NUMERICAL OPTIMAL TRANSPORT AND GEOMETRY

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CONTENTS

Part 1. **Optimal transport theory and duality**

1. Primal problem

1.1. **Monge problem.** The first optimal transport problem was stated by Gaspard Monge, a French engineer and mathematician in 1784, in his famous thesis *"Mémoire sur la théorie des déblais et des remblais"* [7].

Framework:

- We consider two compact sets X and Y of $\mathbb{R}^d$.
- μ and ν probablility measures on X and Y.
- $c : X \times Y \to \mathbb{R}$ a cost function which is continuous.

Monge problem amounts to finding a map that transports X to Y, while minimizing the cost of transport and while preserving the measure. We first need to define what it means to preserve the measure and define the notion of push-forward.

Definition 1 (Pushforward). Let $T : X \to Y$ be a map, μ a measure on X. The pushforward of μ by T is a measure on Y, denoted by $T\sharp\mu$ defined for every Borelien B on Y by

$$T\sharp\mu(B) = \mu(T^{-1}(B)).$$

Definition 2 (Transport map). A $T : X \to Y$ is said to be a transport map between (X, μ) and (Y, ν) if it preserves the mass, namely if one has $T\sharp\mu = \nu$.

Monge problem (1780)**.** Monge problem consists in finding the minimum of

$$(\mathrm{MP}) := \inf_T \int_X c(x, T(x))d\mu(x),$$

over the set of measurable maps $T : X \to Y$ satisfying $T\sharp\mu = \nu$.

Remark that we need the two measures to have the same global mass, since we want the preservation of measure.

Example 1 (Continuous setting). By continuous setting, we mean the case where $\mu(x) = f(x)dx$ and $\nu(x) = g(x)dx$ are two absolutely continuous mesures on $\mathbb{R}^d$, with densities f

and g. In this case, if we assume that T is a smooth bijection, the fact of being a transport map to solving the following jacobian equation:

$$f(x) = g(T(x))|\det(DT(x))|,$$

where $DT(x)$ is the Jacobian matrix of T at x.

Proof. The proof is a direct consequence of the change of variable formula. When $T : X \to Y$ is a diffeomorphism, the change of variable formula reads for every Borelian $B \subset X$

$$\nu(B) := \int_B g(y)\mathrm{d}y = \int_{A=T^{-1}(B)} g(T(x))\Big|\det(DT(x))\Big|\mathrm{d}x.$$

Therefore, one has

$$\nu(B) = \mu(T^{-1}(B)) \quad \Leftrightarrow \quad \int_{T^{-1}(B)} g(T(x))|\det(DT(x))|\mathrm{d}x = \int_{T^{-1}(B)} f(x)\mathrm{d}x.$$

$\square$

Example 2 (Discrete setting). In the discrete setting $X = \{x_1, \cdots, x_n\}$ and $Y = \{y_1, \cdots, y_m\}$. We consider tow probability measures $\mu = \sum_{x \in X} \mu_x \delta_x$ and $\nu = \sum_{y \in Y} \nu_y \delta_y$. In this case, the problem amounts to finding a map $T : X \to Y$ that minimizes

$$\sum_{x \in X} c(x, T(x))\mu_x,$$

under the mass preservation constraint constraint

$$\forall y \in Y \; \nu_y = \sum_{x \in T^{-1}(y)} \mu_x.$$

Uniform case. In the particular case where the two sets have the same cardinal ($m = n$), and the two probability measures are uniform ($\mu_x = \nu_y = 1/n$), the mass conservation constraint enforces T to be a one-to-one map. Therefore, the Monge problem amounts to finding a one-to-one map $T : X \to Y$ that minimizes

$$\sum_{x \in X} c(x, T(x)).$$

Example 3 (Semi-discrete setting). In the semi-discrete setting, we suppose that the source is continuous and the target discrete. More precisely, we assume $X \subset \mathbb{R}^d$ is a compact set (it can be more general), that $\mu(x) = \rho(x)\mathrm{d}x$ is an absolutely continuous measure with respect to the Lebesgue measure. The set $Y = \{y_1, \cdots y_m\}$ is discrete with a measure $\nu = \sum_y \delta_y \nu_y$. A map $T : X \to Y$ is a transport map if one has

$$T\sharp\mu = \nu \quad \iff \quad \forall y \in Y, \; \nu_y = \mu(T^{-1}(y)).$$

The Monge problem in that case reads

$$\inf_T \sum_i \int_{T^{-1}(y)} c(x, y) \, \rho(x)\mathrm{d}x \; \text{ under the constraint } T\sharp\mu = \nu.$$

Example of bakeries in a town. Let X be a town and ρ be the density of population. Let $Y = \{y_1, \cdots, y_m\}$ be a set of bakeries. Each bakery has an amount of bread ν_i. We assume that the total amount of bread $\nu(Y)$ is equal to the quantity of bread needed by the whole population $\mu(X)$. We denote by $c(x, y)$ the distance to go to a bakery y. The problem is to affect globally the people depending on their location x to bakeries y_i such that the sets of trajectories is minimized. This corresponds to exactly solve the Monge problem.
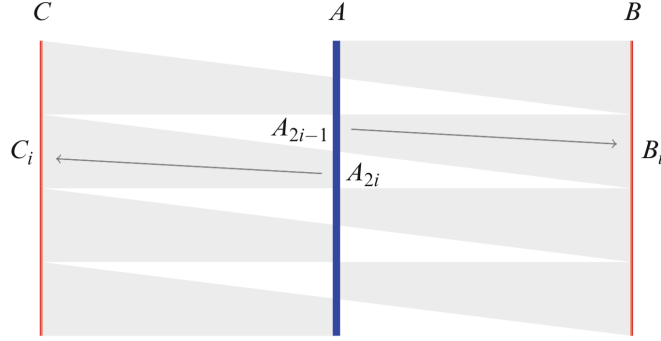
FIGURE 1. Counter-example: $X = [0, 1] \times \{0\}$; $\mu = \mathcal{H}^1_{|X}$; $Y = [0, 1] \times \{-1\} \cup [0, 1] \times \{1\}$ and $\nu = \mathcal{H}^1_{|Y}/2$ and quadratic cost: no optimal transport map exist.

No existence of transport map.
− Example 1: discrete uniform measures where $|X| = 4$ and $|Y| = 3$: no transport map.
− Example 2: if μ has an atom and ν is absolutely continuous : no transport map

No existence of optimal transport map (when transport maps exist).
− Example 3: $X = [0, 1] \times \{0\}$; $\mu = \mathcal{H}^1_{|X}$; $Y = [0, 1] \times \{-1\} \cup [0, 1] \times \{1\}$ and $\nu = \mathcal{H}^1_{|Y}/2$ and quadratic cost: no optimal transport map exist. Indeed:

Proof. **1)** The minimum cost is more than 1.
Indeed, for every $x, y \in X \times Y$ $c(x, y) \geqslant 1$, so for every map $T : X \to Y$

$$\int_X c(x, T(x)) \mathrm{d}\mu(x) \geqslant \int_X \mathrm{d}\mu(x) = \mathcal{H}^1(X) = 1.$$

2) The infimum is equal to 1. We build $T_n : X \to Y$ by subdividing into intervals, $T_n \in \Gamma(\mu, \nu)$. One can show that for every x $c(x, T_n(x)) \to 0$ and so

$$\int_X c(x, T_n(x)) \mathrm{d}\mu(x) \to 1.$$

3) The infimum is not reached. Suppose there exists a solution $T : X \to Y$. Then almost everywhere $c(x, y) = 1$, so T maps horizontally. Define $Y^- = [0, 1] \times \{-1\}$, $Y^+ = [0, 1] \times \{1\}$, $X^- = T^{-1}(Y^-)$. Then by the conservation of mass, one has

$$\mathcal{H}^1(X^-) = \mu(X^-) = \mu(T^{-1}(Y^-)) = \nu(Y^-) = \frac{1}{2}.$$

We denote $\tilde{Y}$ the orthogonal projection of X^- onto Y^+. Then

$$\mathcal{H}^1(\tilde{Y}) = \mathcal{H}^1(X^-) = 1/2.$$

Also, since T is horizontal, $T^{-1}(\tilde{Y}) = \emptyset$ so that

$$\mu(T^{-1}(\tilde{Y})) = \mu(\emptyset) = 0 \neq \nu(\tilde{Y}) = \mathcal{H}^1(\tilde{Y})/2 = 1/4.$$

$\square$

In general, we need regularity assumptions on μ to get existence of optimal transport maps.

Non linearity. The Monge problem is obviously non linear.

We will see that when we relax this problem, it becomes linear and we have existence of a solution under mild assumptions. (For instance, in the above example, if we allow for instance to split the mass, then there exists a solution.)

1.2. Kantorovitch relaxation.

Definition 3 (Marginals). The *marginals* of a measure γ on a product space $X \times Y$ are the measures $\Pi_{X\#}\gamma$ and $\Pi_{Y\#}\gamma$, where $\Pi_X : X \times Y \to X$ and $\Pi_Y : X \times Y \to Y$ are their projection maps.

Definition 4 (Transport plan). A transport plan between two probability measures μ, ν on two metric spaces X and Y is a probability measure γ on the product space $X \times Y$ whose marginals are μ and ν. The space of transport plans is denoted $\Gamma(\mu, \nu)$, i.e.

$$\Gamma(\mu, \nu) = \{\gamma \in \mathcal{P}(X \times Y) \mid \Pi_{X\#}\gamma = \mu, \ \Pi_{Y\#}\gamma = \nu\}.$$

Remark 1.
− The conditions on the marginals means :

$$\mu(A) = \Pi_{X\#}\gamma(A) = \gamma(\Pi_X^{-1}(A)) = \gamma(A \times Y).$$

$$\nu(B) = \gamma(X \times B).$$

− Note that $\Gamma(\mu, \nu)$ is a convex set.
− Note that the set of transport plans $\Gamma(\mu, \nu)$ is never empty, as it contains the measure $\mu \otimes \nu$.

Definition 5 (Kantorovich's problem). Consider two compact metric spaces X, Y, two probability measures $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$ and a *cost function* $c \in \mathcal{C}^0(X \times Y)$. *Kantorovich's problem* is the following optimization problem

$$(1.1) \qquad (\mathrm{KP}) := \inf\left\{\int_{X\times Y} c(x,y)\mathrm{d}\gamma(x,y) \mid \gamma \in \Gamma(\mu, \nu)\right\}$$

Remark 2. The infimum in Kantorovich's problem is less than the infimum in Monge's problem:

$$(\mathrm{KP}) \leqslant (\mathrm{MP}).$$

Indeed, for T be a transport map between μ and ν.
− we have the map $(\mathrm{id}, T) : X \to X \times Y$
− we put $\gamma_T = (\mathrm{id}, T)_{\#}\mu$. One can easily check that $\Pi_{X\#}\gamma_T = \mu$ and $\Pi_{Y\#}\gamma_T = \nu$ so that $\gamma_T \in \Gamma(\mu, \nu)$ is a transport plan between μ and ν.

$$\Pi_{X\#}\gamma_T(A) = \gamma_T(A \times Y) = \mu((\mathrm{id}, T)^{-1}(A \times Y)) = \mu(A \cap T^{-1}(Y)) = \mu(A)$$

− Moreover, by the definition of push-forward,

$$\int_{X\times Y} c(x,y)\mathrm{d}\gamma_T(x,y) = \int_X (c \circ (\mathrm{id}, T))(x)\mathrm{d}\mu(x) \int_X c(x, T(x))\mathrm{d}\mu(x)$$

thus showing that $(\mathrm{KP}) \leqslant (\mathrm{MP})$.

Proposition 1. *Kantorovich's problem* (KP) *admits a minimizer.*

Proof.

1) $\mathcal{P}(X \times Y)$ is weakly compact (it is known by Banach-Alaoglu).

Indeed, Banach-Alaoglu tells that if E is a topological vector space, E' its dual, then any bounded subset $B' \subset E'$ is compact for the weak topology. By definition, $L_n \in E'$ converges weakly to L if it simply converges.

In our case, the set of measures $\mathcal{M}(X \times Y)$ is identified to $\mathcal{C}^0(X \times Y)'$ (by Riesz theorem with $\gamma \mapsto (L_\gamma : \varphi \mapsto \int \varphi \mathrm{d}\gamma)$); $\mathcal{P}(X \times Y) \subset \mathcal{M}(X \times Y)$ is bounded (for $\|L_\gamma\| := \sup_\varphi L_\gamma(\varphi)$); So by Banach-Alaoglu, it is compact for the weak topology

2) The set of transport plans $\Gamma(\mu, \nu) \subseteq \mathcal{P}(X \times Y)$ is weakly closed, so weakly compact.

Indeed, the definition of $\Pi_{X\#}\gamma = \mu$ can be expanded into

$$\varphi \in \mathcal{C}^0(X), \int_{X \times Y} \varphi(x)\mathrm{d}\gamma(x, y) = \int_X \varphi(x)\mathrm{d}\mu(x).$$

Take a sequence $\gamma_n \in \Gamma(\mu, \nu)$ converging (for the weak topology) to $\gamma \in \mathcal{P}(X \times Y)$ which is weakly compact. Then by the previous equation

$$\forall \varphi \in \mathcal{C}^0(X), \int_{X \times Y} \varphi(x)\mathrm{d}\gamma_n(x, y) = \int_X \varphi(x)\mathrm{d}\mu(x)$$

is constant so converges to the same value. Therefore $\Pi_{X\#}\gamma = \mu$. Therefore $\gamma \in \Gamma(\mu, \nu)$. Hence $\Gamma(\mu, \nu)$ is weakly closed

3) We conclude the existence proof by remarking that the functional that is minimized in (KP), namely

$$F : \gamma \in \Gamma(\mu, \nu) \mapsto \int c(x, y)\mathrm{d}\gamma(x, y),$$

is weakly continuous by definition (for every $\gamma_n \to \gamma$ in a weak sense, then $F(\gamma_n) \to F(\gamma)$ by definition). □

2. DISCRETE CASE

In this section, I am going to give and prove the results in the discrete case. The framework is much simpler and gives a nice intuition of what happens.

2.1. **Kantorovitch relaxation.** We consider two probability measures μ and ν supported on two finite sets X and Y: $\mu = \sum_{x \in X} \mu_x \delta_x$ and $\nu = \sum_{y \in Y} \nu_y \delta_y$. One is also given a cost function, namely a map $c : X \times Y \to \mathbb{R}$. The idea of the relaxation is to allow the mass at a location x to be split. More precisely, we allow μ_x to be sent to several y, each μ_y receiving a quantity $\gamma_{x,y}$. The relaxation of the optimal transport problem then mounts to finding

$$\min_\gamma \sum_{x \in X, y \in Y} c(x, y)\gamma_{xy},$$

where $\gamma : X \times Y \to \mathbb{R}^+$ is such that

$$\forall x \in X \sum_{y \in Y} \gamma_{xy} = \nu_x \quad \text{and} \quad \forall y \in Y \sum_{x \in X} \gamma_{xy} = \mu_y.$$

We assume $\mu_x > 0$ and $\nu_y > 0$ for every x, y.

Remark 3.

- Note that in this problem, the function to be minimized is linear (in γ) and that the constraints are also linear. This is called a linear program.

Matrix notation. Since the problem is linear, we can express it with matrices. We denote $X = \{x_1, \cdots, x_n\}$, $Y = \{y_1, \cdots, y_m\}$ and

$$P = \begin{pmatrix} P_{1,1} & \cdots & P_{1,m} \\ \vdots & & \\ P_{n,1} & \cdots & P_{n,m} \end{pmatrix} \quad \mathbf{1}_m = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \quad \mu = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_n \end{pmatrix} \quad \nu = \begin{pmatrix} \nu_1 \\ \vdots \\ \nu_m \end{pmatrix}$$

We denote by $\langle A|B \rangle$ the scalar product between two matrices A and B (if we see the matrices as vectors of size nm). With these notations, the problem reads

$$\min_{P \in \Gamma(\mu,\nu)} \langle P|C \rangle,$$

where $\Gamma(\mu, \nu)$ is the set of transport plans between μ and ν given by

$$\Gamma(\mu, \nu) := \{P \geqslant 0, \quad P\mathbf{1}_m = \mu \quad \text{and} \quad P^t \mathbf{1}_n = \nu\}.$$

Economic interpretation (Mines and factories). A natural problem that illustrates the Kantorovitch relaxation is the following well known ressource allocation problem. We consider an operator that runs a set of warehouses and of fctories. Here
$X = \{x_1, \cdots, x_n\}$ is a <u>set of warehouses</u>
$Y = \{y_1, \cdots, y_m\}$ is a <u>set of factories</u>.
The factories y_j need a certain amount ν_j of a material. All the warehouse x_i have an amount μ_i of this material.
The <u>cost of transport to move a unity of material between x_i to y_i is given by $C_{i,j} = c(x_i, y_j)$.</u>
Hence the cost to transport a quantity $\gamma_{i,j}$ between x_i and y_j is exactly $\gamma_{i,j} c_{i,j}$. The total cost of transporting the material for the operator is thus exactly $\langle \mathcal{P}|C \rangle$ and the operator wants to find the transport plan P that minimizes this quantity.

2.2. **Assignment problem: a particular case.**

Definition 6 (Assignment problem)**.** We assume X and Y have the same cardinal. The assignment problem amounts to finding a bijection $\sigma : X \to Y$ that minimizes

$$(\text{AP}) = \min_{\sigma:X \to Y} \sum_{x \in X} c(x, \sigma(x)).$$

<u>Assignment problem = Monge problem</u> : if we take μ and ν to be uniform measures (i.e. $\mu_x = \nu_y = \frac{1}{n}$) and $T : X \to Y$. Then we remark that T is a bijection iff T is a transport map.

$$(\text{AP}) = (\text{MP})$$

Definition 7. A bistochastic matrix γ is a square matrix with coefficients in $[0, 1]$ such that the sum of each raw and of each columns equals 1.

