Matching, multi-marginals problems and barycenters in the Wasserstein space

Guillaume CARLIER [a]

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[a] CEREMADE, Université Paris Dauphine

Introduction

- Optimal transport with several marginals : Gangbo- Święch (1996), and more recently a series of papers by Pass
- motivation (discretization of) Brenier's Least-Action formulation for the incompressible Euler equation,
- natural in so-called matching problems in economics
- related topic : nonlinear interpolation between more than two probability measures (e.g. interpolation of textures in image processing, Peyré, Delon, Bernot, Rabin);

Outline

① Equilibria, matching and optimal transport

② Barycenters in the Wasserstein space : existence, uniqueness and characterization

③ Link with multi-marginals problems and regularity

④ Examples

⑤ Convexity along barycenters

⑥ Concluding remarks

Matching

Indivisible good that comes in different qualities. The quality good z requires the formation of a *team* (say, one buyer, and a set of producers that have to gather to make the quality good available, a typical example is the market for houses). The different populations that constitute the teams are heterogeneous.

The data of the model are:

- a compact metric space Z, the *quality* space Z,
- compact metric spaces X_j, $j = 0, ..., N$, for the different populations, $x_j \in X_j$: agent type affecting her cost function, each X_j is equipped with a Borel probability μ_j measure, distribution of type x_j in population j,

- continuous cost functions $c_j : X_j \times Z \to \mathbf{R}$, $c_j(x_j, z)$ is the cost of an agent of population j with type x_j when participating to a team that produces $z \in Z$,
- costs are all quasi-linear, which means that an agent of population j with type x_j who participates a team that produces z and gets monetary transfer w_j has total cost:

$$c_j(x_j, z) - w_j.$$

One can think for instance that $j = 0$ corresponds to buyers and $j = 1, ..., N$ to producers (mason, plumber etc... in the case of houses). In this case, for $j \geq 1$, w_j is the wage received by member j of the team and w_0 is minus the total price paid by the consumer, at equilibrium we shall require that are self-financing which will be expressed by the fact that the sum of all transfers is 0.

We are now looking for a sytem of (quality dependent) monetary transfers that clears the market for the quality good. A system of price transfers is a family of function $\varphi_j : Z \to \mathbf{R}$ that it is balanced i.e.

$$\sum_{j=0}^{N} \varphi_j(z) = 0, \ \forall z \in Z.$$

For given transfers, optimal qualities for type x_j are determined by

$$\varphi_j^{c_j}(x_j) := \inf_{z \in Z} \{c_j(x_j, z) - \varphi_j(z))\}. \qquad (1)$$

which is the least cost that type x_j derives from the transfer φ_j.

$\varphi_j^{c_j}$ is the c_j-concave transform of the transfer function φ_j. For every $(x_j, z) \in X_j \times Z$, one has the so-called *Young's inequality*

$$\varphi_j^{c_j}(x_j) + \varphi_j(z) \leq c_j(x_j, z)$$

and cost-minimizing qualities are characterized by

$$\varphi_j^{c_j}(x_j) + \varphi_j(z) = c_j(x_j, z). \tag{2}$$

This induces for each j, couplings $\gamma_j \in \mathcal{M}_1^+(X_j \times Z)$ such that (2) holds γ_j a.e..

The interpretation of $\gamma_j(A_j \times B)$ is the probability that an agent with type in A_j has an optimal quality choice in B (given the transfer scheme φ_j). Of course, the first marginal of the coupling γ_j, $\pi_{X_j\,\#}\gamma_j$ should be μ_j. The last equilibrium requirement is that the demand distribution for the quality good should be the same for any population. In other words the marginal on Z of the coupling γ_j should be independent of j (this common distribution is an equilibrium quality line).

Putting everything together, this leads to

Definition 1 *A* matching equilibrium *consists of a family of transfers* $\varphi_j \in C(Z, \mathbf{R})$*, a family of probabilities* $\gamma_j \in \mathcal{M}_1^+(X_j \times Z)$*,* $j = 0, ..., N$ *and a quality line* $\nu \in \mathcal{M}_1^+(Z)$ *such that:*

1. *For all* $z \in Z$*:*
$$\sum_{j=0}^{N} \varphi_j(z) = 0, \tag{3}$$
2. $\gamma_j \in \Pi(\mu_j, \nu)$ *for every* $j = 0, ..., N$*,*
3. *for every* $j = 0, ..., N$*, one has:*
$$\varphi_j^{c_j}(x_j) + \varphi_j(z) = c_j(x_j, z) \qquad \gamma_j\text{-a.e. on } X_j \times Z.$$

Digression: a short reminder on the Monge-Kantorovich problem

All this is very much related to the Monge-Kantorovich optimal transport problem:

$$W_c(\mu, \nu) := \inf_{\gamma \in \Pi(\mu,\nu)} \int_{X \times Y} c(x, y) d\gamma(x, y)$$

where X and Z are compact metric spaces (say), $c \in C(X \times Z)$ is the transport cost (per unit of mass), μ and ν are probability measures on X and Z respectively and $\Pi(\mu, \nu)$ is the set of transport plans between μ and ν i.e. the set of probability measures on $X \times Z$ having μ and ν as marginals.

