Multimarginal optimal transportation: the one dimensional symmetric case

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(in collaboration with Maria Colombo and Luigi De Pascale)

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Introduction

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- Description of the multi marginal problem and physical motivation;

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- Description of the multi marginal problem and physical motivation;
- Classical results with 2 marginals in dimension 1;
- Symmetric multimarginal case in dimension 1: existence of an optimal map and uniqueness of the symmetric optimal plan.

General minimization problem

We are interested in the following minimum problem:

$$\min_{f \in L^2((\mathbb{R}^d)^n;\mathbb{C}), \|f\|_2=1} \int_{(\mathbb{R}^d)^n} (c|\nabla f|^2 + V_{ee}|f|^2 + V_{ext}|f|^2)\,\mathrm{d}x,$$

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where

- V_{ee} is the Coulombian interaction potential between the electrons:

$$V_{ee}(x_1,\ldots,x_n) = \sum_{1\leq i<j\leq n} \frac{1}{|x_i - x_j|};$$

- V_{ext} is an external potential (due to the nucleus), which is the same for every electron: $V_{ext}(x_1,\ldots,x_n) = V(x_1) + \cdots + V(x_n)$;

Hohenberg e Kohn formulation(HK)

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In order to solve the previous problem, the idea is to fix the density ρ and minimize only the (kinetic + interaction) part under the density constraint. Then one tries to solve the main problem as

$$\min_{\rho \in \mathcal{P}(\mathbb{R}^d)} \left\{ F(\rho) + n \int V(x) \, \mathrm{d}\rho \right\},$$

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Another way is to see it as the strictly correlated regime, in which we neglect the kinetic part (Gori Giorgi).

Mathematical formulation

We are interested in the problem

$$\min_{\pi \in \Gamma(\mu_1, \ldots, \mu_n)} \int_{X^n} c(x_1, \ldots, x_n) \, \mathrm{d}\pi.$$

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- When $n = 2$ we obtain the Kantorovich formulation of optimal transport;
- this isn't exactly a trasport problem but more a coupling problem;
- symmetries: impossibility for uniqueness.

Multimarginal optimal transport

Notations:

- given $\sigma \in S_n$ define $\sigma : X^n \to X^n$ as
$$\sigma : (x_1, \dots, x_n) \mapsto (x_{\sigma(1)}, \dots, x_{\sigma(n)});$$
- $\Gamma_{sym}(\rho)$ is the set of probabilities π which have all marginals equal to ρ and such that $\sigma_\sharp \pi = \pi$ for all $\sigma \in S_n$. The natural projection into symmetric plans is
$$\pi^S = \frac{1}{n!} \sum_{\sigma \in S_n} \sigma_\sharp \pi;$$
- $T_{sym}(\rho)$ is the set of Borel maps $T : X \to X$ such that $T_\sharp \rho = \rho$ e $T^{(n)}(x) = x$ for ρ-almost every x.

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From now on we'll call (K_{sym}) e (M_{sym}) the following two problems:

$$\min_{\pi \in \Gamma_{sym}(\rho)} \int_{X^n} c(x_1, \dots, x_n) \, \mathrm{d}\pi$$

$$\inf_{T \in T_{sym}(\rho)} \int_X c(x, T(x), T(T(x)), \dots, T^{(n-1)}(x)) \, \mathrm{d}\rho$$

Existence of the map

Conjecture

There exists an optimal symmetric map, in particular (M_{sym}) *is a minimum. Furthermore this minimum is equal to* (K_{sym}).

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The goal of this studies is to investigate the equality $(K_{sym}) = (M_{sym})$, the presence of an optimal map and eventually the characterization of optimal (symmetric) plans.

Known results

- (Colombo - D.M.) In the symmetric case is true in general that $(K_{sym}) = (M_{sym})$, in every complete and separable metric space, with a symmetric l.s.c. cost, continuous in its finiteness domain, when ρ is without atoms;

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- (Pass, Pass - Kim) in the non-symmetric case, if a modifed twist condition on the cost holds true and ρ is absolutely continuous with respect to Lebesgue measure, then there exists a unique optimal plan, which is induced by an optimal map (as in the two marginal case);

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Theorem (Buttazzo - De Pascale - Gori Giorgi)

There exists a minimizer of (K_{sym}). Furthermore, the following duality formula holds true

$$(K_{sym}) = n \sup \left\{ \int_X \phi \, \mathrm{d}\rho \ : \ \phi(x_1) + \ldots + \phi(x_n) \leq c(x_1, \ldots, x_n) \right\}$$

Let $X = \mathbb{R}$, and let $c(x_1, \ldots, x_n) = \sum_{1 \le i < j \le n} \phi(|x_i - x_j|)$, where ϕ is a convex and decreasing function on $\mathbb{R}^+$.