Clearly, if $\gamma : X \to Y$ is a transport plan between two uniform probability measures, then $n\gamma$ is a represented by bistochastic matrix.

Theorem 2 (Birkoff)**.** *The set of bistochatic matrices is a convex polytope in the space of matrices of dimensions $n \times n$, whose extremal points are exactly permutation matrices.*

As a direct corollary, one has

> **Corollary 3.** *The Kantorovitch transport problem is equivalent to an assignment problem*
> $$(AP) = (MP) = (KP)$$

Proof. We minimize a linear function on a convex set. The minimum is not unique, but there always exists a minimum that is an extremal point (make a drawing). $\square$

This means that there exists a bijection that solves the Kantorovitch problem. In other words, that there always exists a Monge solution to the Kantorovitch problem. However, there is no uniqueness in general, and all solution are not maps.

2.3. **Formal derivation of Kantorovitch duality.**
This kind of derivation is classical and is using the Lagrangian. The Lagragian associated to the Kantorovitch relaxation is given by

$$L(\varphi, \psi) := \sum_{x \in X, y \in Y} c(x,y)\gamma_{xy} + \sum_{x \in X} \left(\mu_x - \sum_{y \in Y} \gamma_{x,y} \right) \varphi(x) - \sum_{y \in Y} \left(\nu_y - \sum_{x \in X} \gamma_{x,y} \right) \psi(y)$$

Step 1. Remark that

$$\sup_{\varphi, \psi} L(\varphi, \psi) = \begin{cases} \sum_{x \in X, y \in Y} c(x,y)\gamma_{xy} & \text{if } \gamma \text{ is a transport plan} \\ +\infty & \text{otherwise} \end{cases}$$

Indeed, if one of the constraint is not satisfied, then by choosing appropriately φ and ψ, the supremum is infinite. We deduce from this that

$$(KP) = \inf_{\gamma \in \Gamma(\mu,\nu)} \sum_{x \in X, y \in Y} c(x,y)\gamma_{xy} = \inf_{\gamma \geqslant 0} \sup_{\varphi, \psi} L(\varphi, \psi)$$

Step 2. We admit here that we can exchanging the inf and sup. In fact, this a consequence of *Fenchel-Rockafellar theorem* (as in the book of Villani for instance) or the proof can be done with the Karush-Kuhn-Tucken Theorem. Therefore one gets

$$(KP) = \sup_{\varphi, \psi} \inf_{\gamma \geqslant 0} L(\varphi, \psi)$$

Step 3. Remark that

$$L(\varphi, \psi) = \sum_{x \in X, y \in Y} c(x,y)\gamma_{xy} + \sum_{x \in X} \mu_x \varphi(x) - \sum_{y \in Y} \nu_y \psi(y) + \sum_{x \in X, y \in Y} (\psi(y) - \varphi(x))\gamma_{x,y}$$

$$= \sum_{x \in X, y \in Y} (c(x,y) - \varphi(x) + \psi(y)) \gamma_{xy} + \sum_{x \in X} \mu_x \varphi(x) - \sum_{y \in Y} \nu_y \psi(y).$$

By replacing these in the Lagrangian function one gets:

$$\begin{aligned} &(KP) \\ =\ & \sup_{\varphi, \psi} \inf_{\gamma \geqslant 0} L(\varphi, \psi) \\ =\ & \sup_{\varphi, \psi} \inf_{\gamma \geqslant 0} \sum_{x \in X, y \in Y} (c(x,y) - \varphi(x) + \psi(y)) \gamma_{xy} + \sum_{x \in X} \mu_x \varphi(x) - \sum_{y \in Y} \nu_y \psi(y) \\ =\ & \sup_{\varphi - \psi \leqslant c} \sum_{x \in X} \mu_x \varphi(x) - \sum_{y \in Y} \nu_y \psi(y) \end{aligned}$$

Remark that in this equation the inf is equal to $-\infty$ if $c(x,y) - \varphi(x) + \psi(y) < 0$ for some x, y (and is equal to 0 otherwise). This enforces the constraint $\varphi(x) - \psi(y) \leqslant c(x,y)$. Hence one has

$$(KP) = \sup_{\varphi - \psi \leqslant c} \sum_{x \in X} \mu_x \varphi(x) - \sum_{y \in Y} \nu_y \psi(y).$$

We therefore have the following definition

Definition 8 (Kantorovitch dual)**.** The dual problem is given by

$$(DP) = \sup \varphi, \psi \sum_{x \in X} \varphi(x)\mu_x - \sum_{y \in Y} \psi(y)\nu_y,$$

where $\varphi : X \to R$ and $\psi : Y \to \mathbb{R}$ are function satisfying $\varphi(x) - \psi(y) \leqslant c(x, y)$.

2.4. **Strong duality.**

Proposition 4. *Weak duality holds.*

$$(KP) \geqslant (KD)$$

Proof. Let $\gamma \in \Gamma(\mu, \nu)$ and φ and ψ be such that $\varphi(x) - \psi(y) \leqslant c(x, y)$.

$$\sum_{x \in X, y \in Y} c(x, y)\gamma_{xy} \geqslant \sum_{x \in X, y \in Y} (\varphi(x) - \psi(y))\gamma_{xy}$$

$$= \sum_{x \in X} \varphi(x) \sum_{y \in Y} \gamma_{xy} - \sum_{y \in Y} \psi(y) \sum_{x \in X} \gamma_{xy}$$

$$= \sum_{x \in X} \varphi(x)\mu_x - \sum_{y \in Y} \psi(y)\nu_y$$

$\square$

We now need to define the notion of c-transform:

Definition 9 (c-Transform)**.** The c-transform of a function $\psi : Y \to \mathbb{R} \cup \{+\infty\}$ (resp. $\varphi : X \to \mathbb{R} \cup \{+\infty\}$) is defined as

$$(2.2) \qquad\qquad \psi^c : x \in X \mapsto \inf_{y \in Y} c(x, y) + \psi(y)$$

$$(2.3) \qquad\qquad \varphi^c : y \in Y \mapsto \sup_{x \in X} -c(x, y) + \varphi(x)$$

> **Theorem 5** (Kantorovitch duality)**.**
> - *Strong duality holds*
> $$(KP) = (KD)$$
> - *The dual problem is reached for a pair of functions (φ, ψ) that satisfies $\varphi = \psi^c$ and $\psi = \varphi^c$*

Economic interpretation (Mines and Factories). Let us consider again the example of Mines and factories. To understand the dual problem, one considers that the operator is outsourcing the transport to an external seller. The seller is in contact with each warehouse x_i and each factory y_j. For a given unity of material the vendor fixes a price of pickery φ_i to a warehouse and a price of delivery ψ_j to the factory.
The goal of the seller is obviously to maximize its profit $\langle \varphi | \mu \rangle + \langle \psi | \nu \rangle$.
The operator wants to be sure that the price of the seller is not too expensive. To do so, he should solve the optimal problem and compare it to the outcome of the seller. However it is too complicated, so he only does it for each delivery between x_i and y_j. He checks that the price of the seller $\varphi_i + \psi_j$ is less than what it costs to him $C_{i,j}$. So the operator adds a constraint $\varphi_i + \psi_j \leqslant C_{i,j}$, and we assume that the seller is aware of this constraint. So the goal of the seller is exactly to solve the dual problem.
We change put $\psi := -\psi$ and get the same result.

We now turn to the proof of the Kantorovitch duality.

Proposition 6. *Let $\gamma \in \Gamma(\mu, \nu)$ and let $(\varphi, \psi) \in \mathcal{C}^0(X) \times \mathcal{C}^0(Y)$ such that $\varphi(x) - \psi(y) \leqslant c(x, y)$. Then, the following statements are equivalent:*

- $\gamma_{xy} \neq 0 \Rightarrow \varphi(x) - \psi(y) = c(x, y)$
- γ *minimizes* (KP), (φ, ψ) *maximizes* (DP) *and* (KP) = (DP).

Proof. Assume that $\varphi \ominus \psi = c$ γ-a.e. Then,

$$(\text{KP}) \leqslant \sum_{x,y} c(x,y)\gamma_{x,y} = \sum_{x,y}(\varphi(x) - \psi(y))\gamma_{x,y} = \sum_x \varphi(x)\mu_x - \sum_y \psi(y)\nu_y \leqslant (\text{DP})$$

Since in addition (KP) $\geqslant$ (DP), all inequalities are equalities, which implies that (KP) = (DP), γ miminizes (KP) and (φ, ψ) maximizes (DP). Conversely, if (KP) = (DP), γ miminizes (KP) and (φ, ψ) maximizes (DP), then

$$\langle \varphi | \mu \rangle - \langle \psi | \nu \rangle = (\text{DP}) = (\text{KP}) = \langle c | \gamma \rangle \geqslant \langle \varphi \ominus \psi | \gamma \rangle = \langle \varphi | \mu \rangle - \langle \psi | \nu \rangle,$$

implying that $\varphi \ominus \psi = c$ γ a.e. $\qquad \square$

We first recall Karush-Kuhn-Tucken

Theorem 7 (KKT). *Let $f : \mathbb{R}^d \to \mathbb{R}$ be convexe $\mathcal{C}^1$, g_i and h_j be N affine constraints and $K = \{x \in \mathbb{R}^d, \ g_i(x) \leqslant 0 \ h_j(x) = 0\}$. Then x is a minimizer of f on K iff there exists Lagrange multipliers a_i and b_j such that*

$$\begin{cases} x \in K \\ -\nabla f(x) = \sum_i a_i \nabla g_i(x) + \sum_j b_j h_j(x) \\ a_i \geqslant 0 \\ a_i g_i(x) = 0. \end{cases}$$

Proof of Theorem 5. The primal problem is the linear programming problem

$$(\text{KP}) = \min\left\{ \sum_{i,j} \gamma_{ij} c(x_i, y_j) \mid \gamma_{ij} \geqslant 0, \sum_j \gamma_{ij} = \mu_i, \sum_i \gamma_{ij} = \nu_j \right\},$$

which admits a solution which we denote γ. By Karush-Kuhn-Tucker theorem, there exists Lagrange multipliers $(\varphi_i)_{1 \leqslant i \leqslant N}, (\psi_j)_{1 \leqslant j \leqslant M}$ and $(\pi_{ij})_{1 \leqslant i \leqslant N, 1 \leqslant j \leqslant M}$ such that

$$\begin{cases} \varphi_i - \psi_j - c(x_i, y_j) = \pi_{ij} \\ \gamma_{ij}\pi_{ij} = 0 \\ \pi_{ij} \leqslant 0 \end{cases}$$

In particular, $\varphi_i - \psi_j \leqslant c(x_i, y_j)$ with equality if $\gamma_{ij} > 0$. Now, define $\varphi(x_i) = \varphi_i$ and $\psi(y_j) = \psi_j$. Then one has $\varphi(x) - \psi(y) \leqslant c(x, y)$ with equality when $\gamma_{xy} \neq 0$, so that (KP) = (DP) by Proposition 6.

Step 2. Let $i \in \{1, \cdots, N\}$. Since $\mu_i = \sum_j \gamma_{ij} \neq 0$, there exists $j \in \{1, \dots, M\}$ such that $\gamma_{ij} > 0$. Using $\gamma_{ij}\pi_{ij} = 0$, we deduce that so that $\varphi_i - \psi_j = c(x_i, y_j)$, giving

$$\varphi(x_i) = c(x_i, y_j) + \psi_j = \min_{k \in \{1, \dots, N\}} c(x_i, y_k) + \psi_k = \psi^c(x_i)$$

Similarly, since $\nu_j \neq 0$, one also has the existence of i such that

$$\psi(y_j) = -c(x_i, y_j) + \varphi(x_i) = \max_{k \in \{1,\dots,N\}} -c(x_k, y_j) + \varphi(x_k) = \varphi^c(y_j)$$

$\square$

2.5. **Kantorovitch functional.** Since the dual problem is reached for a pair of functions (ψ^c, ψ), one introduces the Kantorovitch functional

Definition 10 (Kantorovitch functional)**.**

$$\mathcal{K}(\psi) := \sum_{x \in X} \min_{y \in Y}(c(x,y) + \psi(y))\mu_x - \sum_{y \in Y} \psi(y)\nu_y,$$

where $\psi : Y \to \mathbb{R}$ is any function.

Solving an optimal transport problem amounts to fining the maximum of the Kantorovitch functional $\mathcal{K}$.

$$(\text{KP}) = (\text{KD}) = \max_{\psi:Y \to \mathbb{R}} \mathcal{K}(\psi).$$

Remark 4 (Numerical interest)*.*
- (KP) amounts to minimize a function of N^2 variables with $2N$ constraints.
- (KD) amounts to maximize of function of $2N$ variables with N^2 constraints.
- There is no constraint in the maximization of $\mathcal{K}$ and N variables. However, the constraints are hidden in ψ^c.

3. Semi-discrete setting in the quadratic case

In the semi-discrete setting, we suppose that the source is continuous and the target discrete. More precisely, we assume $X \subset \mathbb{R}^d$ is a compact set (it can be more general), that $\mu(x) = \rho(x)\mathrm{d}x$ is an absolutely continuous measure with respect to the Lebesgue measure. The set $Y = \{y_1, \cdots y_m\}$ is discrete with a measure $\nu = \sum_i \delta_{y_i}\nu_i$. For convenience, we assume here that the cost is quadratic, namely $c(x,y) = \|x - y\|^2$, but the results hold in a more general setting.

3.1. **Monge problem.** We recall that the Monge problem reads

$$\min_T \sum_i \int_{T^{-1}(y_i)} c(x, y_i)\rho(x)\mathrm{d}x \quad \text{under the constraint } T\sharp\mu = \nu.$$

3.2. **Laguerre cells and transport maps.** To introduce the notions, let us use again the example of bakeries, but we motivate by looking at the interest of people. Suppose that all the bread prices $\psi(y_i)$ are the same. If someone leaves a location x, its interest is to go to the closest bakery, hence to look for the bakery $\operatorname{argmin}_i \|x - y_i\|^2$. This naturally decomposes the space X into Voronoi cells

$$\operatorname{Vor}(y_i) := \{x \in X, \ \|x - y_i\|^2 \leqslant \|x - y_j\|^2 \forall j\}.$$

The set of Voronoi cells is called a *Voronoi diagram.*

Proposition 8 (Reminder on Voronoi diagrams)**.**
- *The Voronoi diagram forms a partition of the space $\mathbb{R}^d$ almost everywhere.*
- *Each cell $\operatorname{Vor}(y_i)$ is a convex polyedron.*

In particular, the amount of people going to a bakery y_i is exactly $\mu(\mathrm{Vor}(y_i)) = \int_{\mathrm{Vor}(y_i)} \rho(x)\mathrm{d}x$. Unfortunately, there is no reason why this quantity is exactly equal to the bread capacity ν_i. If a bakery receives to many people, its interest is to increase the Bread price $\psi(y_i)$, and the interest of people leaving at a location x is to minimize the the cost of transport plus the cost of bread , hence to look for $\mathrm{argmin}_i \|x - y_i\|^2 + \psi(y_i)$. This naturally decomposes the space X into Laguerre cells

$$\mathrm{Lag}_{y_i}(\psi) := \{x \in X, \ \|x - y_i\|^2 + \psi_i \leqslant \|x - y_j\|^2 + \psi_j \forall j\}.$$

Proposition 9 (Reminder on Laguerre diagrams)**.**
- *The Laguerre diagram forms a partition of the space $\mathbb{R}^d$ almost everywhere.*
- *Each cell $\mathrm{Lag}_{y_i}(\psi)$ is a convex polyedron.*

We denote by $T_\psi : X \to Y$ the map that associates to a location $x \in \mathrm{Lag}_{y_i}(\psi)$ the most interesting bakery y_i.

Proposition 10.
- *The map T_ψ is defined almost everywhere on X.*
- *The map T_ψ is an optimal transport map between X and Y for the measures μ and $T_\psi \sharp \mu$.*

Proof.
− Clearly, T_ψ is defined, except at x that belong to two Laguerre cells.

$$
\begin{aligned}
x \in \mathrm{Lag}_{y_i}(\psi) \cap \mathrm{Lag}_{y_j}(\psi) &\iff \|x - y_i\|^2 + \psi_i = \|x - y_j\|^2 + \psi_j \\
&\iff 2\langle y_j - y_i | x \rangle = \psi_j - \psi_i + \|y_j\|^2 - \|y_i\|^2
\end{aligned}
$$

This set is an hyperplane, thus is of dimension $d - 1$, hence is negligible.

− By definition, T_ψ is a transport map for the measures μ and $T_\psi \sharp \mu$. Let us show that it is optimal. Let $T : X \to Y$ be any transport plan. Then by definition of the Laguerre cells

$$\forall x \in X \|x - T_\psi(x)\|^2 + \psi(T_\psi(x)) \leqslant \|x - T(x)\|^2 + \psi(T(x))$$

By integrating over, one has:

$$\int_X \|x - T_\psi(x)\|^2 + \psi(T_\psi(x))\mathrm{d}\mu(x) \leqslant \int_X \|x - T(x)\|^2 + \psi(T(x))\mathrm{d}\mu(x)$$

Since $T_\sharp \mu = \nu$, the change of variable formula gives

$$\int_X \psi(T_\psi(x))\mathrm{d}\mu(x) = \int_Y \psi(y)\mathrm{d}\nu(y).$$

This can also be done directly. Indeed

$$\int_X \psi(T_\psi(x))\mathrm{d}\mu(x) = \sum_{i=1}^n \int_{\mathrm{Lag}_{y_i}} \psi(y_i)\mathrm{d}\mu = \sum_{i=1}^n \psi(y_i)\mu(\mathrm{Lag}_{y_i}) = \sum_{i=1}^n \psi(y_i)\nu_i.$$

This is also true for the map T, so we get

$$\int_X \|x - T_\psi(x)\|^2 \mathrm{d}\mu(x) \leqslant \int_X \|x - T(x)\|^2 \mathrm{d}\mu(x).$$

which shows that T_ψ is optimal. $\square$

The optimal transport problem amounts to solve the reverse:

OT problem. Let (X, μ) and (Y, ν). The OT problem amounts to finding an optimal transport plan $T = T_\psi$ such that $T \sharp \mu = \nu$.