$\gamma \in \Pi(\mu, \nu)$ thus means

$$\gamma(A \times Z) = \mu(A),\ \gamma(X \times B) = \nu(B),\ \forall A, B \text{ Borel}$$

or, put differently, $\forall (\psi, \varphi) \in C(X) \times C(Z)$:

$$\int_{X \times Z} (\psi(x) + \varphi(z)) d\gamma(x, z) = \int_X \psi d\mu + \int_Z \varphi d\nu.$$

Convenient to write the constraint $\gamma \in \Pi(\mu, \nu)$ as $\gamma \geq 0$ and

$$\sup_{(\psi,\varphi)} (\int_X \psi d\mu + \int_Z \varphi d\nu - \int_{X \times Z} (\psi(x) + \varphi(z)) d\gamma(x, z)) = 0.$$

Lagrangian form of $W_c(\mu, \nu)$:

$$W_c(\mu, \nu) = \inf_{\gamma \geq 0} \sup_{(\psi, \varphi)} L(\gamma, \psi, \varphi)$$

with $L(\gamma, \psi, \varphi) = \int_{X \times Z} (c - (\psi \oplus \varphi)) d\gamma + \int_X \psi d\mu + \int_Z \varphi d\nu$. The dual reads as

$$\sup_{(\psi, \varphi)} \inf_{\gamma \geq 0} L(\gamma, \psi, \varphi)$$

but obviously

$$\inf_{\gamma \geq 0} L(\gamma, \psi, \varphi) = \begin{cases} \int_X \psi d\mu + \int_Z \varphi d\nu & \text{if } \psi \oplus \varphi \leq c \\ -\infty & \text{otherwise} \end{cases}$$

Applying a sutable minmax theorem gives

$$W_c(\mu,\nu) = \sup\{\int_X \psi d\mu + \int_Z \varphi d\nu \ : \ \psi(x) + \varphi(z) \leq c(x,z)\}$$

the constraint can be rewritten as

$$\psi(x) \leq \min_z\{c(x,z) - \varphi(z)\} := \varphi^c(x)$$

(φ^c is the so-called c-transform of φ) and since the criterion is nondecreasing in ψ,

$$W_c(\mu,\nu) = \sup_{\varphi \in C(Z)} \{\int_X \varphi^c d\mu + \int_Z \varphi d\nu\}$$

this is the Kantorovich duality formula.

Primal dual relations: let $\gamma \in \Pi(\mu, \nu)$ and $\varphi \in C(Z)$, γ solves $W_c(\mu, \nu)$ and φ solves its dual formulation if and only if

$$\varphi^c(x) + \varphi(z) = c(x, z) \text{ for } \gamma\text{-a.e. } (x, z).$$

Thanks to the Kantorovich duality formula

$$W_{c_j}(\mu_j,\nu) := \inf_{\gamma_j\in\Pi(\mu_j,\nu)} \int_{X_j\times Z} c_j(x_j,z)d\gamma_j(x,z)$$
$$= \sup_{\varphi_j\in C(Z)} \left\{ \int_{X_j} \varphi_j^{c_j} d\mu_j + \int_Z \varphi_j d\mu_j \right\}$$

we see that requirements 2 and 3 in the definition of an equilibrium exactly mean that γ_j is an optimal plan for the optimal transport problem $W_{c_j}(\mu_j,\nu)$ and that φ_j solves its dual.

Let us assume now that $(\varphi_j, \gamma_j, \nu)$ is a matching equilibrium. We thus have

$$W_{c_j}(\mu_j, \nu) = \int_{X_j \times Z} c_j(x_j, z) d\gamma_j(x_j, z) = \int_{X_j} \varphi_j^{c_j} d\mu_j + \int_Z \varphi_j d\nu.$$

Summing these equalities and using the balance condition (3) then yields:

$$\sum_{j=0}^{d} W_{c_j}(\mu_j, \nu) = \sum_{j=0}^{d} \int_{X_j} \varphi_j^{c_j} d\mu_j \tag{4}$$

Now let $\psi_j \in C(Z, \mathbf{R})$ be another balanced family of transfers:

$$\sum_{j=0}^{N} \psi_j(z) = 0, \ \forall z \in Z. \tag{5}$$

The Monge-Kantorovich duality formula yields:

$$W_{c_j}(\mu_j,\nu) \geq \int_{X_j} \psi_j^{c_j} d\mu_j + \int_Z \psi_j d\nu \tag{6}$$

summing these inequalities and using (5) we then get:

$$\sum_{j=0}^{N} W_{c_j}(\mu_j,\nu) \geq \sum_{j=0}^{d} \int_{X_j} \psi_j^{c_j} d\mu_j. \tag{7}$$

With (4), we deduce that the transfers φ_j's solve the following (concave) program:

$$(\mathcal{P}) \ \sup \left\{ \sum_{j=0}^{N} \int_{X_j} \varphi_j^{c_j} d\mu_j \ : \ \sum_{j=0}^{d} \varphi_j = 0 \right\}.$$

Take now some $\eta \in \mathcal{M}_1^+(Z)$. With the Monge-Kantorovich duality formula, the balance condition (3) and (4), we get

$$\sum_{j=0}^{d} W_{c_j}(\mu_j,\eta) \geq \sum_{j=0}^{d} \left(\int_{X_j} \varphi_j^{c_j} d\mu_j + \int_Z \varphi_j d\eta \right)$$
$$= \sum_{j=0}^{d} \int_{X_j} \varphi_j^{c_j} d\mu_j = \sum_{j=0}^{d} W_{c_j}(\mu_j,\nu)$$

So that ν solves

$$(\mathcal{P}^*) \;\; \inf \left\{ \sum_{j=0}^{d} W_{c_j}(\mu_j,\nu) \, : \, \nu \in \mathcal{M}_1^+(Z) \right\}.$$

At this point, we haven't proven anything about the existence of equilibria, but have discovered that if $(\varphi_j, \gamma_j, \nu)$ is a matching equilibrium then: the transfers φ_j's solve $(\mathcal{P})$, the quality line ν solves $(\mathcal{P}^*)$, and for each j, γ_j solves $W_{c_j}(\mu_j, \nu)$.

It turns out that in fact, we have much more (simple convex duality):

Theorem 1 *The supremum in* $(\mathcal{P})$ *and the infimum in* $(\mathcal{P}^*)$ *are attained and the two values are equal. Moreover* $(\varphi_j, \gamma_j, \nu)$ *is a matching equilibrium if and only if:*

- *the transfers* φ_j*'s solve* $(\mathcal{P})$*,*
- *the quality line* ν *solves* $(\mathcal{P}^*)$*,*
- *for each* j*,* γ_j *solves* $W_{c_j}(\mu_j, \nu)$*.*

In particular matching equilibria exist.