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Theorem

Let ρ be a diffuse probability measure on $\mathbb{R}$ (such that $(K) < \infty$). Let $-\infty = d_0 < d_1 < \ldots < d_N = +\infty$ be such that

$$\rho([d_i, d_{i+1}]) = 1/N \qquad \forall i = 0, \ldots, N-1. \tag{1}$$

Let $T : \mathbb{R} \to \mathbb{R}$ be the unique function (up to ρ-null sets) that is increasing on every interval $[d_i, d_{i+1}]$, $i = 0, ..., N-1$, and such that

$$T_\sharp 1_{[d_i, d_{i+1}]}\rho = 1_{[d_{i+1}, d_{i+2}]}\rho \quad \forall i = 0, \ldots, N-1. \tag{2}$$

Then T is an admissible map for (M_{sym}) and

$$(K) = \int_{\mathbb{R}} c(x, T(x), T^2(x), \ldots, T^{(N-1)}(x))\, d\rho. \tag{3}$$

Moreover there exists a unique symmetric optimal plan, that is the symmetrization of the one induced by T.

c-monotonicity

Definition (c-monotonicity)

A set $A \subset X \times X$ is c-monotone if for every two points $(x_1, y_1), (x_2, y_2) \in A$ we have

$$c(x_1, y_1) + c(x_2, y_2) \leq c(x_1, y_2) + c(x_2, y_1)$$

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Let c be a nonnegative l.s.c. cost, continuous in its finiteness domain; then if the optimal cost is finite, the support of every optimal plan is c-monotone.

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Proof.

Consider neighborhoods of the points where inequality fails and rearrange the plan. □

Geometric characterization in $\mathbb{R}$, convex cost

In dimension 1, in the case $c(x,y)=\phi(x-y)$, with ϕ strictly convex function we have: if A is c-monotone, the for every couple $(x_1,y_1),(x_2,y_2)\in A$, if $x_1<x_2$ then $y_1\leq y_2$.

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Proof.

Suppose $y_1 > y_2$. Then we have that $x_1 - y_1 < x_2 - y_1 < x_2 - y_2$, so there exists $t \in (0,1)$ such that

$$x_2 - y_1 = t(x_1 - y_1) + (1-t)(x_2 - y_2)$$

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□

Corollary

The support of an optimal plan is "monotone".If ρ_1 and ρ_2 are diffuse then an optimal plan is induced by a map.

multimarginal c-monotonicity

We can adapt the definition to the multi marginal case. Given $P \subseteq \{1, \dots, n\}$ and two points $x, y \in X^n$ we define the P-mixing as

$$(P(x,y))_i = \begin{cases} x_i & \text{if } i \in P \\ y_i & \text{otherwise.} \end{cases} \qquad (P^c(x,y))_i = \begin{cases} y_i & \text{if } i \in P \\ x_i & \text{otherwise.} \end{cases} .$$

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A set $A \subset X^n$ is c-monotone if for every $x, y \in A$ and every $P \subseteq \{1, \dots, n\}$ one has

$$c(x) + c(y) \leq c(P(x,y)) + c(P^c(x,y))$$

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Theorem (Pass)

Let c be a nonnegative l.s.c. cost, continuous in its finiteness domain; then the support of an optimal plan with finite cost is necessarily c-monotone.

The proof uses Gangbo theorem applied to the spaces $X^{|P|}$ e $X^{|P^c|}$.

symmetric c-monotonicity

If we add symmetry we can define c-monotonicity in the following equivalent way. We first define the "cumulative coordinate" of two points $x, y \in X^n$ as

$$C(x,y) = \sum_{i=1}^{n} \delta_{x_i} + \delta_{y_i}$$

Definition (c-monotonicity)

A symmetric set $A \subset X^n$ is c-monotone if for every points $x, y \in A$ and every points x', y' such that $C(x,y) = C(x',y')$ we have that

$$c(x) + c(y) \leq c(x') + c(y')$$

From now on we'll have $X = \mathbb{R}$ and $c(x) = \sum_{i<j} \phi(|x_i - x_j|)$. The crucial geometrical characterization is:

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Lemma

Given a set T consisting of $2n$ coordinates counted with multiplicities, i.e., there exist $t_1 \leq t_2 \leq \cdots \leq t_{2n}$ such that $T = \sum \delta_{t_i}$, let x, y be points in X^n that minimize the problem

$$\min\{c(x') + c(y') \ : \ C(x', y') = T\}.$$

Then, up to swap x and y and up to re-arrange the coordinates increasingly, we have that $x_i = t_{2i}$ and $y_i = t_{2i-1}$.

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Equivalently, x, y are minimizers iff, defining x^*, y^* the increasing rearrangement of the coordinates, one has

$$x_1^* \leq y_1^* \leq x_2^* \leq \cdots x_n^* \leq y_n^*;$$

in this case the points are *well ordered*.