This is done in the following subsection.

3.3. **Dual formulation.**

The following theorem gives directly the concave formulation of the Kantorovitch duality. It ensures that any semi-discrete optimal transport problem admits such a solution. In other words, for any continuous probability measure $\mu(x) = \rho(x)\mathrm{d}x$ on X and any probability measures μ on Y there exists a function ψ on Y such that $T_{\psi\#}\mu = \nu$. The proof of this theorem was first given in [1] for the quadratic cost, but has been generalized to other costs [5].

Theorem 11. *Let $X \subset \mathbb{R}^d$ be a compact set, $\mu(x) = \rho(x)\mathrm{d}x$ an absolutely continuous measure whose density ρ is continuous, $\nu = \sum_i \delta_{y_i} \nu_i$ a probability measure on $Y = \{y_1, \cdots y_m\}$, and $c(x, y) = \|x - y\|^2$ the quadratic cost. Then, the function*

$$\mathcal{K}(\psi) := \int_X (\min_{y \in Y} c(x, y) + \psi(y))\rho(x)\mathrm{d}x - \sum_{y \in Y} \psi(y)\nu_y$$

(3.4)
$$= \sum_{y \in Y} \int_{\mathrm{Lag}_y(\psi)} (c(x, y) + \psi(y))\rho(x)\mathrm{d}x - \sum_{y \in Y} \psi(y)\nu_y$$

is concave, C^1-smooth, and its gradient is

(3.5)
$$\nabla \mathcal{K}(\psi) = \left(\mu(\mathrm{Lag}_{y_i}(\psi)) - \nu_i\right)_{1 \leqslant i \leqslant m}$$

This functional is also called the *Kantorovitch functional.*

Corollary 12. *The following statements are equivalent:*

(i) $\psi : Y \to \mathbb{R}$ is a global maximizer of $\mathcal{K}$;
(ii) T_ψ is an optimal transport map between ρ and ν ;
(iii) $T_{\psi\#}\mu = \nu$, or equivalently,

(MA)
$$\forall y_i \in Y, \ \mu(\mathrm{Lag}_Y^\psi(y_i)) = \nu_i$$

Proof. Since $\mathcal{K}$ is concave and C^1, one has

$$\begin{aligned}
\psi \text{ is a maximum} \quad &\Leftrightarrow \quad \nabla \mathcal{K}(\psi) = 0 \\
&\Leftrightarrow \quad \mu(\mathrm{Lag}_{y_i}(\psi)) = \nu_i \ \forall i \\
&\Leftrightarrow \quad T_{\psi\#}\mu = \nu \\
&\Leftrightarrow \quad T_\psi \text{ is an optimal transport map between } \mu \text{ and } \nu
\end{aligned}$$

$\square$

Remark 5. Note that both this functional and its gradient are invariant by addition of a constant.

$$\mathcal{K}(\psi + t\mathbf{1}_Y) = \mathcal{K}(\psi) \quad \text{and} \quad \nabla\mathcal{K}(\psi + t\mathbf{1}_Y) = \nabla\mathcal{K}(\psi)$$

The end of this subsection is devoted to the proof of this theorem. For that, we just need some ingredients of convex analysis.
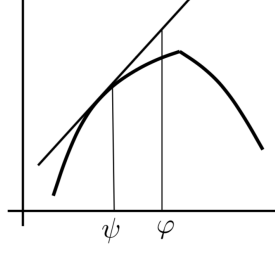
3.4. **Proof of Theorem 11.**

FIGURE 2. Concave functions:

Reminder of properties of concave functions.
- An infimum of linear functions is concave.
- A concave function is differentiable almost everywhere.
- The Supdifferentials of a function $\mathcal{K} : \mathbb{R}^d \to \mathbb{R}$ is defined by

$$\partial^+ \mathcal{K}(\psi) = \{v \in \mathbb{R}^d, \quad \mathcal{K}(\varphi) \leqslant \mathcal{K}(\psi) + \langle \varphi - \psi | v \rangle \quad \forall \varphi \in \mathbb{R}^d\}.$$

- The function $\mathcal{K}$ is concave iff

$$\forall \psi \in \mathbb{R}^d \ \partial^+ \mathcal{K}(\psi) \neq \emptyset.$$

- If $\mathcal{K}$ is differentiable at ψ iff $\partial^+ \mathcal{K}(\psi) = \{\nabla \mathcal{K}(\psi)\}$.
- ψ maximum of $\mathcal{K} \Leftrightarrow 0 \in \partial^+ \mathcal{K}(\psi)$
- The supergradient $\partial^+ \mathcal{K}(\varphi)$ of a concave function is characterized by [8, Theorem 25.6]

$$\partial^+ \mathcal{K}(\varphi) = \text{conv} \left\{ \lim_{n \to \infty} \nabla \mathcal{K}(\varphi_n) \mid (\varphi_n) \in S \right\},$$

where conv denotes the convex envelope and S the set of sequences (φ_n) converging to φ such that $\mathcal{K}$ is differentiable at φ_n.

Continuity of the area of Laguerre cells. We first denote by $G(\psi) := (\mu(\text{Lag}_{y_i}(\psi))_{1 \leqslant i \leqslant m}$ the area vector of the Laguerre cells.

Lemma 13. *The function $G : \mathbb{R}^m \to \mathbb{R}^m$ is continuous. More precisely, each $G_i : \mathbb{R}^m \to \mathbb{R}$ is L-Lipschitz with*

$$L = N \frac{\text{diam}(X)^{d-1} \text{Vol}(B_{d-1}(1)) \|\rho\|_\infty}{2 \inf_{i \neq j} \|y_i - y_j\|}.$$

Proof. Let us show the continuity of G_i. Let $\psi \in \mathbb{R}^m$ and $\varphi = \psi + e_j \varepsilon$ (we just change the jth coordinate). Then the symmetric difference $D := \text{Lag}_{y_i}(\psi) \Delta \text{Lag}_{y_i}(\varphi)$ lies in set delimited by two parallel hyperplanes. Let us bound its volume.

$$x \in \text{Lag}_{y_i}(\psi) \cap \text{Lag}_{y_j}(\psi) \quad \Rightarrow \quad 2\langle y_j - y_i | x \rangle = \psi_j - \psi_i + \|y_j\|^2 - \|y_i\|^2$$
$$x' \in \text{Lag}_{y_i}(\varphi) \cap \text{Lag}_{y_j}(\varphi) \quad \Rightarrow \quad 2\langle y_j - y_i | x' \rangle = \psi_j - \psi_i + \|y_j\|^2 - \|y_i\|^2 + \varepsilon$$

This implies that $2\langle y_j - y_i | x - x' \rangle = \varepsilon$ and that the distance δ between the two hyperplanes satisfies $\delta = \varepsilon/(2\|y_i - y_j\|)$, and then

$$\text{Vol}(D) \leqslant \frac{\varepsilon}{2\|y_i - y_j\|} \text{diam}(X)^{d-1} \text{Vol}(B_{d-1}(1)).$$

We then have

$$|G_i(\psi) - G_i(\psi + e_j\varepsilon)| \leqslant \frac{\mathrm{diam}(X)^{d-1}\mathrm{Vol}(B_{d-1}(1))\|\rho\|_\infty}{2\inf_{i\neq j}\|y_i - y_j\|}\varepsilon.$$

Doing the same thing with all the $j \in \{1, \cdots, m\}$, and using the triangular inequality wet get the same result for any ψ and the Lipschitz constant for G_i. $\square$

Proof of concavity. We consider the following function Ψ:

$$\Psi(\psi) := \sum_{y_i \in Y} \int_{\mathrm{Lag}_{y_i}(\psi)} (\|x - y_i\|^2 + \psi(y_i))d\mu(x).$$

For every map $T : X \to Y$, one has by definition of the Laguerre cells that

$$\Psi(\psi) \leqslant \Psi_T(\psi) := \int_{\mathbb{R}^2} (\|x - T(x)\|^2 + \psi(T(x)))d\mu(x).$$

Furthermore, the infimum is reached: $\Psi(\psi) = \Psi_{T_\psi}(\psi)$. Therefore Ψ_T is linear in ψ and that $\Psi(\psi) = \inf_{T:X\to Y} \Psi_T(\psi)$. The functional Ψ is thus a minimum of linear function, hence is concave and differentiable almost everywhere. Since $\mathcal{K}$ only defers from Ψ by a linear term, it is also concave and differentiable almost everywhere.

Proof of regularity and gradient. Note that at the point ψ one has $\Psi(\psi) = \Psi_{T_\psi}(\psi)$. Let now take any function $\varphi : Y \to \mathbb{R}$. From the previous inequality with $T = T_\varphi$, one gets

$$
\begin{aligned}
\Psi(\psi) \ & \leqslant \Psi_{T_\varphi}(\psi) \\
& = \int_{\mathbb{R}^2}(\|x - T_\varphi(x)\|^2 + \psi(T_\varphi(x)))d\mu(x) \\
& = \int_{\mathbb{R}^2}(\|x - T_\varphi(x)\|^2 + \varphi(T_\varphi(x)))d\mu(x) + \int_{\mathbb{R}^2}\psi(T_\varphi(x))) - \varphi(T_\varphi(x)))d\mu(x) \\
& = \Psi(\varphi) + \sum_{i=1}^n \int_{\mathrm{Lag}_{y_i}(\varphi)} \psi(y_i) - \varphi(y_i)d\mu(x) \\
& = \Psi(\varphi) + \sum_{i=1}^n G_i(\varphi)(\psi_i - \varphi_i) \\
& = \Psi(\varphi) + \langle G(\varphi)|\psi - \varphi\rangle
\end{aligned}
$$

Using the fact $\mathcal{K}(\psi) = \Psi(\psi) - \langle\psi|\nu\rangle$ and $\mathcal{K}(\varphi) = \Psi(\varphi) - \langle\varphi|\nu\rangle$, one gets

$$\mathcal{K}(\psi) \leqslant \mathcal{K}(\varphi) + \langle G(\varphi) - \mu|\psi - \varphi\rangle$$

This proves that the superdifferential $\partial^+\mathcal{K}(\varphi)$ of $\mathcal{K}$ at φ contains $G(\varphi) - \nu$, thus establishing again the concavity. By Lemma 13, the map G is continuous, meaning that we have constructed a continuous selection of a supergradient in the superdifferential of the concave function $\mathcal{K}$. Using standard arguments from convex analysis (mentioned above), this proves that

$$\partial^+\mathcal{K}(\varphi) = \mathrm{conv}\left\{\lim_{n\to\infty}\nabla\mathcal{K}(\varphi_n)\right\} = \mathrm{conv}\left\{\lim_{n\to\infty}G(\varphi_n) - \nu\right\} = \{G(\varphi) - \nu\}.$$

This proves that $\mathcal{K}$ is C^1, and that $\nabla\mathcal{K}(\varphi) = G(\varphi) - \nu$.

Remark 6. It could formally happen that the gradient of the concave function does not vanish (think of the concave function $x \mapsto -e^x$), but in any case this equivalence still holds.

4. GENERAL CASE

The goal here is just to give an overview that optimal transport can be stated in a more general setting. We consider here $X \subset \mathbb{R}^d$ and $Y \subset \mathbb{R}^{d'}$ two compact sets.

4.1. **Duality in the general case.**

> **Theorem 14.** *[Kantorovitch duality] Let μ and ν be two probability measures on two compact sets $X \subset \mathbb{R}^d$ and $Y = \mathbb{R}^{d'}$ and $c : X \times Y \to \mathbb{R}^+ \cup \{+\infty\}$ a continuous cost function. Then*
>
> $$\inf_{\gamma \in \Gamma(\mu,\nu)} \int_{X \times Y} c(x,y)\ d\gamma(x,y) = \sup_{(\varphi,\psi)} \int_X \varphi d\mu\ + \int_Y \psi d\nu,$$
>
> *where $(\varphi, \psi) \in C^0(X) \times C^0(Y)$ satisfies $\varphi(x) + \psi(y) \leqslant c(x, y)$.*

The existence of solutions is obtained in a very general framework. The solutions corresponds to pairs of c-concave functions that satisfy the dual problem.

4.2. **About c-concave functions.**

Definition 11 (c-transform)**.**
− The c-transform of a function $\varphi : X \to \mathbb{R}$ is the function $\varphi^c : Y \to \mathbb{R}$ defined by

$$\varphi^c(y) = \sup_{x \in X} -c(x, y) + \varphi(x).$$

− The c-transform of a function $\psi : Y \to \mathbb{R}$ is the function $\psi^c : X \to \mathbb{R}$ defined by

$$\psi^c(x) = \inf_{y \in Y} c(x, y) + \psi(y).$$

   This leads to the following definition

Definition 12.
− A function $\varphi : X \to \mathbb{R}$ is c-concave if there exists $\psi : Y \to \mathbb{R}$ such that $\varphi = \psi^c$.
− A function $\psi : Y \to \mathbb{R}$ is c-concave if there exists $\varphi : Y \to \mathbb{R}$ such that $\psi = \varphi^c$.

Proposition 15.

- $\varphi^{cc} \geqslant \varphi$
- $\varphi^{ccc} = \varphi^c$
- $\varphi^{cc} = \varphi$ iff φ is c-concave.

Definition 13 (c-superdifferential)**.**

- The *c-superdifferential* of a c-concave function φ is

$$\partial^c \varphi \ := \Big\{ (x, y) \in X \times Y, \quad \forall z \in X \quad \varphi(z) \leqslant \varphi(x) + [c(z, y) - c(x, y)] \Big\}$$

- The *c-superdifferential* of a c-concave function φ at x is

$$\partial^c \varphi(x) := \Big\{ y \in Y, \quad (x, y) \in \partial^c \varphi \Big\}$$

   These definitions are symmetric in X and Y.

4.3. **Relation between Kantorovitch dual and transport plan.** Dans un cas assez général, on a existence d'une solution qui s'exprime comme une paire de fonctions c-concaves. Par ailleurs, les plans de transport optimaux sont caractérisés par leur support ! Interestingly, the knowledge of a Kantorovitch function (also Kantorovitch potential) allows to recover (at least partially) transport plan. As in the discrete and semi-discrete setting, we define

Theorem 16. *Under the same assumptions of Theorem 14, we have*
- *A maximizer (φ, ψ) of the dual Kantorovitch problem is of the form (φ, φ^c) or (ψ^c, ψ).*
- *An optimal transport plan γ is supported on the set*

$$\{(x, y) \in X \times Y, \ \varphi(x) - \psi(y) = c(x, y)\}.$$

Support of a measure. We recall that the support of a measure μ is given by

$$\mathrm{spt}(\mu) := \bigcap \{A \subseteq X \mid A \text{ closed and } \mu(X \setminus A) = 0\}.$$

A point x belongs to $\mathrm{spt}(\mu)$ iff for every $r > 0$ one has $\mu(\mathbb{B}(x, r)) > 0$.

Remark 7. We consider the couple (φ, ψ) solution of the dual problem, with $\varphi(x) := \psi^c(x) = \min_{z \in Y}(c(x, z) + \psi(z))$ and the transport plan γ solution to the primal problem. According to Theorem 16,

$$
\begin{aligned}
(x, y) \text{ belongs to the support of } \gamma &\iff y \in \mathrm{argmin}_{z \in Y}(c(x, z) + \psi(z)) \\
&\iff (x, y) \in \partial^c \varphi \\
&\iff y \in \partial^c \varphi(x) \\
&\iff x \in \partial^c \psi(y)
\end{aligned}
$$

In the semi-discrete setting $T = \partial^c \varphi$ is to the optimal transport plan and $\partial^c \psi$ is the Laguerre cell.

4.4. **Brenier theorem in the quadratic case.**

Theorem 17 (Brenier theorem). *Let μ and ν be two probability measures on $\mathbb{R}^d$, $c(x, y) = \frac{1}{2}\|x - y\|^2$ and μ be absolutely continuous. Then*
- *There exists a unique (a.e.) measurable map $T : X \to Y$ such $T = \nabla f$ where $f : X \to \mathbb{R}$ is a convex function and $T \sharp \mu = \nu$.*
- *Such a map is the unique optimal transport map between μ and ν (and γ_T is the unique transport plan).*

Such a map is called a *Brenier map*. The initial Brenier result was assuming that both μ and ν had moments of order two finite. This results was refined later on by Mc Cann without that assumption.