Key role played by the convex but nonlinear problem

$$(\mathcal{P}^*) \ \inf \left\{ \sum_{j=0}^{d} W_{c_j}(\mu_j, \nu) \, : \, \nu \in \mathcal{M}_1^+(Z) \right\}.$$

there is a (linear) reformulation in terms of multi-marginal optimal transport. Define the least cost

$$\overline{c}(x) := \overline{c}(x_0, ..., x_N) := \inf \left\{ \sum_{j=0}^{N} c_j(x_j, z), \ z \in Z \right\}.$$

For the sake of simplicity, let us assume that for every $x = (x_0, ..., x_N) \in X$ there is a unique cost-minimizing quality $z =: \overline{z}(x)$:

$$\overline{c}(x) = \sum_{j=0}^{N} c_j(x_j, \overline{z}(x)).$$

Now let us consider the multi-marginal Monge-Kantorovich problem

$$\inf_{\gamma \in \Pi(\mu_0,...,\mu_N)} \int_{X_0 \times ... \times X_N} \overline{c}(x_0, ..., x_N) d\gamma(x_0, ..., x_N) \qquad (8)$$

where $\Pi(\mu_0, ..., \mu_N)$ denotes the set of probability measures on $X_0 \times ... \times X_N$ having $\mu_0, ..., \mu_N$ as marginals. The connection between the multi-marginal Monge-Kantorovich problem (8) and $(\mathcal{P}^*)$ is:

Proposition 1 *Under the previous assumptions, one has:*

1. *the infimum in (8) is attained and its value coincide with* $\inf(\mathcal{P}^*)$*,*
2. *if* $\overline{\gamma}$ *solves (8) then* $\overline{\nu} := \overline{z} \sharp \gamma$ *solves* $(\mathcal{P}^*)$*,*
3. *if* $\overline{\nu}$ *solves* $(\mathcal{P}^*)$ *then there exists a solution of (8),* $\overline{\gamma}$*, such that* $\overline{\nu} := \overline{z} \sharp \overline{\gamma}$*.*

Barycenters in the Wasserstein space

Taking quadratic costs in the previous matching problem leads to the a minimization problem of the form

$$\inf_{\nu} \sum_{i=1}^{p} \lambda_i W_2^2(\nu_i, \nu)$$

where W_2^2 is the squared 2-Wasserstein distance:

$$W_2^2(\mu, \nu) := \inf_{\gamma \in \Pi(\mu,\nu)} \int_{\mathbf{R}^d \times \mathbf{R}^d} |x - y|^2 d\gamma(x, y)$$

By analogy with the euclidean case, a minimizer will be called a barycenter of the measures ν_i with weights λ_i.

The quadratic OT problem has received a considerable attention since the seminal work of Brenier in the late 80's/early 90's:

- if μ and ν have second moments and μ is absolutely continuous (or more generally does not charge Lipschitz hypersurfaces), there is a unique optimal plan it is induced by an optimal transport map that is the gradient of a convex function : $\gamma = (\mathrm{id}, \nabla u)\sharp\mu$ with u convex,
- Connection with the Monge-Ampère equation:

$$\det(D^2 u)\nu(\nabla u) = \mu$$

  for which a deep regularity theory was developed by Caffarelli (see also the work of Urbas).

The set of probability measures with second moments equipped with the 2-Wasserste distance, viewed as a (complete) metric space, is a nice geometric object:

- formal Riemannian structure (Otto) in which geodesics are given by McCann's interpolation, or Benamou-Brenier dynamic formulation,
- natural notion of convexity, gradient flows of semi convex functionals: for instance, the heat flow is the gradient flow of the Boltzmann entropy for this Riemannian-like structure, the GF theory was investigated in depth in the book of Ambrosio, Gigli and Savaré,
- strong connections with functional and geometric inequalities....

Application : a four line proof of the isoperimetric inequality

Let B be the unit ball of $\mathbf{R}^d$ and A be another (regular enough) domain. Let $T = \nabla u$ be the Brenier transport between $|A|^{-1}\chi_A$ and $|B|^{-1}\chi_B$ so that

$$\det(DT) = \det(D^2 u) = \frac{|B|}{|A|}.$$

Since by construction $DT = D^2 u$ is diagonalizable with nonnegative eigenvalues, the arithmetico-geometric inequality gives

$$\det(DT)^{1/d} \leq \frac{1}{d}\mathrm{div}(T) = \frac{1}{d}\Delta u$$

integrating, we obtain

$$|B|^{1/d}|A|^{1-1/d} \leq \frac{1}{d}\int_A \Delta u = \frac{1}{d}\int_{\partial A} \nabla u \cdot n$$

and since $T = \nabla u \in B$, we get

$$|B|^{1/d}|A|^{1-1/d} \leq \frac{1}{d}\mathrm{Per}(A) = |B|\frac{\mathrm{Per}(A)}{\mathrm{Per}(B)}$$

that is

$$\frac{|A|^{1-1/d}}{\mathrm{Per}(A)} \leq \frac{|B|^{1-1/d}}{\mathrm{Per}(B)}.$$

The notion of a barycenter as a minimizer of an averaged squared distance is not new and has already been investigated in depth by Sturm in the framework of nonpositively curved metric spaces. It turns out, however, that the Wasserstein space is not nonpositively curved as illustrated by an example in the book of Ambrosio, Gigli, and Savaré, and that much less is known on the existence, uniqueness, and properties of barycenters outside of the nonpositively curved case. See, however, the recent article of Ohta for the case of Alexandrov spaces of curvature bounded from below.

