

If \( \pi_0 \) solves the OT+interaction problem, then

1. \( \pi_0 \) is supported in the set of \( c_{\pi_0} \)-minimal paths
2. The joint probability measure

\[(e_0, e_1) \# \pi_0\]

solves the Kantorovich problem for \( \mu_0, \mu_1 \) 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 $(\rho, v)$ such that

$$\partial_t \rho + \text{div}(\rho v) = 0, \ \rho_0 = \mu_0, \ \rho_1 = \mu_1$$
Benamou-Brenier with interaction effects

Basics of the proof

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

$$(\rho, v) \rightarrow (\rho, E)$$

where $E = v\rho$

and obtain a convex functional in $(\rho, E)$

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

This convexity of the functional allows us to work with smooth approximations.
In terms of the variables \((\rho, E)\) we can regularize via convolutions

\[ \rho^{(\varepsilon)} := \rho \ast \eta_\varepsilon, \quad E^{(\varepsilon)} := E \ast \eta_\varepsilon, \quad v^{(\varepsilon)} := \frac{E_\varepsilon}{\rho^\varepsilon} \]

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

\[ \partial_t \rho^{(\varepsilon)} + \text{div} (\rho^{(\varepsilon)} v^{(\varepsilon)}) = 0 \]
Benamou-Brenier with interaction effects
Basics of the proof

Take a smooth vector field \( v(x, t) \).
The flow of \( v \), \( \Gamma : \mathbb{R}^n \times [0, 1] \rightarrow \mathbb{R}^n \) is characterized by
\[
\partial_t \Gamma_t(x) = v(\Gamma_t(x), t), \quad \Gamma_0(x) = x \forall x.
\]
Equivalently, the flow defines a map \( \Gamma : \mathbb{R}^n \rightarrow \Omega \).

\( x \rightarrow \gamma(t) = \Gamma_t(x) \)
Benamou-Brenier with interaction effects

Basics of the proof

With $\Gamma$ and $\mu_0$, we can create measures

$$\pi := \Gamma \# \mu_0, \quad \rho_t := (e_t) \# \pi$$

Then, observe

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

$$= \frac{1}{2} \int_{\mathbb{R}^n} \int_0^1 |\partial_t \Gamma_t(x)|^2 \, dt \, d\rho_0(x)$$

$$= \frac{1}{2} \int_0^1 \int_{\mathbb{R}^n} |v(\Gamma_t(x), t)|^2 \, d\rho_0(x) \, dt$$

$$= \frac{1}{2} \int_0^1 \int_{\mathbb{R}^n} |v(y, t)|^2 \, d\rho_t(y) \, dt$$
Benamou-Brenier with interaction effects
Basics of the proof

On the other hand,

\[
\int_{\Omega} \int_{\Omega} U(\gamma_1, \gamma_2) \, d\pi(\gamma_1) d\pi(\gamma_2)
\]

\[
= \int_{\Omega} \int_{\Omega} \int_{0}^{1} K(\gamma_1(t) - \gamma_2(t)) \, dt \, d\pi(\gamma_1) d\pi(\gamma_2)
\]

\[
= \int_{0}^{1} \left( \int_{\Omega} \int_{\Omega} K(\gamma_1(t) - \gamma_2(t)) \, d\pi(\gamma_1) d\pi(\gamma_2) \right) dt
\]

\[
= \int_{0}^{1} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} K(x - y) \, d\rho_t(x) d\rho_t(y) dt
\]
Therefore, for $\pi = \Gamma \# \mu_0$ and $\rho_t = (e_t) \# \pi$, 

$$
\int_\Omega c(\gamma) \, d\pi + \int_\Omega \int_\Omega U(\gamma, \sigma) d\pi(\gamma) d\pi(\sigma) \\
= \frac{1}{2} \int_0^2 \int_\Omega |v(x, t)|^2 \rho_t(\, dx) \, dt + \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(x - y) \, d\rho_t(x) d\rho_t(y) \, dt
$$
Benamou-Brenier with interaction effects
Hamilton-Jacobi equation

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

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

$$
\partial_t \rho = \text{div}(\rho \nabla \phi)
$$

$$
\partial_t \phi = \frac{1}{2}|\nabla \phi|^2 - K * \rho
$$
A numerical experiment
A numerical experiment
An artistic rendering!
A two-phase problem

We have begun studying the problem of minimizing

\[
E(\rho^{(1)}, \rho^{(2)}, v^{(1)}, v^{(2)})
\]

\[
:= \frac{1}{2} \int_0^1 \int_{\mathbb{R}^d} |v^{(1)}(x, t)| d\rho_t^{(1)}(x) dt
\]

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

\[
+ \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} K(x - y) \ d\rho_t^{(1)}(x) d\rho_t^{(2)}(y) dt
\]

constrained to initial/final time constraints and

\[
\partial_t \rho^{(i)} + \text{div}(\rho^{(i)} v^{(i)}) = 0 \text{ for } i = 0, 1.
\]
Problems

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

\[ \mathcal{U} : \mathcal{P}(\Omega) \rightarrow \mathbb{R} \]

which are “lifted” from functions \( \mathcal{P}(\mathbb{R}^n) \rightarrow \mathbb{R} \)?
5. (serious question!) What else is this hammer good for?
\[ \ddot{r} = -\nabla V(r) \]

Thank you!

Questions / Comments / Suggestions:
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