Remark 8 (Monge Ampère equation). In the continuous setting (μ and ν are absolutely continuous), the fact of having a transport map corresponds to

$$g(T(x))|\det(DT(x))| = f(x).$$

The fact of having a map that is optimal gives $T = \nabla h$ which leads to

$$g(\nabla h(x))|\det(\nabla^2 h(x))| = f(x).$$

4.5. **Wasserstein distance.**
For this part, the best is probably to look at Filippo's book [9]. Let $X \subset \mathbb{R}^d$ be any $\underline{\text{compact set}}$, $p \in [1, +\infty[$. We define for any probability measure μ and ν on X

$$W_p(\mu, \nu) := \left(\inf_{\gamma \in \Gamma(\mu, \nu)} \int_{X \times X} \|x - y\|^p \mathrm{d}\gamma(x, y) \right)^{\frac{1}{p}}$$

Proposition 18. *For any $p > 0$, W_p is a distance on the set of probability measures.*

The notion of weak convergence is associated to a space of functions, usually the set of continuous functions $f : X \to \mathbb{R}$ that vanish at infinity and denoted $C^c(X)$. Since X is compact, we do not need such an assumption here.

Definition 14 (Weak convergence). A sequence of probability measures μ_n weakly converges to a probability measure μ, and we denote $\mu_n \rightharpoonup \mu$ if

$$\forall f :\in C^c(X) \quad \lim_{n \to \infty} \int_X f \mathrm{d}\mu_n = \int_X f \mathrm{d}\mu.$$

Proposition 19. *Let $X \subset \mathbb{R}^d$ be a compact set and $p \in [1, +\infty[$.*

$$\mu_n \rightharpoonup \mu \Leftrightarrow \lim_{n \to \infty} W_p(\mu_n, \mu) = 0.$$

4.6. **Mac Cann interpolation. Reminder on geodesics.**
Make a drawing with a surface, show the example of segments in the plane and great circles on spheres.

Proposition 20. *Let μ and ν be two probabilities measures on the compact set $X \subset \mathbb{R}^d$ and let $T : X \to Y$ be a transport map for the cost $c(x,y) = \|x - y\|^p$ ($p \in [0, +\infty[$). Then*

- *The probability measures $\mu_t = T_t \sharp \mu$ (with $t \in [0, 1]$) is a geodesic in the set of probability measures, where $T_t := (1 - t)Id + tT$.*
- *The map $T_t : X \to X$ is an optimal transport map for the cost c.*

Remark 9 (Discrete case). Let us look at the Mac Cann interpolation in the discrete setting for the quadratic cost. Here clearly, the mass is sent through segments that do not cross.

Remark 10 (Semi-discrete case). Let us look at the Mac Cann interpolation in the semi-discrete setting. Let $y_i \in Y$. We know that $\mathrm{Lag}_{y_i}(\psi) = T^{-1}(y_i)$. We get

$$T_t(\mathrm{Lag}_{y_i}) = \{(1 - t)x + ty_i, \ x \in \mathrm{Lag}_{y_i}(\psi)\}.$$

In practice, if we suppose in addition that ν is an absolutely continuous measure on X. We consider a point set $Y \subset X$ and choose to discretize ν by setting $\nu_y = \nu(\mathrm{Vor}_y)$. Therefore a Laguerre cell is transformed in a point y_i then spread into a Voronoi cell Vor_{y_i}. The underlying idea is therefore to directly go from the Laguerre cell to the Voronoi cell by interpolating the weights.

FIGURE 3. Mac Cann interpolation between Monge and Riemann

5. Gradient of Kantorovitch functional in the discrete case

Proposition 21. *Let X be a compact space, Y be finite, $c \in \mathcal{C}^0(X \times Y)$ and $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$. Then, for all $\psi_0 \in \mathbb{R}^Y$,*

$$(5.6) \qquad \partial^+ \mathcal{K}(\psi_0) = \{\Pi_{Y\#}\gamma - \nu \mid \gamma \in \Gamma_{\psi_0}(\mu)\} \quad \text{with} \quad \Pi_{X\#}\gamma = \Big(\sum_x \gamma_{x,y}\Big)_{y \in Y}$$

where $\Gamma_{\psi_0}(\mu)$ is the set of probability measures on $X \times Y$ with first marginal μ and supported on the c-subdifferential $\partial^c \psi_0$, i.e.

$$(5.7) \qquad \Gamma_{\psi_0}(\mu) = \{\gamma \in \mathcal{P}(X \times Y) \mid \Pi_{X\#}\gamma = \mu \text{ and } \mathrm{spt}(\gamma) \subseteq \partial^c \psi_0\}$$

Proof. Let $\gamma \in \Gamma_{\psi_0}(\mu)$. Then, for all $\psi \in \mathbb{R}^Y$,

$$\begin{aligned}
\mathcal{K}(\psi) &= \sum_x \psi^c(x)\mu_x - \sum_y \psi(y)\nu_y \\
&= \sum_{x,y} \psi^c(x)\gamma_{x,y} - \sum_y \psi(y)\nu_y \\
&\leqslant \sum_{x,y} c(x,y) + \psi(y)\gamma_{x,y} - \sum_y \psi(y)\nu_y,
\end{aligned}$$

where we used $\Pi_{X\#}\gamma = \mu$ to get the first equality and $\psi^c(x) \leqslant c(x,y) + \psi(y)$ to get the first inequality. Note also that <u>equality holds if $\psi = \psi_0$, by assumption on the support of γ</u>. Hence,

$$\begin{aligned}
\mathcal{K}(\psi) &\leqslant \mathcal{K}(\psi_0) + \sum_{x,y}(\psi(y) - \psi_0(y))\gamma_{x,y} - \sum_y (\psi(y) - \psi_0(y))\nu_y \\
&= \mathcal{K}(\psi_0) + \sum_y \Big(\sum_x \gamma_{x,y} - \nu_y\Big)(\psi(y) - \psi_0(y)) \\
&= \mathcal{K}(\psi_0) + \langle \Pi_{Y\#}\gamma - \nu | \psi - \psi_0 \rangle.
\end{aligned}$$

This implies by definition that $\Pi_{Y\#}\gamma - \nu$ lies in the superdifferential $\partial^+ \mathcal{K}(\psi_0)$, giving us the inclusion

$$D(\psi_0) := \{\Pi_{Y\#}\gamma - \nu \mid \gamma \in \Gamma_{\psi_0}(\mu)\} \subseteq \partial^+ \mathcal{K}(\psi_0).$$

Note also that the superdifferential of $\mathcal{K}$ is non-empty at any $\psi_0 \in \mathbb{R}^Y$, so that $\mathcal{K}$ is concave. As a concave function, $\mathcal{K}$ is differentiable almost everywhere and one has $\partial \mathcal{K}^+(\psi) = \{\nabla \mathcal{K}(\psi)\}$ at differentiability points.

We now show that $\partial \mathcal{K}^+(\psi_0) \subset D(\psi_0)$, using the characterization of the subdifferential recalled in the Appendix:

$$\partial \mathcal{K}^+(\psi_0) = \mathrm{conv}\Big\{\lim_{n\to\infty} \nabla \mathcal{K}(\psi^n) \mid (\psi^n)_{n\in\mathbb{N}} \in S\Big\},$$

where S is the set of sequences $(\psi^n)_{n\in\mathbb{N}}$ that converge to ψ_0, such that $\nabla \mathcal{K}(\psi^n)$ exist and admit a limit as $n \to +\infty$. Let $v = \lim_{n\to\infty} \nabla \mathcal{K}(\psi^n)$, where $(\psi^n)_{n\in\mathbb{N}}$ belongs to the set S. For every n, there exists $\gamma^n \in \Gamma_{\psi^n}(\mu)$ such that $\nabla \mathcal{K}(\psi^n) = v^n := \Pi_{Y\#}\gamma^n - \nu$. By compactness of $\mathcal{P}(X \times Y)$, one can assume (taking a subsequence if necessary) that γ^n weakly converges to some γ, and it is not difficult to check that $\gamma \in \Gamma_{\psi_0}(\mu)$, ensuring that the sequence v^n converges to some $v \in D(\psi_0)$. Thus,

$$\Big\{\lim_{n\to\infty} \nabla \mathcal{K}(\psi^n) \mid (\psi^n)_{n\in\mathbb{N}} \in S\Big\} \subseteq D(\psi_0).$$

Taking the convex hull and using the convexity of $D(\psi_0)$, we get $\partial^+ \mathcal{K}(\psi_0) \subseteq D(\psi_0)$ as desired. $\qquad\square$

As a corollary, we obtain an explicit expression for the left and right partial deriatives of $\mathcal{K}$, and a characterization of its differentiability. Using the terminology used in the semi-discrete setting, we will refer to the c-subdifferential at $y \in Y$ as *Laguerre cell associated to y* and we will denote it by $\mathrm{Lag}_y(\psi)$.

$$\mathrm{Lag}_y(\psi) := \{x \in X \mid \forall z \in Y, c(x,y) + \psi(y) \leqslant c(x,z) + \psi(z)\}.$$

We also need to introduce the *strict Laguerre cell* $\mathrm{SLag}_y(\psi)$:

$$\mathrm{SLag}_y(\psi) := \{x \in X \mid \forall z \in Y, c(x,y) + \psi(y) < c(x,z) + \psi(z)\}.$$

Corollary 22 (Directional derivatives of $\mathcal{K}$). *Let $\psi \in \mathbb{R}^Y$, $y \in Y$ and define $\kappa(t) = \mathcal{K}(\psi^t)$ where $\psi^t = \psi + t\mathbf{1}_y$. Then, κ is concave and*

$$\partial^+\kappa(t) = [\mu(\mathrm{SLag}_y(\psi^t)) - \nu_y, \mu(\mathrm{Lag}_y(\psi^t)) - \nu_y]$$

In particular $\mathcal{K}$ is differentiable at $\psi \in \mathbb{R}^Y$ iff $\mu(\mathrm{Lag}_y(\psi) \setminus \mathrm{SLag}_y(\psi))$ for all $y \in Y$, and in this case

$$\nabla\mathcal{K}(\psi) = \Big(\mu(\mathrm{Lag}_y(\psi)) - \nu_y\Big)_{y \in Y}.$$

Proof. Using Hahn-Banach's theorem, one can easily relate the super-differential of κ to the one of $\mathcal{K}$: $\partial^+\kappa(t) = \{\langle \pi | \mathbf{1}_y \rangle \mid \pi \in \partial^+\mathcal{K}(\psi^t)\}$. Combining with the previous proposition we get

$$\partial^+\kappa(t) = \{\langle \Pi_{X\#\gamma} - \nu | \mathbf{1}_y \rangle \mid \gamma \in \Gamma_{\psi^t}(\mu)\}$$

$$= \left\{\sum_x \gamma_{x,y} - \nu_y \mid \gamma \in \Gamma_{\psi^t}(\mu)\right\}$$

Let $\gamma \in \Gamma_{\psi^+}(\mu)$.

Step 1. We first remark that $x \in SLag_y(\psi^+)$ then $\gamma_{x,y} = \mu_x$.

$$\forall z \neq y \quad \gamma_{x,z} = 0$$

$$\Rightarrow \quad \gamma_{x,y} = \sum_z \gamma_{x,z} = \nu_x \quad \text{since } \Pi_\sharp \gamma = \mu.$$

We deduce that

$$\sum_{x \in SLag_y(\psi^+)} \gamma_{x,y} = \mu(SLag_y(\psi^+)).$$

Step 2. We also remark that $x \in Lag_y(\psi) \setminus SLag_y(\psi^+)$ then $\gamma_{x,y}$ can take any value in $[0, \mu_x]$. This implies that

$$\left\{\sum_x \gamma_{x,y} \mid \gamma \in \Gamma_{\psi^t}(\mu)\right\} = [0, \mu(Lag_y(\psi) \setminus SLag_y(\psi^+))].$$

Conclusion. We conclude since if $x \notin Lag_y(\psi)$, the $\gamma_{x,y} = 0$. $\square$

Part 2. **Numerical optimal transport**

6. Overview of some methods

Continuous methods I will not speak about these methods here.
- Benamou-Brenier algorithm
- stencil methods.

Discrete methods

- Linear programming methods: simplex method (cubic complexity),...
- Bertseka's auction algorithm (quite efficient, even costly) $\rightsquigarrow$ *Studied*
- Entropic regularization (simple algorithm, very efficient in some cases, solves an approximation of the result) $\rightsquigarrow$ *Studied*

Semi-discrete methods

- Oliker-Prussner algorithm : 1990's, analysis of convergence but slow (complexity cubic) $\rightsquigarrow$ *Studied*
- Quasi Newton (efficient, but no analyses)
- Damped newton algorithm (more recent, fast and certified) $\rightsquigarrow$ *Studied*

7. Auction algorithm for linear assignment method

The Bertsekas Auction's algorithm [3] is a primal dual method that allows to solve linear assignment problem <u>when the cost has integer values</u>. This algorithm remains one of the most performant for assignment problems. More precisely, its complexity is $O(N^3 C)$, where $C = \max c(x, y)$ and $N = |X| = |Y|$ [2]. There also exists a scaled version which is fast and well used in practice.

7.1. **Problem and its dual formulation.** We recall that the linear assignment problem amounts to finding a bijection $\gamma : X \to Y$ that minimizes

$$\min_{\gamma : X \to Y} \sum_{x \in X} c(x, \gamma(x)).$$

The idea of Auctions' algorithm is to use the dual formulation of the Kantorovitch functional

$$\mathcal{K}(\psi) := \frac{1}{N} \left(\sum_{x \in X} \min_{y \in Y} (c(x, y) + \psi(y)) - \sum_{y \in Y} \psi(y) \right).$$

We following proposition is just a recast of the Kantorovitch duality theorem.

Proposition 23. *The following statements are equivalent*

- *ψ is a global maximizer of the Kantorovitch functional $\mathcal{K}$*
- *There exists a bijection $\gamma : X \to Y$ that satisfies*

$$\forall x \in X \quad c(x, \gamma(x)) + \psi(\gamma(x)) = \min_{y \in Y} c(x, y) + \psi(y).$$

Moreover a bijection γ satisfying this last equation is a solution to the linear assignment problem.

The idea of Auction algorithm is to

(1) increase iteratively the weights $\psi(y)$ so as to reach a maximizer of $\mathcal{K}$. It is therefore a coordinate-wise ascent for $\mathcal{K}$. It is well known that in such a case, one can get stuck at points that are not maximizers. A local increment will allow to tackle this problem.

(2) Furthermore, the idea is to build an injective map $\gamma : S \subset X \to Y$ (*partial matching*) that will converge to a bijection.

7.2. Best bid (increase of price).

The idea is to modify the prices one after another in order to reach a maximum of the function $\mathcal{K}$. Remark that for a given $y \in Y$, when we increase its price $\psi(y)$, then its Laguerre cell reduces. Since we want a matching, we need its Laguerre cell to be non empty. We can increase $\mathcal{K}$ if we increase $\psi(y)$ without emptying the Laguerre cell. The best price is given by the following lemma [6].

Lemma 24. *Let $\psi : Y \to \mathbb{R}$ be a price function and $y \in Y$. We assume that the (discrete) Laguerre cell $\mathrm{Lag}_y(\psi) = \{x \in X, \ y \in \mathrm{argmin}_{z \in Y} \, c(x, z) + \psi(z)\}$ is not empty. Then the maximum of the function $t \to \mathcal{K}(\psi + t\mathbf{1}_y)$ is reached at*

$$p_y = \max\{bid_x, \ x \in \mathrm{Lag}_y(\psi)\}, \quad where \quad bid_x := \left(\min_{z \in Y \setminus y} c(x, z) + \psi(z) \right) - (c(x, y) + \psi(y)).$$

Economic interpretation. Assume that Y is a set of houses owned by one seller and X is a set of customers that want to buy a house. Let y_0 be a given house. The cost $c(x, y)$ represents the interest for x to have the house y (independently of its price). The customer x wants to minimize $c(x, y) + \psi(y)$. The seller wants to maximize his profit, hence to increase $\psi(y)$ as much as possible. Suppose that one customer x is already interested, meaning that $x \in \mathrm{Lag}_{y_0}(\psi)$. The second best house for x is $y_1 \in \mathrm{argmin}_{z \neq y_0}(c(x, z) + \psi(z))$. The difference of interest between the two houses is exactly bid_x. Since the seller wants only one customer, the best increase of price he can take is exactly p_{y_0}.

Proof of Lemma 24.
• We have $\mathrm{Lag}_y(\psi) \neq \emptyset$. When we increase a price $\psi(y)$, the its Laguerre cell $\mathrm{Lag}_y(\psi)$ decreases. More precisely one has for $t > 0$ $\mathrm{Lag}_y(\psi + t\mathbf{1}_y) \subset \mathrm{Lag}_y(\psi)$.
• Remark also that for $x \in \mathrm{Lag}_y(\psi)$, one has

$$\begin{aligned}
x \in \mathrm{Lag}_y(\psi + t\mathbf{1}_y) \quad &\Leftrightarrow \quad \forall z \neq y \quad c(x, y) + \psi(y) + t \leqslant c(x, z) + \psi(z) \\
&\Leftrightarrow \quad t \leqslant \left(\min_{z \in Y \setminus y} c(x, z) + \psi(z) \right) - (c(x, y) + \psi(y)) \\
&\Leftrightarrow \quad t \leqslant bid_x
\end{aligned}$$

This implies that

$$\mathrm{Lag}_y(\psi + t\mathbf{1}_y) \neq \emptyset \Leftrightarrow t \leqslant p_y = \max_x bid_x.$$

• Therefore, when $0 \leqslant t \leqslant p_y$ increases, since the Laguerre cell contains at least one element x, then $\mathcal{K}(\psi + t\mathbf{1}_y)$ does not decrease. When $t > p_y$, then it strictly decreases (because the first sum does not vary). This implies the result. □

Alternate proof of Lemma 24-third bullet.
• By Corollary 22, the upper-bound of the superdifferential $\partial^+ \kappa(t)$ of the function $\kappa(t) = \mathcal{K}(\psi + t\mathbf{1}_y)$ is $\mu(\mathrm{Lag}_y(\psi^t)) - \frac{1}{N}$. It is $\geqslant 0$ (non-negative) for $t \in [0, \mathrm{bid}_y(\psi)]$ and < 0 for $t > \mathrm{bid}_y(\psi)$. This directly implies (for instance using the same characterization at the limit) that $\underline{0 \in \partial^+ \kappa(\mathrm{bid}_{y_0}(\psi))}$, so that the largest maximizer of κ is $\mathrm{bid}_{y_0}(\psi)$.