Duality

Define $Y := (1 + |\,.\,|^2)C_b(\mathbf{R}^d)$ and $X := (1 + |\,.\,|^2)C_0(\mathbf{R}^d)$, given an integer $p \geq 2$, p probability measures $\nu_1, ..., \nu_p$ in $X' \cap \mathcal{M}_+^1(\mathbf{R}^d)$ and p real numbers $\lambda_1, ...\lambda_p$ such that $\lambda_i > 0$ and $\sum_{i=1}^p \lambda_i = 1$, we are thus interested in the following problem:

$$(\mathcal{P}) \quad \inf_{\nu \in \mathcal{M}_+^1(\mathbf{R}^d) \cap X'} J(\nu) = \sum_{i=1}^{p} \frac{\lambda_i}{2} W_2^2(\nu_i, \nu). \tag{9}$$

Duality

Dual of $(\mathcal{P})$:

$$(\mathcal{P}^*) \quad \sup\left\{F(f_1,...,f_p) = \sum_{i=1}^{p} \int_{\mathbf{R}^d} S_{\lambda_i} f_i d\nu_i \ : \sum_{i=1}^{p} f_i = 0,\ f_i \in Y\right\} \tag{10}$$

where

$$S_\lambda f(x) := \inf_{y\in\mathbf{R}^d} \left\{\frac{\lambda}{2}|x-y|^2 - f(y)\right\},\ \ \forall x \in \mathbf{R}^d,\ f \in Y,\ \lambda > 0. \tag{11}$$

Both the infimum in $(\mathcal{P})$ and the supremum in $(\mathcal{P}^*)$ are attained and $\min(\mathcal{P}) = \max(\mathcal{P}^*)$.

Optimality conditions

Let $(f_1, ..., f_p)$ be a solution of $(\mathcal{P}^*)$ and define the convex potentials:

$$\lambda_i \phi_i(x) := \frac{\lambda_i}{2}|x|^2 - S_{\lambda_i} f_i(x), \tag{12}$$

by duality, if ν solves $(\mathcal{P})$ and γ_i is an optimal transport plan between ν_i and ν then:

- the support of γ_i is included in $\partial\phi_i$,
- $\sum_i \phi_i^*(y) \leq \frac{1}{2}|y|^2$ for all $y \in \mathbf{R}^d$ with an inequality on the support of ν.

Uniqueness

We then deduce the following uniqueness result and characterization of the barycenter:

Proposition 2 *Assume that there is an index* $i \in \{1, ...p\}$ *such that* ν_i *vanishes on small sets. Then* $(\mathcal{P})$ *admits a unique solution* ν *which is given by* $\nu = \nabla\phi_i \sharp \nu_i$ *where* ϕ_i *is the convex potential defined by (12).*

As soon as one of the ν_i's vanishes on small sets , this therefore enables one to define unambiguously the barycenter $(\text{bar}(\nu_i, \lambda_i)_{i=1,\dots,p})$ of the ν_i's with weights λ_i.

Characterization

Proposition 3 *Assume that ν_i vanishes on small sets for every $i = 1, .., p$, and let $\nu \in \mathcal{M}_+^1(\mathbf{R}^d) \cap X'$. Then the following conditions are equivalent:*

1. *ν solves $(\mathcal{P})$.*
2. *$\nu = \nabla\phi_i \sharp \nu_i$ for every i, where ϕ_i is defined by (12).*
3. *There exist convex potentials ψ_i such that $\nabla\psi_i$ is the Brenier's map transporting ν_i to ν, and a constant C such that*

$$\sum_{i=1}^{p} \lambda_i \psi_i^*(y) \leq C + \frac{|y|^2}{2}, \ \forall y \in \mathbf{R}^d, \text{ with equality } \nu\text{-a.e.} \quad (13)$$

$T_i := \nabla\psi_i^*$ is the optimal transport between the unknown barycenter ν and the vertex ν_i the previous characterization implies

$$\sum_{i=1}^{p} \lambda_i T_i = \mathrm{id} \;\; \nu\text{-a.e.}$$

and if the previous condition holds on the whole of $\mathbf{R}^d$ then ν is the barycenter of the ν_i's with weights λ_i.

Link with multi-marginals problems

$(\mathcal{P})$ is in fact equivalent to a problem of multi-marginal optimal transportation type similar to the one solved by Gangbo and Święch. For $x := (x_1, ..., x_p) \in (\mathbf{R}^d)^p$, define the euclidean barycenter

$$T(x) := \sum_{i=1}^{p} \lambda_i x_i. \tag{14}$$

Multi-marginal optimal transportation problem

$$\inf \left\{ \int_{\mathbf{R}^d} \Big(\sum_{i=1}^{p} \frac{\lambda_i}{2} |x_i - T(x)|^2 \Big) d\gamma(x_1, ...x_p),\ \gamma \in \Pi(\nu_1, ..., \nu_p) \right\} \tag{15}$$

$\Pi(\nu_1, ..., \nu_p)$: probab. on $(\mathbf{R}^d)^p$ having $\nu_1, ..., \nu_p$ as marginals.

Of course equivalent to

$$(\mathcal{Q})\ \sup\left\{\int\Big(\sum_{1\le i<j\le p}\lambda_i\lambda_j x_i\cdot x_j\Big)d\gamma(x_1,...x_p),\ \gamma\in\Pi(\nu_1,...,\nu_p)\right\}. \tag{16}$$

that has been solved by Gangbo and Święch. As usual, a key tool is the dual problem

$$(\mathcal{Q}^*)\ \inf\left\{\sum_{i=1}^p\int_{\mathbf{R}^d} g_i d\nu_i,\ \sum_{i=1}^p g_i(x_i)\ge\sum_{1\le i<j\le p}\lambda_i\lambda_j x_i\cdot x_j,\ \forall x\right\}. \tag{17}$$

In $(\mathcal{Q}^*)$, one can restrict to potentials that satisfy

$$g_i(x_i) = \sup_{(x_j)_{j\neq i}} \left\{ \frac{1}{2} \sum_{1\leq k\neq j\leq p} \lambda_k \lambda_j x_k \cdot x_j - \sum_{j\neq i} g_j(x_j) \right\} \qquad (18)$$

hence are convex. Secondly, the duality relation between $(\mathcal{Q})$ and $(\mathcal{Q}^*)$ expresses that, γ solves $(\mathcal{Q})$ and $(g_1, ..., g_p)$ solves $(\mathcal{Q}^*)$ if and only if

$$\sum_{i=1}^{p} g_i(x_i) = \frac{1}{2} \sum_{1\leq i\neq j\leq p} \lambda_i \lambda_j x_i \cdot x_j, \ \ \gamma\text{-a.e..} \qquad (19)$$