How to conclude

Given the lemma, we can conclude the proof of the theorem:

- prove that the support of an optimal plan doesn't intersect $x_i = x_j$;
- reduce the analysis to the zone $x_1 < x_2 \cdots < x_n = O$;
- consider the numbers

$$d_i^+ = \max\{x_i : x \in O \cap \mathrm{spt}\pi\} \qquad d_i^- = \min\{x_i : x \in O \cap \mathrm{spt}\pi\},$$

  and prove $d_i^+ \leq d_{i+1}^-$ and consequently $\rho([d_i^+, d_{i+1}^+]) = 1/n$;
- conclude as in the 2 dimensional case, with monotone maps.

Case with 3 marginals: by hands

We have 6 points on the real line (that represent T). In what way I can group in two groups of three points such that the interaction potential is minimal? $\binom{6}{3}/2 = 10$ cases.

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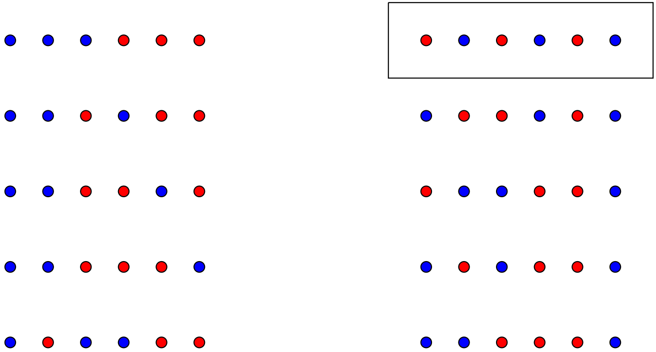

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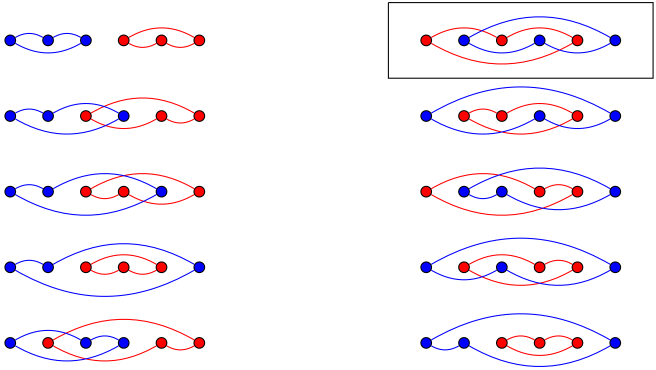

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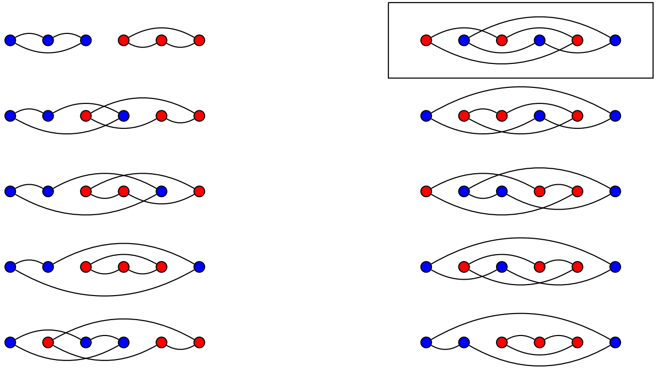

n-marginals symmetric case

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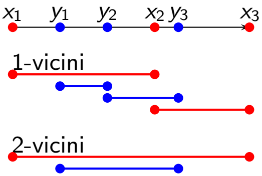

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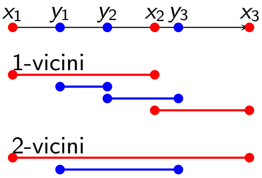

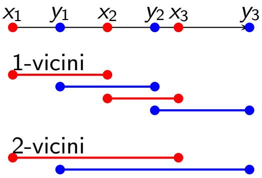

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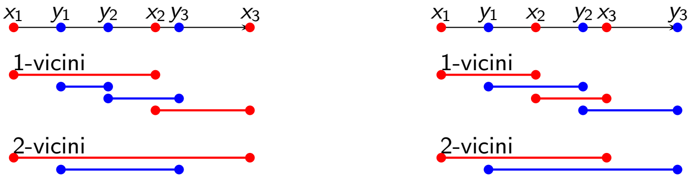

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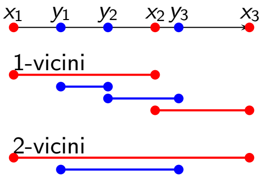

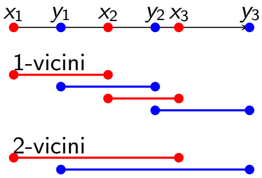

- Step 1 (convexity of ϕ): use the one-dimensional result for 2 marginals on k-neighbors (with fixed k);
- Step 2 (monotonicity of ϕ): stretch in the right way the segments to get the "well ordered" situation.

Future development

- one-dimensional symmetric case with a cost that is concave or concave-convex;

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- sufficiency of multimarginal c-monotonicity (other possible definitions?).

Thanks for the attention