□

7.3. Bertsekas (original) Auction's algorithm.
We first need the following definitions
- A *partial assignment* is a pair (γ, S) where $S \subset X$ and $\gamma : S \to Y$ is injective.
- A partial assignment (γ, S) and a vector price ψ satisfy the ε-complementary slackness condition if

$$c(x, \gamma(x)) + \psi(\gamma(x) \leqslant \min_{y \in Y} c(x, y) + \psi(y) + \varepsilon$$

Remark 11. If the cost is integer-valued, if $(\gamma, S = X)$ is a partial assignment (bijective) that satisfies the ε-complementary slackness condition, and if $\varepsilon < 1/N$, then $\gamma : X \to Y$ is a optimal matching. Indeed

$$\sum_{x \in X} c(x, \gamma(x)) \leqslant \min_{\sigma \text{permutation}} \sum_{x \in X} c(x, \sigma(x)) + N\varepsilon.$$

The goal of Auction algorithm is to increase the prices by the bids, and to maintain a partial matching "that increases".

Auctions algorithm (let $\varepsilon > 0$) :
- **Initialization.** $S = \emptyset \subset X$ (no point of X is assigned)
            $\psi(y) = 0$ (prices are equal to 0).
- **Step 1.** We pick $x \in X \setminus S$ and calculate

    $y_0 \leftarrow \text{argmin}_{y \in Y} \, c(x, y) + \psi(y)$ house that minimizes the cost
    $y_1 \leftarrow \text{argmin}_{y \in Y \setminus y_0} \, c(x, y) + \psi(y)$ second best house

- **Step 2.** if y_0 was already assigned to x', then $S \leftarrow S \setminus \{x'\}$
- **Step 3.** Update:
    - $\psi(y_0) \leftarrow \psi(y_0) + (c(x, y_1) + \psi(y_1)) - (c(x, y_0) + \psi(y_0)) + \varepsilon$ (increase the price of the $bid_x + \varepsilon$)
    - $S \leftarrow S \cup \{x\}$.
    - We assign x to y_0 ($\gamma(x) = y_0$).
    If $S \neq X$, we go to Step 1.

7.4. **Analyses.** The following lemma is by construction.

Lemma 25. *Along the algorithm, one has*
- *The image $\pi(S)$ is increasing.*
- *$(\pi, S), \psi$ satisfies the ε-complementary slackness condition*
- *the price increments in $\psi(Y)$ are at least of ε.*

Proof. Step 2 ensures that we have an injective map.
Step 3 ensures an increment of at least ε.
Note that the image $\pi(S)$ is not strictly increasing.   □

Proposition 26. *The number of steps in Auction algorithm is at most $N(C/\varepsilon + 1)$, where $C = \max_{x,y} c(x, y)$.*

Proof. For simplicity, we assume that the cost is positive.
- Suppose that after i step, the algorithm has not stopped (the prices are denoted $\psi_i(y)$). Then it means that there exists y_0 that does not belong to $\pi(S)$ (since $\pi : S \to Y$ injective). Therefore $\psi_i(y_0) = 0$.
- Suppose that there exists y_1 whose price has been raised more than $n > C/\varepsilon + 1$. Then for every $x \in X$

$$\psi_i(y_0) + c(x, y_0) = c(x, y_0) \leqslant C < (n-1)\varepsilon = n\varepsilon - \varepsilon \leqslant \psi_i(y_1) - \varepsilon \leqslant \psi_i(y_1) + c(x, y_1) - \varepsilon$$

This contradicts the fact the price $\psi_l(y_1) \leqslant \psi_i(y_1) - \varepsilon$ was raised at a previous iteration l. Indeed if it was the case, then we had to have

$$\exists x \in X, s.t. \quad \psi_l(y_1) + c(x, y_1) \leqslant \psi_i(y_1) - \varepsilon + c(x, y_1) \leqslant \psi_l(y_0) + c(x, y_0) = c(x, y_0),$$

which is not true.

• We deduce that the prices of each y has been raised at most $C/\varepsilon + 1$ times. Since there are N such y, we conclude. □

Using the remark before, in order to solve the assignment problem, we need to put $\varepsilon = 1/(N+1)$. There are $O(N/\varepsilon)$ steps. The complexity of each step is $O(N)$ (a loop to determine y_0 and y_1). We then get

Theorem 27. *The (worst case) complexity of Auction's algorithm is $O(N^3 C)$, where $C = \max_{x,y} c(x,y)$.*

7.5. **Scaling technique.** The idea of scaling is used in several algorithms and usually speeds up drastically the time. In the case of Auction's algorithm, it is as follows. We denote by $\text{Auction}(\psi_k, \varepsilon_k)$ the Auction algorithm with input error ε_k and intial weights ψ_k and that output the final weights ψ_{k+1}. The algorithm just consist in starting with $\psi_0 = 0$ and the computing recursively $\psi_{k+1} = \text{Auction}(\psi_k, C/2^k)$.

Theorem 28. *The (worst case) complexity of the scaled Auction's algorithm is $O(N^3 \log(NC))$, where $C = \max_{x,y} c(x,y)$.*

Proof. ADMITTED. □

8. Semi-discrete case

8.1. **Problem and Kantorovitch functional in the quadratic case.** We recall that the Kantorovicth functional is the function

$$\mathcal{K}(\psi) = \sum_{y \in Y} \int_{\text{Lag}_y(\psi)} (c(x,y) + \psi(y))\rho(x)\mathrm{d}x - \sum_{y \in Y} \psi(y)\nu_y$$

and that we have the following corollary:

Corollary 29. *The following statements are equivalent:*
   (i) $\psi : Y \to \mathbb{R}$ is a global maximizer of $\mathcal{K}$;
   (ii) T_ψ is an optimal transport map between ρ and ν ;
   (iii) $T_{\psi\#}\mu = \nu$, or equivalently,

$$\text{(MA)} \qquad\qquad \forall y_i \in Y, \ \mu(\text{Lag}_{y_i}(\psi)) = \nu_i$$

8.2. **Oliker-Prussner algorithm.** The Oliker-Prussner algorithm is an increment-wise algorithm (such as Auction's algorithm) whose goal is to obtain *(iii)*. It is also based on the observation that when a price $\psi(y_i)$ decreases, then its Laguerre cell $\text{Lag}_{y_i}(\psi) = \{x, \|x - y_i\| + \psi(y_i) \leqslant \|x - y_j\| + \psi(y_j)\}$ increases. The idea is to start with all the prices that are too small, except for y_0, and to iteratively increase the prices of the $y_i \neq y$.

Oliker-Prussner algorithm
   • **Input.**
      - Two probability measures $\mu(x) = \rho(x)\mathrm{d}x$ and $\nu = \sum_{y \in Y} \nu_y \delta_y$.
      - Parameter $\delta > 0$
   • **Initialization of the weights.**
      - $\psi_0(y_0) = 0$
      - $\psi_0(y_i) = \max_{x,y} c(x,y) - \min_{x,y} c(x,y)$ for every $i \neq 0$.
      - $k = 0$.

- **While there exists $y_i \in Y \setminus \{y_0\}$ such that** $\mu(\mathrm{Lag}_{y_i}(\psi_k) \leqslant \nu_i - \delta$
  - Calculate $t_i \geqslant 0$ so that $\mu(\mathrm{Lag}_{y_i}(\psi_k - t_i e_i)) \in [\nu_i, \nu_i + \delta]$
  - Calculate the new price $\psi_{k+1} = \psi_k - t_i e_i$.
  - $k = k + 1$.

Remark 12. At the end of the algorithm, one has

$$\forall y_i \in Y \setminus \{y_0\} \quad \mu(\mathrm{Lag}_{y_i}(\psi_k)) \in [\nu_i, \nu_i + \delta].$$

Therefore, since we have two probability measures, if one takes $\delta = \varepsilon/N$, where $N = \sharp Y$, one has

$$|\nu_0 - \mu(\mathrm{Lag}_{y_0}(\psi_k))| \leqslant \left| \sum_i \nu_i - \mu(\mathrm{Lag}_{y_i}(\psi_k)) \right| \leqslant \delta N = \varepsilon.$$

This implies that at the end of the algorithm, one has

$$\forall y_i \in Y \quad \left| \nu_i - \mu(\mathrm{Lag}_{y_i}(\psi_k)) \right| \leqslant \varepsilon.$$

8.3. **Analysis of Oliker-Prussner algorithm.** Remark that the algorithm will terminate in a finite number of steps if there is a minimal increment on the t_is. This will be the case if the functions $G_i(\psi) := \mathrm{Lag}_{y_i}(\psi)$ are Lipschitz. We recall that in Lemma 13, we show that the functions G_i are L-Lipschitz with $L = O(N)$.

Theorem 30. *Let $\varepsilon > 0$. The Oliker-Prussner with $\delta = \varepsilon/N$ converges in $0(N^3/\varepsilon)$ steps.*

Proof. We assume that the algorithm stops at step k.
- Since there exists $x \in \mathrm{Lag}_{y_0}(\psi)$, one has

$$\|x - y_0\|^2 = \|x - y_0\|^2 + \psi_k(y_0) \leqslant \|x - y_i\|^2 + \psi_k(y_i),$$

which implies that $\psi_k(y_i) \geqslant -C$ where $C = \max_{x,y} c(x, y)$.
- Now, for a given y_i, since G_i is L-Lipschitz (see Lemma 13), one has

$$\delta \leqslant |G_i(\psi_k + t_i e_i) - G_i(\psi_k)| \leqslant L t_i,$$

hence one has $t_i \geqslant \delta/L$. Let N_s^i be the number of times the price of y_i has changed. One has

$$N_s^i \frac{\delta}{L} \leqslant \text{variation of } \psi(y_i) \leqslant C,$$

which leads to $N_s^i \leqslant CL/\delta$. Since there are N points y_i the total number of steps is

$$N_s \leqslant N \frac{CL}{\delta} \leqslant N^2 \frac{CL}{\varepsilon}$$

using $\delta = \varepsilon/N$.
- We conclude by using the fact that the Lipschitz constant is $O(N)$. $\qquad\square$

8.4. **Hessian of Kantorovitch functional.** In order to use a Newton method, one needs to evaluate the Hessian of the Kantorovitch functional and to show its C^2-continuity. For this purpose, we also need the following notion of genericity.

Definition 15.
- A set Y is said to be in generic position if it does not contain any triplet of aligned points.
- Y is said to be generic with respect to X if it is generic and if for any y_i and y_j in Y and any hyperplane H orthogonal to $y_i - y_j$ $H \cap \partial X$ is Lebesgues negligible.

Theorem 31. *Suppose that the density $\rho : X \to \mathbb{R}$ is continuous and that Y is in generic position with respect to X. Then the Kantorovitch functional is of class C^2 one has*

$$\frac{\partial^2 \mathcal{K}}{\partial \psi_i \psi_j}(\psi) = \int_{\mathrm{Lag}_{i,j}(\psi)} \frac{\rho(x)}{2\|y_i - y_j\|} \mathrm{d}x.$$

where $\mathrm{Lag}_{i,j}(\psi) = \mathrm{Lag}_{y_i}(\psi) \cap \mathrm{Lag}_{y_j}(\psi)$. Moreover

$$\frac{\partial^2 \mathcal{K}}{\partial \psi_i^2}(\psi) = -\sum_{j \neq i} \int_{\mathrm{Lag}_{i,j}(\psi)} \frac{\rho(x)}{2\|y_i - y_j\|} \mathrm{d}x.$$

Remark 13. Note that the genericity condition allows to show that Ψ is of class C^2 on the whole $\mathbb{R}^N$. It can be replaced by imposing that the Laguerre cells have positive mass and belong to the set [5].

$$\mathcal{K}^+ = \{\psi : Y \to \mathbb{R}, \mu(\mathrm{Lag}_{y_i}(\psi)) > 0 \; \forall y_i \in Y\}$$

Remark 14. Note that $\nabla \mathcal{K} = G$ is invariant by addition of a constant, namely $G(\psi + \mathrm{cste}\mathbf{1}_N) = G(\psi)$, where $G_i(\psi) = \mu(\mathrm{Lag}_{y_i}(\psi))$. This implies that $\mathbf{1}_N = (1, \cdots, 1)$ belongs to the Kernel of $DG(\psi)$, hence to the Hessian of $\mathcal{K}$ at ψ. In particular, the Hessian is not invertible.

Remark 15. Let μ be the uniform probability measure on $X = [0,1]^2 \subseteq \mathbb{R}^2$, and let $y_1 = (\frac{1}{2}, 0)$, $y_2 = (-\frac{1}{2}, 0)$ and $y_3 = (1, 0)$. Set $\psi^t = (0, t, 0)$. Then,

$$\frac{\partial G_1}{\partial \psi_3}(\psi^t) = \mathrm{length}(K \cap \mathrm{Lag}_1(\psi^t) \cap \mathrm{Lag}_3(\psi^t)) = \begin{cases} 0 & \text{when } t > \frac{-6}{4} \\ 1 & \text{when } t < \frac{-6}{4}, \end{cases}$$

thus showing that G is not globally C^1.

Remark 16. We see that if a Laguerre $\mathrm{Lag}_{y_i}(\psi)$ cell is empty, then $\frac{\partial G_i}{\partial \psi_{-j}}(\psi) = 0$ for every j, meaning than the correspondin raws and columns in $DG(\psi)$ vanishes.

8.5. **Reminder on Coarea formula.** We consider two Riemannian sub-manifolds M and N, respectively of dimensions m and n, of two Euclidean spaces and assume that $n \leqslant m$. Let $\Phi : M \to N$ be a function of class C^1 between the two manifolds. The *Jacobian determinant* of $\Phi : E \subseteq M \to N$ at x is defined by

(8.8) $$J_\Phi(x) = \sqrt{\det(\mathrm{D}\Phi(x)\mathrm{D}\Phi(x)^T)}$$

Note that if $M = \mathbb{R}^m$, $N = \mathbb{R}^n$ and $\Phi = (\Phi_1, \ldots, \Phi_n)$, one has

$$\mathrm{D}\Phi(x)\mathrm{D}\Phi(x)^T = (\langle \nabla \Phi_i(x) | \nabla \Phi_j(x) \rangle)_{1 \leqslant i, j \leqslant n}.$$

In particular, for $n = 1$, one has $J\Phi(x) = \|\nabla \Phi_1(x)\|$, and for $n = 2$ one gets

$$J\Phi(x)^2 = \|\nabla \Phi_1(x)\|^2 \|\nabla \Phi_2(x)\|^2 - \langle \nabla \Phi_1(x) | \nabla \Phi_2(x) \rangle^2$$

which by Cauchy-Schwarz's inequality is always non-negative and vanishes iff $\nabla \Phi_1(x)$ and $\nabla \Phi_2(x)$ are collinear.

Theorem 32 (Coarea formula)**.** *Let $\Phi : M \to N$ be a function of class C^1. For every $\mathcal{H}^m$-measurable function $u : M \to \mathbb{R}$, one has*

$$\int_M u(x) J_\Phi(x) \mathrm{d}\mathcal{H}^m(x) = \int_N \int_{\Phi^{-1}(y)} u(x) \mathrm{d}\mathcal{H}^{m-n}(x) \mathrm{d}\mathcal{H}^n(y).$$

If $J_\Phi(x)$ does not vanish on a measurable subset $E \subset M$, then

$$(8.9) \qquad \int_M u(x) \mathrm{d}\mathcal{H}^m(x) = \int_N \int_{\Phi^{-1}(y)} \frac{u(x)}{J_\Phi(x)} \mathrm{d}\mathcal{H}^{m-n}(x) \mathrm{d}\mathcal{H}^n(y).$$

In particular, if $m = n$ and $\Phi : M \to N$ is an homeomorphism of class C^1, letting $v = u \circ \Phi^{-1} : N \to \mathbb{R}$, one recovers the change of variable formula

$$(8.10) \qquad \int_M v(\Phi(x)) J_\Phi(x) \mathrm{d}\mathcal{H}^m(x) = \int_N v(y) \mathrm{d}\mathcal{H}^n(y).$$

8.6. **Proof of the C^2-continuity of $\mathcal{K}$ (Theorem 31).** We recall that the Kantorovitch functional $\mathcal{K}$ is of class C^1 and that one has $\nabla \mathcal{K} = (G_i)_{1 \leqslant i \leqslant n}$ where $G_i(\psi) = \int_{\mathrm{Lag}_{y_i}(\psi)} \rho(x) \mathrm{d}x$.