so that, if, in addition the potentials g_i's are differentiable γ-a.e., then one can deduce from (18) and (19) that for γ-a.e. $x = (x_1, ..., x_d)$, one has

$$\nabla g_i(x_i) = \lambda_i \sum_{j \neq i} \lambda_j x_j$$

which can be rewritten as

$$\nabla\Big(\frac{\lambda_i}{2}|\ .\ |^2 + \frac{g_i}{\lambda_i}\Big)(x_i) = \sum_{j=1}^{p} \lambda_j x_j = \nabla\Big(\frac{\lambda_1}{2}|\ .\ |^2 + \frac{g_1}{\lambda_1}\Big)(x_1)$$

or in a more explicit way

$$x_i = \nabla\Big(\frac{\lambda_i}{2}|\ .\ |^2 + \frac{g_i}{\lambda_i}\Big)^* \circ \nabla\Big(\frac{\lambda_1}{2}|\ .\ |^2 + \frac{g_1}{\lambda_1}\Big)(x_1).$$

This yields that the optimal γ is in fact supported by the graph of a map of the form
$x_1 \mapsto (x_1, \nabla u_i^*(\nabla u_1(x_1)), ..., \nabla u_p^*(\nabla u_1(x_1)))$ for some potentials u_i such that $u_i - \lambda_i| \, . \,|^2/2$ is convex (so that u_i^* is $C^{1,1}$).
Gangbo and Święch proved:

Theorem 2 *Assume that ν_i vanishes on small sets for $i = 1, .., p$. Then $(\mathcal{Q})$ admits a unique solution $\gamma \in \Pi(\nu_1, ..., \nu_p)$. Moreover, γ is of the form $\gamma = (T_1^1, ..., T_p^1)\sharp\nu_1$ with $T_i^1 = \nabla u_i^* \circ \nabla u_1$ for $i = 1, ..., p$ where the u_i's are strictly convex potentials defined by*

$$u_i(x) := \frac{\lambda_i}{2}|x|^2 + \frac{g_i(x)}{\lambda_i}, \ \forall x \in \mathbf{R}^d \tag{20}$$

and $(g_1, ..., g_p)$ are convex potentials that solve $(\mathcal{Q}^*)$.

In the sequel, we will refer to the maps T_i^1 of the previous theorem as the Gangbo-Święch maps between ν_1 and ν_i. Note that the Gangbo-Święch maps a priori depend on the whole collections of the ν_i's and the weights λ_i's. These maps are transport maps in the sense that $T_i^1 \sharp \nu_1 = \nu_i$. Of course, by permuting the indices, one can similarly define the Gangbo-Święch maps $T_i^j := \nabla u_i^* \circ \nabla u_j$ between a reference measure ν_j and ν_i.

Precise relationship between our initial barycenter problem $(\mathcal{P})$ and the multi-marginals problem $(\mathcal{Q})$:

Proposition 4 *Assume that ν_i vanishes on small sets for $i = 1, .., p$. Then the solution of $(\mathcal{P})$ is given by $\overline{\nu} = T\sharp\gamma$, where T is defined by (14) and γ is the solution of $(\mathcal{Q})$.*

Combining Theorem 2 and Proposition 4 yields:

$$\overline{\nu} := \Big(\sum_{i=1}^{p} \lambda_i T_i^1\Big)\sharp\nu_1 = \Big(\sum_{i=1}^{p} \lambda_i T_i^j\Big)\sharp\nu_j \tag{21}$$

where the T_i^j are the Gangbo-Święch maps between ν_j and ν_i which are given by $T_i^j = \nabla u_i^* \circ \nabla u_j$, where the u_j's are strictly convex potentials defined by (20). Immediate consequences : support of $\mathrm{bar}((\nu_i, \lambda_i)_i) \subset \sum_{i=1}^p \lambda_i \mathrm{supp}(\nu_i)$ and the center of mass of $\mathrm{bar}((\nu_i, \lambda_i)_i)$ is $\sum_{i=1}^p \lambda_i \int_{\mathbf{R}^d} x d\nu_i(x)$.

Another consequence of this structure of the barycenter is that the internal energy $E_\Phi : \nu \mapsto \int \Phi(\nu(x))dx$ (with Φ convex and $\Phi(0) = 0$) is convex along barycenters in the sense that $E_\Phi(\text{bar}((\nu_i, \lambda_i)) \leq \sum_i \lambda_i E_\Phi(\nu_i)$ as soon as Φ satisfies the McCann displacement convexity condition that requires $\lambda \mapsto \lambda^d \Phi(\lambda^{-d})$ to be convex nonincreasing on $(0, +\infty)$. I'll be more precise later on and will recall what displacement convexity means.

This kind of convexity arguments implies in particular that if all the ν_i's are in L^q with $q > 1$, then so is their barycenter:

$$\|\mathrm{bar}((\nu_i, \lambda_i))\|_{L^q}^q \leq \sum \lambda_i \|\nu_i\|_{L^q}^q$$

(thus yielding the case $p = \infty$ by a limit argument). The next result gives an L^∞ bound on the barycenter as soon as one of the measures has a bounded density with a direct proof.

Finally, the relation between the barycenter and the Gangbo-Święch maps easily enables us to obtain a regularity result on the barycenter.

Theorem 3 *Let* $(\nu_1, ..., \nu_p)$ *be probability measures with finite second moments and let* $(\lambda_1, ..., \lambda_p)$ *be positive reals that sum to* 1*. If* $\nu_1 \in L^\infty$*, then* $\overline{\nu} := \mathrm{bar}((\nu_i, \lambda_i)) \in L^\infty$ *and more precisely:*

$$\|\overline{\nu}\|_{L^\infty} \leq \frac{1}{\lambda_1^d} \|\nu_1\|_{L^\infty}. \tag{22}$$

Recall that $\overline{\nu} = \overline{T}\sharp\nu_1$ where

$$\overline{T} = \sum_{i=1}^{p} \lambda_i \nabla u_i^* \circ \nabla u_1 = \lambda_1 \,\mathrm{id} + \sum_{i=2}^{p} \lambda_i \nabla u_i^* \circ \nabla u_1$$

and the potentials u_i satisfy

$$D^2 u_i \geq \lambda_i \,\mathrm{id},\; D^2 u_i^* \leq \frac{1}{\lambda_i}\,\mathrm{id}\,. \tag{23}$$

regularize u_1 in the previous formula and get

$$D\overline{T}^{\varepsilon}(x) = \lambda_1 \,\mathrm{id} + \sum_{i=2}^{p} \lambda_i D^2 u_i^* (\nabla u_1^{\varepsilon}(x)) D^2 u_1^{\varepsilon}(x)$$

that is of the form $\lambda_1 \,\mathrm{id} + AB$ where both matrices A and B are symmetric and positive definite, thus, the eigenvalues of $D\overline{T}^{\varepsilon}$ are all real and bounded from below by λ_1, the desired estimate easily follows.