Step 1. We want to show that

$$\frac{\partial G_i}{\partial \psi_j} = \int_{\mathrm{Lag}_{i,j}(\psi)} \frac{\rho(x)}{2\|y_i - y_j\|} \mathrm{d}x.$$

We introduce the set

$$L := L_{y_i}(\psi) := \{x \in \mathbb{R}^d, \ \forall k \neq j \|x - y_i\|^2 + \psi_i \leqslant \|x - y_k\|^2 + \psi^k\} \supset \mathrm{Lag}_{y_i}(\psi).$$

Note that the boundary of this set coincides with the one of $\mathrm{Lag}_{y_i}(\psi)$ except along $\mathrm{Lag}_{i,j}(\psi)$. First recall that

$$x \in \mathrm{Lag}_{i,j}(\psi + te_j) \iff \|x - y_i\|^2 + \psi_i = \|x - y_j\|^2 + \psi_j + t$$
$$\iff u(x) := 2\langle y_j - y_i | x \rangle - \psi_j + \psi_i - \|y_j\|^2 + \|y_i\|^2 = t$$

Suppose $t \geqslant 0$. Therefore, by construction one has

$$\mathrm{Lag}_{y_i}(\psi + te_j) \Delta \mathrm{Lag}_{y_i}(\psi) = L \cap u^{-1}(]0, t]).$$

This implies by the Coarea formula that

$$\begin{aligned}
\frac{G(\psi + te_j) - G(\psi)}{t} &= \frac{1}{t} \int_{L \cap u^{-1}([0,t])} \rho(x) \mathrm{d}x \\
&= \frac{1}{t} \int_0^t \int_{L \cap u^{-1}(s)} \frac{\rho(x)}{\|\nabla u(s)\|} \mathrm{d}x \mathrm{d}s \\
&= \frac{1}{t} \int_0^t \int_{\mathrm{Lag}_{i,j}(\psi + se_j)} \frac{\rho(x)}{\|\nabla u(s)\|} \mathrm{d}x \mathrm{d}s \\
&= \frac{1}{t} \int_0^t g_{i,j}(\psi + se_j) \mathrm{d}s
\end{aligned}$$

where we introduced the map

$$g_{i,j}(\psi) := \frac{1}{2\|y_i - y_j\|} \int_{\mathrm{Lag}_{i,j}(\psi)} \rho(x) \mathrm{d}x$$

We show below in Lemma 33 that $g_{i,j}$ is continuous. By the fundamental theorem of calculus, one has

$$\frac{\partial G_i}{\partial \psi_j}(\psi) = g_{i,j}(\psi) = \int_{\mathrm{Lag}_{i,j}(\psi)} \frac{\rho(x)}{2\|y_i - y_j\|} \mathrm{d}x.$$

Step 2. Since $G_i(\psi) = 1 - \sum_{j \neq i} G_j(\psi)$, we know that G_i is also differentiable with respect to ψ_i and that we have the required formula. This implies that the partial derivatives are continuous, so that $\nabla \mathcal{K}$ is of class C^1.

Lemma 33. *Assume that Y is generic with respect to ∂X. Then, for any $i \neq j$, the function $g_{i,j}$ defined above is continuous.*

Proof of Lemma 33. Let $f : \Omega_X \to \mathbb{R}$ defined by $f(x) = \|x - y_i\|^2 - \|x - y_j\|^2 = 2\langle y_j - y_i | x \rangle - \|y_j\|^2 + \|y_i\|^2$.

Step 1 (Flow). We consider the vector field $X = \nabla f(x)/\|\nabla f(x)\|^2$ on Ω_X. Let $\Omega_X^1 \subset \Omega_X$ be an open set containing X. By Cauchy-Lipschitz's theory, one can construct a flow $\Phi : [-\varepsilon, \varepsilon] \times \Omega_X^1 \to \Omega_X$, where $\varepsilon > 0$, such that

$$(8.11) \qquad \begin{cases} \Phi(0, x) = x \\ \dot{\Phi}(t, x) = \dfrac{\nabla f(\Phi(t,x))}{\|\nabla f(\Phi(t,x))\|^2}, \end{cases}$$

where $\dot{\Phi}$ is the derivative with respect to t.

$$\frac{\partial}{\partial t} f(\Phi(t, x)) = \nabla f(\Phi(t,x)) \cdot \frac{\nabla f(\Phi(t,x))}{\|\nabla f(\Phi(t,x))\|^2} = 1.$$

This implies that $\underline{f(\Phi(t, x)) = f(\Phi(0, x)) + t}$. Moreover, since $X = \nabla f / \|\nabla f\|$ is of class C^1 on Ω_X, then $\underline{F_t := \Phi(t, \cdot) \text{ simply converges to the identity}}$ and $\underline{DF_t \text{ simply converges to the identity}}$, as $t \to 0$.

Step 2 (Sending the Laguerre cells on $f^{-1}(0)$).
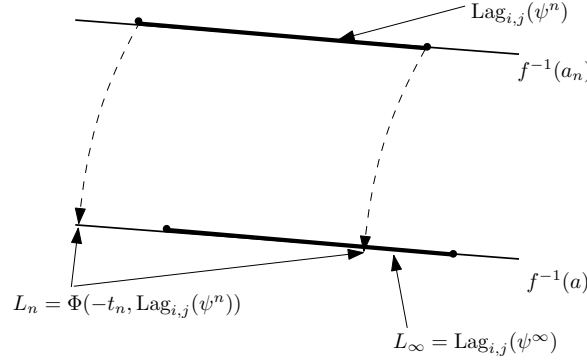

FIGURE 4. Proof of continuity of $g_{i,j} : F_n := \Phi(t_n, \cdot)|_{L_n} : L_n \to \mathrm{Lag}_{i,j}(\psi^n)$ is such that $F_n(L_n) = \mathrm{Lag}_{i,j}(\psi^n)$

Let (ψ^n) be a sequence in $\mathbb{R}^Y$ converging to some $\psi^\infty \in \mathbb{R}^Y$. We put $a_n = \psi_j^n - \psi_i^n$, $a = \psi_j^\infty - \psi_i^\infty$ and $t_n = a_n - a$ and define

$$L_n = \Phi(-t_n, \mathrm{Lag}_{ij}(\psi^n)) \quad \text{and} \quad L_\infty = \mathrm{Lag}_{ij}(\psi^\infty).$$

By definition, one has $f(\mathrm{Lag}_{ij}(\psi^n)) = a_n$ and $f(\mathrm{Lag}_{ij}(\psi^\infty)) = a$. Using the flow property, one gets that both L_n and L_∞ are subsets of the hypersurface $H = f^{-1}(a)$. Denoting F_n the restriction of $\Phi(t_n, \cdot)$ to H, one has $\mathrm{Lag}_{ij}(\psi^n) = F_n(L_n)$. Since the flow is transverse to the hypersurfaces $f^{-1}(cste)$, $F_n : L_N \to \mathrm{Lag}_{ij}(\psi^n)$ is a C^1 diffeomorphism.

Step 2 (Comparing on $f^{-1}(0)$). We now need to consider a continuous extension $\bar{\rho}$ of $\rho_{|X}$ onto Ω_X, since L_n may not be included in X. By a change of variable (see (8.10) for

instance), one gets

$$g_n := g_{i,j}(\psi^n) = \int_{\mathrm{Lag}_{ij}(\psi^n)} \frac{\rho(y)}{2\,\|y_i - y_j\|} \mathrm{d}\mathcal{H}^{d-1}(y)$$

$$= \int_{\mathrm{Lag}_{ij}(\psi^n)} \frac{\overline{\rho}(y)}{2\,\|y_i - y_j\|} \chi_X(y) \mathrm{d}\mathcal{H}^{d-1}(y)$$

$$= \int_H \frac{\overline{\rho}(F_n(x))}{2\,\|y_i - y_j\|} JF_n(x) \chi_{L_n}(x) \chi_X(F_n(x)) \mathrm{d}\mathcal{H}^{d-1}(x),$$

where χ_A is the indicator function of A. Moreover,

$$g_\infty := g_{i,j}(\psi^\infty) = \int_H \frac{\rho(x)}{2\,\|y_i - y_j\|} \chi_{L_\infty \cap X}(x) \mathrm{d}\mathcal{H}^{d-1}(x).$$

Step 3 (Simply convergence of the integrands). By Lebesgue's dominated convergence theorem, to prove that $(g_n)_{n \geqslant 0}$ converges to g_∞, it suffices to prove that the integrand of g_n (seen as a function on H) tends to the integrand of g_∞ $\mathcal{H}^{d-1}$-almost everywhere. Since F_n converges to the identity in a C^1 sense and $\overline{\rho}$ is continuous, it remains to show that $\lim_{n \to \infty} \chi_{L_n}(x) \chi_X(F_n(x)) = \chi_{L_\infty \cap X}(x)$ for almost every $x \in H$ (for the $(d-1)$ Hausdorff measure).

• We first prove that $\limsup_{n \to \infty} \chi_{L_n}(x) \chi_X(F_n(x)) \leqslant \chi_{L_\infty \cap X}(x)$ for every $x \in H$. The limsup is non-zero if and only if there exists a subsequence $\sigma(n)$ such that $x \in L_{\sigma(n)}$ and $F_n(x) \in X$. Then, since $F_{\sigma(n)}(L_{\sigma(n)}) = \mathrm{Lag}_{ij}(\psi_{\sigma(n)})$ we get

$$\begin{cases} \|F_{\sigma(n)}(x) - y_i\|^2 + \psi_{\sigma(n)}(y_i) \leqslant \|F_{\sigma(n)}(x) - y_k\|^2 + \psi_{\sigma(n)}(y_k) & \forall k \\ \|F_{\sigma(n)}(x) - y_i\|^2 + \psi_{\sigma(n)}(y_i) = \|F_{\sigma(n)}(x) - y_j\|^2 + \psi_{\sigma(n)}(y_j). \end{cases}$$

Passing to the limit $n \to +\infty$, we see that x belongs to $\mathrm{Lag}_{ij}(\psi_\infty) = L_\infty$ and to X, thus ensuring

$$\lim_{n \to +\infty} \sup \chi_{L_n}(x) \chi_X(F_n(x)) \leqslant \chi_{L_\infty \cap X}(x).$$

• We now pass to the liminf inequality. Denote

$$S = \left(\bigcup_{k \neq i,j} H_{ijk}(\psi_\infty) \right) \cup \left(H_{ij}(\psi) \cap \partial X \right),$$

where $H_{ij}(\psi) = \{x \in \Omega_X, \|x - y_i\|^2 + \psi_i = \|x - y_j\|^2 + \psi_j\}$, $H_{ijk}(\psi) := H_{ij}(\psi) \cap H_{jk}(\psi)$ which by assumption has zero $(d-1)$ Hausdorff measure.

We now prove that $\liminf_{n \to \infty}(x) \chi_{L_n} \chi_X(F_n(x)) \geqslant \chi_{L_\infty \cap X}$ on $H \setminus S$. If $x \notin L_\infty \cap X$, $\chi_{L_\infty \cap X}(x) = 0$ and there is nothing to prove. We therefore consider $x \in (L_\infty \cap X) \setminus S$, meaning by definition of S that x belongs to the interior $\mathrm{int}(X)$ and that

$$\forall k \neq i,j \; \|x - y_i\|^2 + \psi_i^\infty < \|x - y_k\|^2 + \psi_k^\infty.$$

Since $F_n(x)$ converges to x, this implies that for n large enough one has $F_n(x) \in \mathrm{int}(X)$ and

$$\forall k \neq i,j \; \|F_n(x) - y_i\|^2 + \psi_i^\infty < \|F_n(x) - y_k\|^2 + \psi_k^\infty.$$

By definition, this means that $F_n(x)$ belongs to $\mathrm{Lag}_{ij}(\psi^n)$, and therefore $x \in L_n$ by definition of L_n. Thus

$$\lim_{n \to +\infty} \inf \chi_{L_n}(x) \chi_X(F_n(x)) = 1 \geqslant \chi_{L_\infty \cap X}(x)$$

$\square$

8.7. **Strict concavity of $\mathcal{K}$.** We denote by

$$\mathcal{K}^+ = \{\psi : Y \to \mathbb{R}, \mu(\mathrm{Lag}_{y_i}(\psi)) > 0 \ \forall y_i \in Y\}.$$

> **Theorem 34.** *We assume that X is a convex compact domain of $\mathbb{R}^d$, that $\rho : X \to \mathbb{R}$ is continuous $\mathrm{spt}(\rho) = \mathrm{int}(X)$ and that Y is generic with respect to X and $\rho(\partial X) = 0$. The Kantorovitch $\mathcal{K}$ is strictly concave in the sense that*
>
> $$\forall \psi \in \mathcal{K}^+, \ \forall v \in \{\mathbf{1}_N\}^\perp \ \langle DG(\psi).v|v\rangle < 0$$
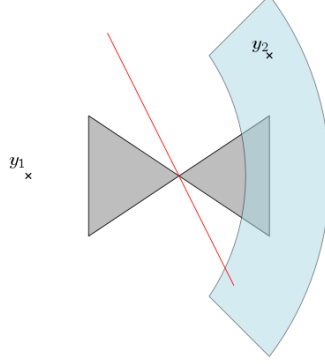

FIGURE 5. Simplex soup where the set of points y_1, y_2 such that $\mu(\mathrm{Lag}_{1,2}(\psi)) = 0$ has not a zero measure.

Remark 17. The assumption can be much more general on X. Some connectedness conditions are required. Let us illustrate the fact that the connectedness of X is not sufficient (i.e. why we require that it is impossible to disconnect the support X of μ by removing a finite number of points). Consider the case where X is made of the two 2-dimensional simplices embedded in $\mathbb{R}^2$, and displayed in grey in Figure 5. We assume that μ is the restriction of the Lebesgue measure to X and that $Y = \{y_1, y_2\}$. Then, the matrix of the differential of G at ψ is the 2-by-2 matrix given by

$$\mathrm{D}G(\psi) = \begin{pmatrix} -a & a \\ a & -a \end{pmatrix} \text{ where } a = \frac{1}{2\|y_1 - y_2\|} \mathrm{length}^1(\mathrm{Lag}_{1,2}(\psi) \cap X).$$

If we fix $y_1 \in \mathbb{R}^2$, it is easy to see that for any y_2 in the blue domain, there exists weights ψ_1 and ψ_2 such that the interface $\mathrm{Lag}_{1,2}(\psi)$ (in red) passes through the common vertex between the two simplices, thus implying that $a = 0$, hence $\mathrm{D}G(\psi) = 0$. In such setting, G is not strictly monotone, the conclusion of Theorem 34 does not hold.

Proof. This theorem will follow using standard arguments, once one has established the connectedness of the graph induced by the Jacobian matrix. Let $\psi \in \mathcal{K}^+$, $H := \mathrm{D}G(\psi)$. Since $\mathcal{K}$ is concave with gradient $\nabla\mathcal{K} = G$, we know that H is symmetric. We have to show that $\mathrm{Ker}(H) = \mathrm{vect}(\{\mathrm{cst}\})$.

Step 1. We consider the graph $\mathcal{G}$ supported on the set of vertices $V = \{1, \ldots, N\}$ and with edges

$$E(\mathcal{G}) := \{(i,j) \in V^2 \mid i \neq j \text{ and } H_{i,j}(\psi) > 0\}.$$

Lemma 35. *The graph $\mathcal{G}$ is connected.*

Proof.
Step 1: We show here that for all $i \in \{1, \ldots, N\}$, $\mathrm{int}(\mathrm{Lag}_{y_i}(\psi) \cap X)$ contains at least a point which we denote x_i.

Indeed, since $\psi \in \mathcal{K}^+$, we know that $\rho(\mathrm{Lag}_{y_i}(\psi)) > 0$. In addition, $\rho(\mathrm{Lag}_{y_i}(\psi) \cap \mathrm{Lag}_{y_j}(\psi)) = 0$ for all $j \neq i$, and $\rho(\partial X) = 0$ by assumption.

Step 2: Let S the union of facets that are common to at least three distinct Laguerre cells, i.e.

$$S = \bigcup_{y_1, y_2, y_3 \text{distinct}} \mathrm{Lag}_{y_1, y_2, y_3}(\psi).$$

Then, $\underline{\mathrm{int}(X) \setminus S \text{ is open and path-connected.}}$ Indeed, by the genericity assumption, we already know that $\mathcal{H}^{d-1}(S) = 0$, and Lemma of chapter (ADMIS) then implies that $\mathrm{int}(X) \setminus S$ is path-connected.

Step 3: Let $x \in \mathrm{int}(X) \setminus S$ be such that $x \in \mathrm{Lag}_{y_i}(\psi) \cap \mathrm{Lag}_{y_j}(\psi)$ for $i \neq j$. Then, $H_{ij} > 0.$ To see this, we note that since x belongs to the complement of S,

$$\begin{cases} c(x, y_i) + \psi(y_i) = c(x, y_j) + \psi(y_j), \\ \forall k \notin \{i, j\}, c(x, y_i) + \psi(y_i) < c(x, y_k) + \psi(y_k). \end{cases}$$

This implies that there exists a ball with radius $r > 0$ around x such that

$$\forall x' \in \mathbb{B}(x, r), \forall k \notin \{i, j\}, c(x, y_i) + \psi(y_i) < c(x, y_k) + \psi(y_k),$$

directly implying that

$$H_{yy'}(\psi) \cap \mathbb{B}(x, r) \subseteq \mathrm{Lag}_{y_i y_j}(\psi).$$

By the twist hypothesis and the inverse function theorem, $H_{yy'}(\psi)$ is a $(d-1)$-dimensional submanifold. In addition, $\rho(x) > 0$ because x belongs to Z. This implies that

$$H_{ij} = \int_{\mathrm{Lag}_{y_i y_j}(\psi)} \frac{\rho(x')}{\|\nabla_x c(x', y_i) - \nabla_x c(x', y_j)\|} \mathrm{d}\mathcal{H}^{d-1}(x')$$

$$\geqslant \int_{H_{y_i y_j}(\psi) \cap \mathbb{B}(x, r)} \frac{\rho(x')}{\|\nabla_x c(x', y_i) - \nabla_x c(x', y_j)\|} \mathrm{d}\mathcal{H}^{d-1}(x') > 0.$$

Step 4: We now fix $i \neq j \in \{1, \ldots, N\}$ and the points x_i, x_j whose existence is established in Step 1:

$$x_i \in \mathrm{int}(\mathrm{Lag}_{y_i}(\psi) \cap X), \quad x_j \in \mathrm{int}(\mathrm{Lag}_{y_j}(\psi) \cap X),$$

so that in particular x_i, x_j belongs to $\mathrm{int}(X) \setminus S$. By Step 2, we get the existence of a continuous path $\gamma \in \mathcal{C}^0([0, 1], \mathrm{int}(X) \setminus S)$ such that $\gamma(0) = x_i$ and $\gamma(1) = x_j$. We define a sequence $i_k \in \{1, \ldots, N\}$ of indices by induction, starting from $i_0 = i$. For $k \geqslant 0$ we define $t_k = \max\{t \in [0, 1] \mid \gamma(t) \in \mathrm{Lag}_{y_{i_k}}\}$. If $t_k = 1$ we are done. If not, $\gamma(t_k)$ belongs to exactly two distinct Laguerre cells, and we define $i_{k+1} \neq i_k$ so that $\gamma(t_k) \in \mathrm{Lag}_{y_{i_k}}(\psi) \cap \mathrm{Lag}_{y_{i_{k+1}}}(\psi)$. By definition of t_i as a maximum, the points $y_1, \ldots, y_k$ must be distinct, so that $t_\ell = 1$ after a finite number of iterations and then $i_\ell = j$. By Step 3, we get that $H_{y_{i_k} y_{i_{k+1}}} > 0$ for any $k \in \{0, \ell - 1\}$, proving that the matrix H is irreducible, thus the graph $\mathcal{G}$ is connected. $\qquad\square$

Step 2. We now want to show that $\mathrm{Ker}(H) = \mathrm{vect}(\{\mathrm{cst}\})$. Let $v \in \mathrm{Ker}(H)$ and let i_0 be an index where v attains its maximum, i.e. $i_0 \in \mathrm{argmax}_{1 \leqslant i \leqslant n} v_i$. Then using $Hv = 0$, hence

$(Hv)_{i_0} = 0$, one has

$$0 = \sum_{i \neq i_0} H_{i,i_0} v_i + H_{i_0,i_0} v_{i_0} = \sum_{i \neq i_0} H_{i,i_0} v_i - \sum_{i \neq i_0} H_{i,i_0} v_{i_0} = \sum_{i \neq i_0} H_{i,i_0} (v_i - v_{i_0}).$$

This follows from $H_{i_0,i_0} = -\sum_{i \neq i_0} H_{i,i_0}$. Since for every $i \neq i_0$, one has $H_{i,i_0} \geqslant 0$ and $v_{i_0} - v_i \geqslant 0$, this implies that $v_i = v_{i_0}$ for every i such that $H_{i,i_0} \neq 0$. By induction and using the connectedness of the graph $\mathcal{G}$, this shows that v has to be constant, i.e. $\mathrm{Ker}(H) = \mathrm{vect}(\{\mathrm{cst}\})$. $\qquad\square$

8.8. **Newton's method.** Let $\varepsilon > 0$. We denote by

$$\mathcal{K}^\varepsilon = \{\psi : Y \to \mathbb{R}, \mu(\mathrm{Lag}_{y_i}(\psi)) > \varepsilon \ \forall y_i \in Y\} \subset \mathcal{K}^+ := \mathcal{K}^0.$$

The idea of the Damped Newton algorithm is to choose a step parameter so as to stay all way long in the admissible set $\mathcal{K}^\varepsilon$.

Algorithm 1 Damped Newton algorithm

Input: A tolerance $\eta > 0$ and an initial $\psi^0 \in \mathbb{R}^Y$ (of mean value 0) such that

$$(8.12) \qquad\qquad \varepsilon := \frac{1}{2} \min \left[\min_{y \in Y} G_y(\psi^0), \ \min_{y \in Y} \nu_y \right] > 0.$$

While: $\left\| G(\psi^k) - \nu \right\|_\infty \geqslant \eta$

    Step 1: Compute the direction d^k satisfying

$$\begin{cases} \mathrm{D}G(\psi^k)d^k = -\left(G(\psi^k) - \nu \right) \\ \sum_{y \in Y} d^k(y) = 0 \end{cases}$$

    Step 2: Determine the minimum $\ell \in \mathbb{N}$ such that $\psi^{k,\ell} := \psi^k + 2^{-\ell} d^k$ satisfies

$$\begin{cases} \forall y \in Y, G_y(\psi^{k,\ell}) \geqslant \varepsilon \\ \left\| G(\psi^{k,\ell}) - \mu \right\| \leqslant (1 - 2^{-(\ell+1)}) \left\| G(\psi^k) - \mu \right\| \end{cases}$$

    Step 3: Set $\psi^{k+1} = \psi^k + 2^{-\ell} d^k$ and $k \leftarrow k + 1$.

Output: A vector ψ^k that satisfies $\left\| G(\psi^k) - \nu \right\|_\infty \leqslant \eta$.

Remark 18. We assume that $\psi^0 \in \mathbb{R}^N \cap \{\mathbf{1}\}^\perp$ is chosen so that

$$\varepsilon = \frac{1}{2} \min \left(\min_i G_i(\psi^0), \min_i \nu_i \right) > 0,$$

and we let $\mathcal{S} := \mathcal{S}_\varepsilon \cap \{\mathbf{1}\}^\perp$. Let $\psi \in \mathcal{S}$. By Theorem 34, the matrix $\mathrm{D}G(\psi)$ is symmetric non-positive, and its kernel is the one-dimensional space $\mathbb{R}\mathbf{1}$. Thus, the equation

$$\begin{cases} \mathrm{D}G(\psi)d = \nu - G(\psi), \\ \sum_i d_i = 0, \end{cases}$$

has a unique solution, which we denote $d(\psi)$, and we let $\psi_\tau = \psi + \tau d(\psi)$.

Theorem 36 (Kitagawa, Mérigot, Thibert). *We assume that X is a convex compact domain of $\mathbb{R}^d$, that $\rho : X \to \mathbb{R}$ is continuous $\mathrm{spt}(\rho) = \mathrm{int}(X)$ (this assumption can be much more general) and that Y is generic with respect to X and $\rho(\partial X) = 0$. Then the damped Newton algorithm converges with linear rate. There exists $\tau^* \in]0, 1]$ such that at every step, one has*

$$\left\| G(\psi^{k+1}) - \nu \right\| \leqslant \left(1 - \frac{\tau^*}{2} \right) \left\| G(\psi^k) - \nu \right\|$$

8.9. **Proof of Theorem 36.** The proof of this theorem relies on the regularity and properties of strict concavity of the Kantorovitch functional.

Estimates. By continuity of $\mathrm{D}G(\psi)$ over the compact domain $\mathcal{S} = \mathcal{S}_\varepsilon \cap \{\mathbf{1}\}^\perp$, the non-zero eigenvalues of $-\mathrm{D}G(\psi)$ lie in $[a, A]$ for some $0 < a \leqslant A < +\infty$. In particular, there exists a constant $M > 0$ such that for all $\psi \in \mathcal{S}$, one has

$$a\|d(\psi)\| \leqslant \|DG(\psi)d(\psi)\| = \|G(\psi) - \nu\| = \|DG(\psi)d(\psi)\| \leqslant A\|d(\psi)\|$$

which implies

(8.13) $$\frac{\|G(\psi) - \nu\|}{A} \leqslant \|d(\psi)\| \leqslant \frac{\|G(\psi) - \nu\|}{a} \leqslant M.$$

In particular, the function $F : (\psi, \tau) \in \mathcal{S} \times [0, 1] \mapsto \psi_\tau = \psi + \tau d(\psi)$ is continuous. Since $\mathcal{S} \times [0, 1]$ is compact, $K := F(\mathcal{S} \times [0, 1])$ is also compact. Then, by uniform continuity of $\mathrm{D}G$ over K, we see that there exists an increasing function ω such that $\lim_{t \to 0} \omega(t) = 0$ and $\|\mathrm{D}G(\psi) - \mathrm{D}G(\psi')\| \leqslant \omega(\|\psi - \psi'\|)$ for all $\psi, \psi' \in K$. Since G is of class $\mathcal{C}^1$, a Taylor expansion in τ gives

$$\begin{aligned} G(\psi_\tau) &= G(\psi + \tau d(\psi)) \\ &= G(\psi) + \tau DG(\psi)d(\psi) + R(\tau) \\ &= G(\psi) + \tau(\nu - G(\psi)) + R(\tau) \\ &= (1 - \tau)G(\psi) + \tau\nu + R(\tau), \end{aligned}$$

(8.14)

where $R(\tau) = \int_0^\tau (\mathrm{D}G(\psi_t) - \mathrm{D}G(\psi))d(\psi)\mathrm{d}t$ is the integral remainder. Then, we can bound the norm of $R(\tau)$ for $\tau \in [0, 1]$:

$$\begin{aligned} \|R(\tau)\| &= \left\| \int_0^\tau (\mathrm{D}G(\psi_t) - \mathrm{D}G(\psi))d(\psi)\mathrm{d}t \right\| \\ &\leqslant \|d(\psi)\| \int_0^\tau \omega(\|\psi_t - \psi\|)\mathrm{d}t \\ &\leqslant \|d(\psi)\| \tau \, \omega(\tau \|d(\psi)\|) \\ &\leqslant M\tau \, \omega(\tau M). \end{aligned}$$

(8.15)

To establish the first inequality, we used that ψ and ψ_t belong to the compact set K and for the second one that ω is increasing and that $t \in [0, \tau]$.

Linear convergence. We first show the existence of $\tau_1^* > 0$ such that for all $\psi \in \mathcal{S}$ and $\tau \in (0, \tau_1^*)$, one has $\psi_\tau \in \mathcal{S}$. By definition of ε, for every $i \in \{1, \ldots, N\}$ one has $\nu_i \geqslant 2\varepsilon$ and $G_i(\psi) \geqslant \varepsilon$. Using (8.14) and (8.15), one deduces a lower bound on $G_i(\psi_\tau)$:

$$\begin{aligned} G_i(\psi_\tau) &\geqslant (1 - \tau)G_i(\psi) + \tau\nu_i + R_i(\tau) \\ &\geqslant (1 + \tau)\varepsilon - \|R(\tau)\| \\ &\geqslant \varepsilon + \tau(\varepsilon - M\omega(\tau M)). \end{aligned}$$

If we choose $\tau_1^* > 0$ small enough so that $M\omega(\tau_1^* M) \leqslant \varepsilon$, this implies that $\psi_\tau \in \mathcal{S}$ for all $\psi \in \mathcal{S}$ and $\tau \in [0, \tau_1^*]$.
We now prove:

$$\exists \tau_2^* > 0, \quad \forall \tau \in [0, \tau_2^*], \quad \|G(\psi_\tau) - \nu\| \leqslant (1 - \tau/2) \, \|G(\psi) - \nu\|.$$

Let $\tau_2^* > 0$ be such that for every $\tau \leqslant \tau_2^*$ one has $\omega(\tau M)/a \leqslant 1/2$. With the upper bound on $R(\tau)$ given in Equation (8.15) combined with the two bounds on $\|d(\psi)\|$ of Equation (8.13), one gets

$$\|R(\tau)\| \leqslant \|d(\psi)\| \tau \; \omega(\tau \|d(\psi)\|) \leqslant \frac{\|G(\psi) - \nu\|}{a} \tau \omega(\tau M) \leqslant \frac{\tau}{2} \|G(\psi) - \nu\|$$

From Equation (8.14), we have $G(\psi_\tau) - \nu = (1 - \tau)(G(\psi) - \nu) + R(\tau)$, and therefore

$$\|G(\psi_\tau) - \nu\| \leqslant (1 - \tau)\|G(\psi) - \nu\| + \frac{\tau}{2} \|G(\psi) - \nu\| \leqslant (1 - \tau/2) \, \|G(\psi) - \nu\|.$$

These two bounds directly imply that the $\tau^{(k)}$ chosen in Algorithm 1 always satisfy $\tau^{(k)} \geqslant \tau^*$ with $\tau^* = \frac{1}{2} \min(\tau_1^*, \tau_2^*)$, so that

$$\left\|G(\psi^{(k+1)}) - \nu\right\| \leqslant \left(1 - \frac{\tau^*}{2}\right) \left\|G(\psi^{(k+1)}) - \nu\right\|.$$

This establishes the linear convergence of Algorithm 1.

8.10. **Numerics.**

9. Entropic regularization

9.1. **Formulation.** In the discrete optimal transport problem, the idea is just to add a regularization term. This term is the entropy function. Let $\varepsilon > 0$. The regularized problem that is considered here is the following

$$(9.16) \qquad (\mathrm{KP})^\varepsilon := \min_\gamma \sum_{x \in X, y \in Y} c(x,y)\gamma_{xy} + \varepsilon \sum_{x \in X, y \in Y} h(\gamma_{x,y}),$$

where $\gamma : X \times Y \to \mathbb{R} \in \overline{\Gamma}(\mu, \nu)$ satisfies the constraints

$$\forall x \in X \; \sum_{y \in Y} \gamma_{xy} = \nu_x \quad \text{and} \quad \forall y \in Y \; \sum_{x \in X} \gamma_{xy} = \mu_y.$$

and $h : \mathbb{R} \to \mathbb{R}$ is the entropy defined by

$$h(t) = \begin{cases} t(\ln(t) - 1) & \text{if } t > 0 \\ 0 & \text{if } t = 0 \\ \infty & \text{if } t \leqslant 0 \end{cases}$$

Remark that an optimal solution has a finite entropy, which directly implies that $\gamma_{x,y} \geqslant 0$. That is why this condition is dropped in the constraints.

Theorem 37. *The problem* (KP^η) *has a unique solution γ, which belongs to $\Gamma(\mu, \nu)$. Moreover, if $\min_{x \in X} \mu_x > 0$ and $\min_{y \in Y} \mu_y > 0$, then*

$$\forall (x, y) \in X \times Y, \; \gamma_{x,y} > 0.$$

Lemma 38. $H : \gamma \in (\mathbb{R}^+)^{X \times Y} \mapsto \sum_{x,y} h(\gamma_{x,y})$ *is 1-strongly convex.*
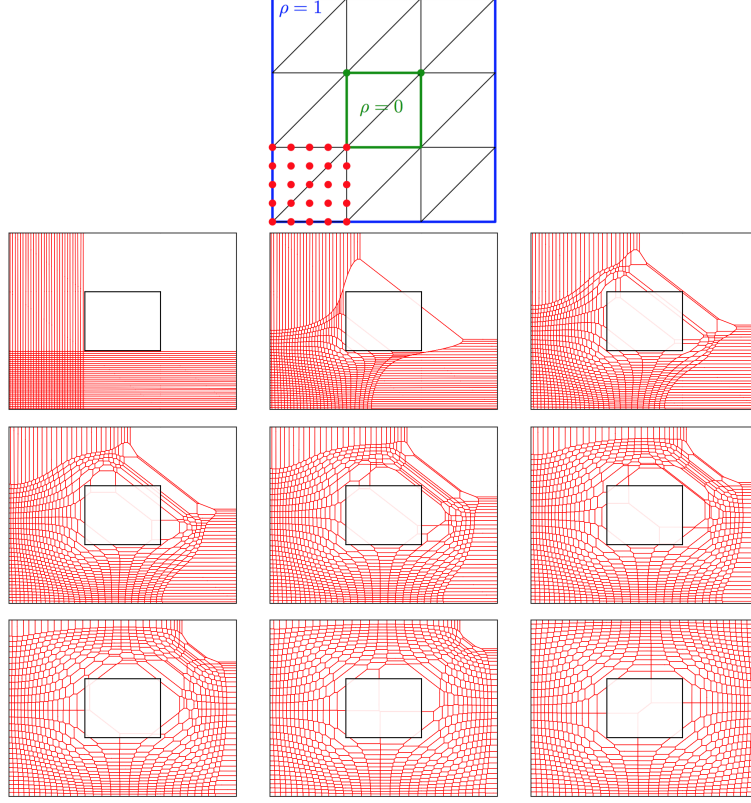
FIGURE 6. Evolution of the Laguerre cells during the execution of the damped Newton algorithm for semi-discrete optimal transport. (Top) The source density ρ is piecewise linear over the domain $X = [0,3]^3$ over the displayed triangulation: it takes value 1 on the boundary of the square $[0,3]^2$ and 0 on the boundary of $[1,2]^2$. The target measure is uniform over a 30^2 uniform grid in $[0,1]^2$. (Bottom) Laguerre cells at steps $k = 0, 2, 6, 9, 12, 15, 18, 21$ and 25.

Proof. Seeing matrices as vectors of $\mathbb{R}^{nm}$, we have $H : \mathbb{R}^{nm} \to \mathbb{R}$. From $h'(t) = \ln(t)$, one gets

$$\frac{\partial H}{\partial \gamma_{x,y}}(\gamma) = h'(\gamma_{x,y}) = \ln(\gamma_{x,y}).$$

We deduce that the Hessian of H is diagonal with diagonal coefficients given by

$$\frac{\partial^2 H}{\partial \gamma_{x,y}^2}(\gamma) = \ln'(\gamma_{x,y}) = 1/\gamma_{x,y} \geqslant 1.$$

since $\gamma_{x,y} \in]0,1]$.   □

Proof.
• First remark that in the regularized problem (KP^η), the minimum can be taken over $\overline{\Gamma}(\mu,\nu) \cap [0,\infty)^{X \times Y}$ instead of $\overline{\Gamma}(\mu,\nu)$. By the previous lemma, the regularized problem (KP^η) amounts to minimizing a coercive and strictly convex function over a closed convex set, thus showing existence and uniqueness.