Examples

The case $d = 1$

When $d = 1$, the description of the barycenter is simple and this is due to the fact that gradient of convex functions are simply nondrecreasing functions, and this property is stable by composition. Let $\nu_1, ..., \nu_p$ be nonatomic probability measures on the real line that have finite second moments, and let $\lambda_1, ..., \lambda_p$ be positive reals that sum to 1. From formula (21), the barycenter $\overline{\nu} := \mathrm{bar}(\nu_i, \lambda_i)_i$ is given by

$$\overline{\nu} = \Big(\sum_{i=1}^{p} \lambda_i T_i^1 \Big) \sharp \nu_1$$

where T_i^1 is the Gangbo-Święch map between ν_1 and ν_i.

Therefore, T_i^1 is a nondecreasing map that pushes ν_1 forward to ν_i, there is only one such map, which is given by the usual rearrangement formula $T_i^1 := F_i^{-1} \circ F_1$, where F_i is the cumulative function of F_i i.e. $F_i(\alpha) = \nu_i((-\infty, \alpha])$, and F_i^{-1} denotes the generalized inverse of F_i,

$$F_i^{-1}(t) := \inf\{\alpha \ : \ F_i(\alpha) \geq t\}.$$

Therefore, $\mathrm{bar}(\nu_i, \lambda_i)_i$ is simply obtained as the image of ν_1 by the linearly interpolated transport map $\sum_i \lambda_i T_i^1$.

Of course, one also has

$$\overline{\nu} = \Big(\sum_{i=1}^{p} \lambda_i T_i^j\Big) \sharp \nu_j$$

where T_i^j is the Brenier's map between ν_j and ν_i. The fact that the resulting measure does not depend on j is very specific to the unidimensional case and does not hold in general in higher dimensions. Also specific to the one-dimensional case is the associativity of barycenters.

The case $p = 2$

In the case of two mesures ν_0 and ν_1 (regular say), and $t \in (0, 1)$, it is reasonable to expect that the barycenter of $(\nu_0, (1-t))$ and (ν_1, t) is McCann's interpolant:

$$\nu_t := ((1-t)\mathrm{id} + t\nabla\phi)\sharp\nu_0 = (t\mathrm{id} + (1-t)\nabla\phi^*)\sharp\nu_1$$

where $\nabla\phi$ is the Brenier's map between ν_0 and ν_1. To see this, it is enough to prove that

$$(1-t)f_t + tg_t = \frac{1}{2}|.|^2 \tag{24}$$

where ∇f_t and ∇g_t are respectively the Brenier's maps between ν_t and ν_0, and ν_t and ν_1, i.e.,

$$f_t = \Big(\frac{(1-t)}{2}|.|^2 + t\phi\Big)^*, \; g_t = \Big(\frac{t}{2}|.|^2 + (1-t)\phi^*\Big)^*.$$

To prove (24), we first write

$$-f_t(p) = \inf_{x\in\mathbf{R}^d}\{(1-t)\frac{|x|^2}{2} - p\cdot x + t\phi(x)\}$$

with the Fenchel-Rockafellar duality theorem, this rewrittes

$$-f_t(p) = \sup_{z\in\mathbf{R}^d}\{-t\phi^*(-z/t) - \frac{1}{2(1-t)}|p+z|^2\}.$$

Therefore

$$\begin{aligned}-(1-t)f_t(p) &= \sup_{y\in\mathbf{R}^d}\{-t(1-t)\phi^*(y) - \frac{1}{2}|p-ty|^2\}\\ &= -\frac{1}{2}|p|^2 + t\sup_{y\in\mathbf{R}^d}\{p\cdot y - (\frac{t}{2}|y|^2 + (1-t)\phi^*(y))\}\\ &= -\frac{1}{2}|p|^2 + tg_t(p).\end{aligned}$$

The gaussian case

Consider now the case where ν_i is a gaussian measure with mean 0 and covariance matrix S_i. We assume that each S_i is positive definite and, given weights $\lambda_i > 0$ that sum to 1, we consider again the barycenter problem. This gaussian case was already considered by Knott and Smith who suggested an almost explicit construction for the barycenter but neither existence nor uniqueness was proved in their paper.

Theorem 4 *In the gaussian framework, there is a unique solution $\overline{\nu}$ to (9). Moreover, $\overline{\nu} = \mathcal{N}(0, \overline{S})$ where $\overline{S}$ is the unique positive definite root of the matrix equation*

$$\sum_{i=1}^{p} \lambda_i \left(S^{1/2} S_i S^{1/2} \right)^{1/2} = S. \qquad (25)$$

Step 1: *existence of a solution to (25).* Let α_i and β_i denote respectively the smallest and largest eigenvalue of S_i, and α and β be such that

$$\beta \geq \Big(\sum_{i=1}^{p} \lambda_i \sqrt{\beta_i}\Big)^2 \geq \sum_{i=1}^{p} \Big(\lambda_i \sqrt{\alpha_i}\Big)^2 \geq \alpha.$$

Let $K_{\alpha,\beta}$ be the (convex and compact) set of symmetric matrices S such that $\beta I \geq S \geq \alpha I$. For $S \in K_{\alpha,\beta}$, define

$$F(S) := \sum_{i=1}^{p} \lambda_i \Big(S^{1/2} S_i S^{1/2}\Big)^{1/2}.$$

It is easy to see that

$$\beta I \geq \sum_{i=1}^{p} \lambda_i \sqrt{\beta\beta_i} I \geq F(S) \geq \sum_{i=1}^{p} \lambda_i \sqrt{\alpha\alpha_i} I \geq \alpha I, \ \ \forall S \in K_{\alpha,\beta}.$$

Then F is a self-map of $K_{\alpha,\beta}$. It is also continuous on $K_{\alpha,\beta}$. The existence of a solution to (25) in $K_{\alpha,\beta}$ then directly follows from Brouwer's fixed-point theorem.