• Let us denote by γ^* the solution of (KP^η). Then, γ^* has a finite entropy, so that it satisfies the constraint $\gamma^*_{x,y} \geqslant 0$. This implies that γ^* is a transport map between μ and ν. We now prove by contradiction that the set $Z := \{(x,y) \mid \gamma^*_{x,y} = 0\}$ is empty. For this purpose, we define a new transport map $\gamma^\varepsilon \in \Gamma(\mu, \nu)$ by $\gamma^\varepsilon = (1 - \varepsilon)\gamma^* + \varepsilon\mu \otimes \nu$, and we give an upper bound on the energy of γ^ε.

1) Let $(x,y) \in Z$. Introducing $C = \min_{x,y} \mu_x\nu_y$, which is strictly positive by assumption, we have (with $\varepsilon \log \varepsilon \leqslant 0$)

$$
\begin{aligned}
h(\gamma^\varepsilon_{x,y}) &= h(\varepsilon\mu_x\nu_y) \\
&= \mu_x\nu_y\varepsilon(\log \varepsilon + \log(\mu_x\mu_y)) - \mu_x\nu_y\varepsilon \\
&\leqslant C\varepsilon \log \varepsilon + O(\varepsilon) \\
&= h(\gamma^*_{x,y}) + C\varepsilon \log \varepsilon + O(\varepsilon)
\end{aligned}
$$

We then get (setting $n = \text{Card}(Z)$)

$$
\sum_{(x,y)\in Z} h(\gamma^\varepsilon_{x,y}) \leqslant \sum_{(x,y)\in Z} h(\gamma^*_{x,y}) + nC\varepsilon \log \varepsilon + O(\varepsilon)
$$

2) We observe that by convexity of $h : r \mapsto r(\log r - 1)$, one has

$$
h(\gamma^\varepsilon_{x,y}) \leqslant (1 - \varepsilon)h(\gamma^*_{x,y}) + \varepsilon h(\mu_x\nu_y) \leqslant h(\gamma^*_{x,y}) + O(\varepsilon),
$$

which implies

$$
\sum_{(x,y)\notin Z} h(\gamma^\varepsilon_{x,y}) \leqslant \sum_{(x,y)\notin Z} h(\gamma^*_{x,y}) + O(\varepsilon)
$$

Summing the two previous estimates over Z and $(X \times Y) \setminus Z$, we get

$$
H(\gamma^\varepsilon) \leqslant H(\gamma^*) + Cn\varepsilon \log \varepsilon + O(\varepsilon).
$$

Since in addition we have by linearity $\langle c|\gamma^\varepsilon \rangle \leqslant \langle c|\gamma^* \rangle + O(\varepsilon)$, we get

$$
\langle c|\gamma^* \rangle + H(\gamma^*) \leqslant \langle c|\gamma^\varepsilon \rangle + H(\gamma^\varepsilon) \leqslant \langle c|\gamma^* \rangle + H(\gamma^*) + Cn\varepsilon \log \varepsilon + O(\varepsilon),
$$

where the lower bound comes from the optimality of γ^*. Thus, $Cn\varepsilon \log \varepsilon + O(\varepsilon) \geqslant 0$, which is possible if and only if $n = \text{Card}(Z)$ vanishes, implying the strict positivity of γ^*. □

Proposition 39 (Convergence).

• *The solution γ^ε of (9.16) converges when ε tends to zero to the optimal transport map that minimizes the entropy (among the set of optimal transport plans).*

$$
\gamma^\varepsilon \longrightarrow_{\varepsilon \to 0} \arg\min_\gamma \{H(\gamma), \gamma \text{ is an optimal transport plan }\}.
$$

• *When ε tends to infinity, the solution tends to the transport plan that minimizes the entropy*

$$
\gamma^\varepsilon \longrightarrow_{\varepsilon \to \infty} (\mu_x\nu_y)_{x\in X, y\in Y}
$$

Proof. The proof of this results can be found in [4].   □

This result was first proved in Sharify 2013 and then Carlier et al showed Γ-convergence in 2017.

9.2. Derivation of the dual problem.

The Lagrangian of the primal problem is given by

$$
\begin{aligned}
L(\varphi, \psi) &= \sum_{x,y} \Big(\gamma_{x,y} c(x,y) + \varepsilon h(\gamma_{x,y}) \Big) + \sum_{x \in X} \varphi(x) \Big(\mu_x - \sum_{y \in Y} \gamma_{x,y} \Big) - \sum_{y \in Y} \psi(y) \Big(\nu_y - \sum_{x \in X} \gamma_{x,y} \Big) \\
&= \sum_{x,y} \gamma_{x,y} \Big(c(x,y) - \varphi(x) + \psi(y) \Big) + \varepsilon h(\gamma_{x,y}) + \sum_{x \in X} \varphi(x) \mu_x - \sum_{y \in Y} \psi(y) \nu_y
\end{aligned}
$$

This follows from $\sum_x \varphi(x) \sum_y \gamma_{x,y} = \sum_{x,y} \varphi(x) \gamma_{x,y}$. Denoting P the primal cost

$$
P = \min_\gamma \sup_{\varphi, \psi} L(\varphi, \psi) = \sup_{\varphi, \psi} \min_\gamma L(\varphi, \psi)
$$

The function $\gamma \mapsto L(\varphi, \psi)$ is strongly convex (affine term minus the entropy). The minimum is reached when its gradient vanishes. Using the fact that $h'(t) = \ln(t)$, one gets

$$
\begin{aligned}
\gamma \text{ is the minimum} &\Leftrightarrow \forall \gamma_{x,y} \quad c(x,y) - \varphi(x) + \psi(y) + \varepsilon \ln(\gamma_{x,y}) = 0 \\
&\Leftrightarrow \forall \gamma_{x,y} \quad \gamma_{x,y} = e^{\frac{-c(x,y) + \varphi(x) - \psi(y)}{\varepsilon}}.
\end{aligned}
$$

Let $\mathcal{K}_\varepsilon(\varphi, \psi)$ be the evaluation of the Lagragian at this minimum. By using the last equation twice, we have

$$
\begin{aligned}
\mathcal{K}_\varepsilon(\varphi, \psi) &= \sum_{x,y} -\varepsilon \gamma_{x,y} \ln(\gamma_{x,y}) + \varepsilon h(\gamma_{x,y}) + \sum_{x \in X} \varphi(x) \mu_x - \sum_{y \in Y} \psi(y) \nu_y \\
&= \sum_{x,y} -\varepsilon \gamma_{x,y} + \sum_{x \in X} \varphi(x) \mu_x - \sum_{y \in Y} \psi(y) \nu_y \\
&= \sum_{x,y} -\varepsilon e^{\frac{-c(x,y) + \varphi(x) - \psi(y)}{\varepsilon}} + \sum_{x \in X} \varphi(x) \mu_x - \sum_{y \in Y} \psi(y) \nu_y
\end{aligned}
$$

Definition 16. The dual problem is defined by

$$
(\mathrm{DP})^\varepsilon := \sup_{\varphi, \psi} \mathcal{K}_\varepsilon(\varphi, \psi),
$$

where

$$
\mathcal{K}_\varepsilon(\varphi, \psi) = -\sum_{x,y} \varepsilon e^{\frac{\varphi(x) - \psi(y) - c(x,y)}{\varepsilon}} + \sum_{x \in X} \varphi(x) \mu_x - \sum_{y \in Y} \psi(y) \nu_y
$$

Remark 19. Remark that in this dual formulation, similarly to the primal formulation, the exponential is a barrier function that imposes when ε tends to zero

$$
\varphi(x) - \psi(y) \leqslant c(x,y)
$$

9.3. Strong duality.

> **Theorem 40** (Strong duality and existence of duals)**.**
> - *There exists φ and ψ such that*
> $$
> (\mathrm{KP})^\varepsilon = (\mathrm{DP})^\varepsilon = \mathcal{K}_\varepsilon(\varphi, \psi).
> $$
> - *A maximizer (φ, ψ) allows to recover an optimal solution γ^ε by the formula*
> $$
> \gamma_{x,y} = e^{\frac{\varphi(x) - \psi(y) - c(x,y)}{\varepsilon}}.
> $$

Proof.
• Weak duality $(\mathrm{KP}^\eta) \geqslant (\mathrm{DP}^\eta)$ always hold. To prove the strong duality, we denote by γ^* the solution to (KP^η), and we note that by Theorem 37, $\gamma_{xy}^* > 0$ for all $(x,y) \in X \times Y$. This implies that the optimized functional $\gamma \mapsto \langle c | \gamma \rangle + \eta H(\gamma)$ is $\mathcal{C}^1$ in a neighborhood of γ^*. Thus, there exists Lagrange multipliers for the equality constrained problem, i.e. $\tilde{\varphi} \in \mathbb{R}^X$ and $\tilde{\psi} \in \mathbb{R}^Y$ such that

$$
\nabla_\gamma L(\gamma^*, \tilde{\varphi}, \tilde{\psi}) = 0.
$$

Since the function $L(\cdot, \tilde{\varphi}, \tilde{\psi})$ is convex, this implies that $\gamma^* = \mathrm{argmin}_\gamma L(\gamma, \tilde{\varphi}, \tilde{\psi})$. Hence

$$(\mathrm{DP}^\eta) = \sup_{\varphi, \psi} \min_\gamma L(\gamma, \varphi, \psi) \geqslant \min_\gamma L(\gamma, \tilde{\varphi}, \tilde{\psi}) = L(\gamma^*, \tilde{\varphi}, \tilde{\psi}) = (\mathrm{KP}^\eta).$$

The last equality follows from the fact that γ^* satisfies the constraints and is a solution to (KP^η). Thus $(\mathrm{DP}^\eta) = (\mathrm{KP}^\eta)$.

• The second point has already been proved. $\square$

9.4. **Sinkorn algorithm.** The numerical resolution of this problem has been addressed by Bregman in 1967 to solve a strictly convex problem by iteratively projecting on two convex sets, by Sinkor and Knopp in 1967 who proposed a converging diagonal scaling technique, and by Cuturi in 2013 who applied these algorithms to the regularized optimal transport problem.

The goal is to optimize the function $\mathcal{K}_\varepsilon$, Sinkorn's algorithm is going to increase it by iteratively changing the dual variables φ and ψ.

Proposition 41. *Let* $u(x) = e^{\frac{\varphi(x)}{\varepsilon}}$, $v(y) = e^{\frac{-\psi(y)}{\varepsilon}}$ *and the Gibbs Kernel* $K(x,y) = e^{\frac{-c(x,y)}{\varepsilon}}$.

$$
1) \quad \varphi \text{ maximizes } \mathcal{K}_\varepsilon(\cdot, \psi) \quad \Leftrightarrow \quad \forall x \quad u(x) = \frac{\mu_x}{\sum_y K(x,y)v(y)}
$$

$$
2) \quad \psi \text{ maximizes } \mathcal{K}_\varepsilon(\varphi, \cdot) \quad \Leftrightarrow \quad \forall y \quad v(y) = \frac{\nu_y}{\sum_x K(x,y)u(x)}
$$

$$
3) \quad (\varphi, \psi) \text{ maximizes } \mathcal{K}_\varepsilon \quad \Leftrightarrow \quad \forall x, y \quad \gamma_{x,y} = u(x)K(x,y)v(y).
$$

Proof. Recall that $\mathcal{K}_\varepsilon$ is given by

$$\mathcal{K}_\varepsilon(\varphi, \psi) = -\varepsilon \Big(\sum_x e^{\frac{\varphi(x)}{\varepsilon}} \sum_y e^{\frac{-\psi(y) - c(x,y)}{\varepsilon}} + \sum_{x \in X} \varphi(x)\mu_x - \sum_{y \in Y} \psi(y)\nu_y \Big)$$

So its gradient with respect to $\varphi_x = \varphi(x)$ is given by

$$\frac{\partial \mathcal{K}_\varepsilon}{\partial \varphi_x}(\varphi, \psi) = -e^{\frac{\varphi(x)}{\varepsilon}} \sum_y e^{\frac{-\psi(y) - c(x,y)}{\varepsilon}} + \mu_x$$

Therefore

$$\frac{\partial \mathcal{K}_\varepsilon}{\partial \varphi_x}(\varphi, \psi) = 0 \Leftrightarrow u(x) \sum_y K(x,y)v(y) = \mu_x,$$

which allows to conclude. The second part is similar. The last point has already been proved. $\square$

Remark 20. Now, if we see u and v as vectors and K as a matrix, this reads $u = \mu/(Kv)$ and $v = \nu/(K^t u)$, where the division is entry-wise. Furthermore, if (φ, ψ) is a maximizer, then the optimal transport plan is given by

$$\gamma = \mathrm{diag}(u)K\mathrm{diag}(v).$$

Remark 21. At every step, Sinkorn algorithm amounts to project the current matrix $P = \mathrm{diag}(u)K\mathrm{diag}(v)$ iteratively onto the sets on constraints $C^1 = \{P, P\mathbf{1}_m = \mu\}$ and $C^2 = \{P, P^t\mathbf{1}_n = \nu\}$. Indeed, given u and v, we consider $P = \mathrm{diag}(u)K\mathrm{diag}(v)$ (Note that P is not an optimal transport plan). Then

$$P \in C^1 \Leftrightarrow P\mathbf{1}_m = \mu \Leftrightarrow \mathrm{diag}(u)K\mathrm{diag}(v)\mathbf{1}_m = \mathrm{diag}(u)Kv = \mu \Leftrightarrow u = \mu/(Kv)$$

Similarly

$$P \in C^2 \Leftrightarrow v = \nu/(K^t u)$$

Algorithm 2 Sinkorn's algorithm

Function: OT_EntropicRegularization$(\mu, \nu, C, \varepsilon)$.

    Initialization: $v^0 = \mathbf{1}_n$; $K = e^{C/\varepsilon}$

    Repeat:

        : $u^{k+1} = \mu/(Kv^k)$

        : $v^{k+1} = \nu/(K^t u^{k+1})$

    Until: stopping criteria

    Return: $\gamma = \text{diag}(u_{k+1})K\text{diag}(v_{k+1})$.

9.5. **Convergence of the algorithm.** The Hilbert projective metric is adapted to state the convergence since we expect the outputs u and v are a solutions up to the multiplication by a scalar. (To be more precise if we multiply u by λ and v by $1/\lambda$, the solution remains unchained.)

Definition 17. The Hilbert projective metric $d_{\mathcal{H}}$ on the space $\mathbb{R}_{+*}^n$ is defined by

$$d_{\mathcal{H}}(u,v) = \ln \max_{i,j} \frac{u_i v_j}{u_j v_i}$$

Theorem 42 (Birkhoff, 1967)**.** *Let $K \in \mathbb{R}_{+*}^{n \times m}$ be a matrix with positive entries, then for every u and v in $\mathbb{R}_{+*}^m$ one has*

$$d_{\mathcal{H}}(Ku, Kv) \leqslant \lambda(K) d_{\mathcal{H}}(u,v) \quad where \quad \begin{cases} \lambda(K) = \frac{\sqrt{\eta(K)}-1}{\sqrt{\eta(K)}+1} < 1 \\ \eta(K) = \max_{i,j,k,l} \frac{K_{i,j} K_{k,l}}{K_{i,k} K_{j,l}} \end{cases}$$

Theorem 43. *Sinkorn algorithm has a linear convergence to the fixed point solution (u^*, v^*), namely*

$$d_{\mathcal{H}}(u_k, u^*) \leqslant \lambda(K)^{2k-1} d_{\mathcal{H}}(v_0, v^*) \quad and \quad d_{\mathcal{H}}(v_k, v^*) \leqslant \lambda(K)^{2k} d_{\mathcal{H}}(v_0, v^*)$$

Proof. First remark that for every u and v, one has

$$d_H(u,v) = d_{\mathcal{H}}(u/v, \mathbf{1}_n) = d_{\mathcal{H}}(1/v, 1/u).$$

This implies that

$$d_{\mathcal{H}}(u_{k+1}, u^*) = d_{\mathcal{H}}\left(\frac{\mu}{Kv_k}, \frac{\mu}{Kv^*}\right) = d_{\mathcal{H}}(Kv_k, Kv^*) \leqslant \lambda(K) d_{\mathcal{H}}(v_k, v^*)$$

Similarly $d_{\mathcal{H}}(v_{k+1}, v^*) \leqslant \lambda(K) d_{\mathcal{H}}(u_k, u^*)$, which allows to conclude. $\qquad\square$

9.6. **Numerics comments. Complexity.** The main complexity is in the product matrix Kv or $K^t u$.

- General cost function. The complexity is $O(n^2)$.
- Wasserstein cost on a regular grid. In that case, we have $K_{x,y} = k_{x-y}$, therefore each product $u = Kv$ is a convolution $u = k \star v$. Note that the matrix has therefore a Toeplitz structure (constant coefficient on each 1st, 2nd, etc diagonals). The complexity of the multiplication with such a matrix is $O(n \ln(n))$.

- Truncating the Gibbs Kernel make it almost diagonal and leads an approximation for which the complexity of the matrix product is $O(n)$.
- Cost $d_M(x, y)^p$ on a manifold M. In that case, d_M can be approximated by using Varadhan's formula (involving the Laplace-Beltrami operator) which leads to a nearly linear multiplication.

Number of steps. When ε decreases, we numerically observe an increase of the number of steps.

Stabilization techniques. When ε tends to zero, K tends to 0, which create some instabilities (u and v might be infinite). Chizat et al 2006, as well as Schmitzer et al in 2006 propose to stabilize by multiplying u and v accordingly at every step. However, this create a new kernel $\tilde{K}$ which is not Toeplitz anymore.

Acceleration techniques. There are also some scaling techniques to accelerate (Schmitzer et al 2006). The scaling technique is then combined with stabilization (papers from Schmitzer).

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