Step 2: *sufficiency*. Set $\overline{\nu} := \mathcal{N}(0, \overline{S})$ where $\overline{S}$ is a positive definite solution of (25). The optimal transport between $\overline{\nu}$ and ν_i is then the linear map

$$T_i = S_i^{1/2}\left(S_i^{1/2}\overline{S}S_i^{1/2}\right)^{-1/2}S_i^{1/2}.$$

Let us now prove that $\sum_{i=1}^{p} \lambda_i T_i = I$ that we already know to be a sufficient condition for $\overline{\nu}$ be the barycenter.

Set $K_i = S_i^{1/2}$ and $\overline{K} := \overline{S}^{1/2}$. Using the identity

$$(\overline{K} K_i^2 \overline{K})^{1/2} = \overline{K} K_i (K_i \overline{K}^2 K_i)^{-1/2} K_i \overline{K}$$

we may rewrite $F(\overline{S}) = \overline{S}$ as

$$\sum_{i=1}^{p} \lambda_i \overline{K} K_i (K_i \overline{K}^2 K_i)^{-1/2} K_i \overline{K} = \overline{K}^2$$

and since $\overline{K}$ is invertible, this yields

$$\sum_{i=1}^{p} \lambda_i K_i (K_i \overline{K}^2 K_i)^{-1/2} K_i = \sum_{i=1}^{p} \lambda_i T_i = I$$

which proves that $\overline{\nu}$ is optimal.

Step 3: We already know that the barycenter is unique and from the previous step, we have that, for any positive definite solution $\overline{S}$ of the matrix equation (25), $\mathcal{N}(0, \overline{S})$ solves a sufficient optimality condition for the barycenter. This proves that (25) has a unique positive definite solution.

We have used Brouwer's fixed point. Can one prove existence and uniqueness in a constructive way (Picard iterations)? Numerical computations most of the time suggest convergence of Picard iterations. Degenerate cases perhaps deserve to be investigated as well.

Convexity of functionals

Let E be a functional defined on the set of probability measures on $\mathbf{R}^d$ our aim is to investigate various convexity properties of E and in particular convexity along Wasserstein barycenters i.e. :

$$E(\mathrm{bar}(\nu_i, \lambda_i)) \leq \sum_{i=1}^{p} \lambda_i E(\nu_i)$$

for p, every weights in the simplex and every $(\nu_1, ..., \nu_p)$ (regular say).

Mc Cann's displacement convexity

A functional E is called displacement convex if for every ν_0 and ν_1, $t \in [0,1] \mapsto E(\nu_t)$ is convex where $\nu_t := ((1-t)\,\mathrm{id} + tT)_\sharp \nu_0$ and T denotes Brenier's optimal transport between ν_0 and ν_1.

Convexity along Wasserstein barycenters is stronger than McCann's displacement convexity (which as seen before corresponds to the case $p = 2$), it is a priori strictly stronger because there is no associativity of the barycenters (except in dimension 1 where the two notions therefore coincide).

Three *typical* examples:

- potential energy:

$$E(\nu) := \int_{\mathbf{R}^d} V(x) d\nu(x)$$

- interaction energy

$$E(\nu) := \int_{\mathbf{R}^d \times \mathbf{R}^d} W(x-y) d\nu(x) d\nu(y)$$

- internal energy:

$$E(\nu) := \int_{\mathbf{R}^d} \Phi(\nu(x)) dx$$

Potential energies

$$E(\nu) := \int_{\mathbf{R}^d} V(x) d\nu(x)$$

if the potential V is convex then E is convex along Wasserstein barycenters. Indeed, recall that

$$\mathrm{bar}(\nu_i, \lambda_i) = (\sum_{i=1}^{p} \lambda_i T_i^1)_{\sharp} \nu_1$$

where T_i^1 is the Gangbo-Święch transport between ν_1 and ν_i.

We thus have

$$E(\mathrm{bar}(\nu_i,\lambda_i)) = \int_{\mathbf{R}^d} V(\sum_{i=1}^{p} \lambda_i T_i^1(x))d\nu_1(x)$$
$$\leq \int_{\mathbf{R}^d} \sum_i \lambda_i V(T_i^1(x))d\nu_1(x)$$
$$= \sum_i \lambda_i \int_{\mathbf{R}^d} V(x)d\nu_i(x) = \sum_i \lambda_i E(\nu_i).$$

Interaction energies

$$E(\nu) := \int_{\mathbf{R}^d} W(x-y)d\nu(x)d\nu(y)$$

if the interaction potential W is convex then E is convex along Wasserstein barycenters. Indeed, using again the expression of the barycenter by the Gangbo-Święch transports, we have by convexity of W:

$$\begin{aligned} E(\mathrm{bar}(\nu_i,\lambda_i)) &= \int_{\mathbf{R}^d\times\mathbf{R}^d} W(\sum_{i=1}^{p}\lambda_i(T_i^1(x)-T_i^1(y)))d\nu_1(x)d\nu_1(y) \\ &\leq \int_{\mathbf{R}^d\times\mathbf{R}^d} \sum_i \lambda_i W(T_i^1(x)-T_i^1(y))d\nu_1(x)d\nu_1(y) \\ &= \sum_i \lambda_i \int_{\mathbf{R}^d\times\mathbf{R}^d} W(x-y)d\nu_i(x)d\nu_i(y) = \sum_i \lambda_i E(\nu_i). \end{aligned}$$

Internal energies

The case of the internal energy

$$E(\nu) := \int_{\mathbf{R}^d} \Phi(\nu(x))dx$$

is more involved (note that in the previous examples we haven't any structural assumptions on the Gangbo-Święch transports). Mc Cann proved that if $\Phi(0) = 0$ and $\nu \mapsto \nu^d \Phi(\nu^{-d})$ is convex nonincreasing on $(0, +\infty)$ then the corresponding internal energy is displacement convex. Let us prove that this condition is in fact also sufficicient for convexity along Wasserstein barycenters.

Set $\nu := \text{bar}(\nu_i, \lambda_i)$ and write ν in the form

$$\nu = (\sum_i \lambda_i \nabla u_i^* \circ \nabla u_1)\sharp\nu_1 = (\sum_i \lambda_i \nabla u_i^*)\sharp\mu$$

where $\mu := \nabla u_1 \sharp \nu_1$ and recall that each u_i^* is convex and that $\nabla u_i^* \sharp \mu = \nu_i$. Also define $T := \sum_i \lambda_i \nabla u_i^*$, T has a symmetric and semi-definite positive Jacobian matrix and satisfies the Jacobian equation

$$\det(DT)\nu(T) = \mu$$

Performing the change of variables $y = T(x)$, we thus have

$$\begin{aligned} E(\nu) &= \int_{\mathbf{R}^d} \Phi(\nu(y))dy \\ &= \int_{\mathbf{R}^d} \Phi(\nu(T(x))\det(DT(x))dx \\ &= \int_{\mathbf{R}^d} \Phi\Big(\frac{\mu(x)}{\det(DT(x))}\Big)\det(DT(x))dx \\ &= \int_{\mathbf{R}^d} \Psi_x((\det DT(x))^{1/d})dx \end{aligned}$$

where $\Psi_x(\alpha) := \alpha^d \Phi(\mu(x)\alpha^{-d})$ (it is convex and nonincreasing by McCann's condition).

Next using $DT = \sum \lambda_i D^2 u_i^*$ and the concavity of $S \mapsto \det(S)^{1/d}$ over the cone of symmetric positive semi-definite matrices, we have

$$\det(DT)^{1/d} \geq \sum \lambda_i \det(D^2 u_i^*)^{1/d}$$

and thus since Ψ_x is nonincreasing and convex

$$\begin{aligned}\Psi_x(\det DT(x)^{1/d}) &\leq \sum \lambda_i \Psi_x((\det D^2 u_i^*(x))^{1/d}) \\ &= \sum \lambda_i \Phi\Big(\frac{\mu(x)}{\det(D^2 u_i^*(x))}\Big) \det D^2 u_i^*(x).\end{aligned}$$

Using the fact that $\nabla u_i^* \sharp \mu = \nu_i$, this finally gives

$$E(\nu) \leq \sum \lambda_i \int_{\mathbf{R}^d} \Phi\Big(\frac{\mu(x)}{\det(D^2 u_i^*(x))}\Big) \det D^2 u_i^*(x) dx$$
$$= \sum \lambda_i \int_{\mathbf{R}^d} \Phi(\nu_i(x)) dx = \sum \lambda_i E(\nu_i)$$

which is the desired convexity estimate. McCann's condition is therefore sufficient for convexity along Wasserstein barycenters of internal energy functionals.

This is useful to obtain integrability estimates for the barycenter. Since for $q > 1$, $\Phi(\nu) = \nu^q$ satisfy Mc Cann's condition we have

$$\int_{\mathbf{R}^d} (\mathrm{bar}(\nu_i, \lambda_i)^q \leq \sum \lambda_i \int_{\mathbf{R}^d} \nu_i^q$$

and taking the $1/q$ power and letting $q \to \infty$, we get

$$\|(\mathrm{bar}(\nu_i, \lambda_i)\|_{L^\infty} \leq \max_i (\|\nu_i\|_{L^\infty}).$$

Another relevant example is when $\Phi(\nu) = \nu \log(\nu)$ in this case if all the ν_i's have finite entropy then so does their barycenter (with an estimate).

It is mainly an open problem to find displacement convex functionals that do not belong to the three classes considered above (for instance functionals depending on derivatives of ν or on solutions of PDE's where ν is a parameter). We therefore do not have here any explicit example of a functional that is displacement convex but not convex along Wasserstein barycenters. This seems difficult to find such an example but this issue deserves in my opinion to be better investigated.

Concluding remarks

Starting from an economic matching problem we have proposed a notion of Wasserstein barycenter. We have established existence, uniqueness and regularity of such barycenters and related them with the quadratic multi marginals optimal problem. We have also considered simple examples and extended the notion of displacement convexity to barycenters and shown that they roughly coincide on large classes of functionals. Still, there remains a lot to do in the analysis of the barycenters and more generally on optimal transport problems with several marginals. Many open questions, let me list a few.

Geometric and global approaches

Given finitely many probability measures, is there an intrinsic characterization of their (Wasserstein) convex hull? Does it solve an abstract minimal surface or harmonic extension problem? This is maybe a starting point to investigate some Sobolev spaces of measure valued maps or PDE's for measure-valued maps...

Similarly can one give a characterization of the potentials e.g. in terms of multi-time Hamilton-Jacobi equations? Seems difficult because of commutation properties.

What can be extended to the case of a Riemannian manifold?

Regularity/qualitative properties

We have seen that the support of the barycenter is included in the corresponding convex combination of the supports of the vertices, when is the converse true? When is the support of the barycenter convex?

This seems very likely that the barycenter of smooth and positive measures is smooth and positive as well but not so straightforward to prove....

Another regularity issues concerns the regularity of the Gangbo-Święch transports: if we had estimates from below on the density of the barycenter or information on the convexity of its support then Caffarelli's theory would apply. The picture is however more complicated here since one has to solve a system of Monge-Ampère equations.

Numerical computation of the barycenter

I haven't addressed this issue but this is probably what is really missing. The LP approach seems inadequate because of the size of the problem, interior points seem to be more promising but still extremely costly, efficient methods probably have to combine interior points and MCMC.