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Katharina Eichinger

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**THÈSE DE DOCTORAT**

**DE L'UNIVERSITÉ PSL**

Préparée à l'Université Paris Dauphine

**Problèmes variationnels pour l'interpolation dans l'espace  
de Wasserstein**

Soutenue par

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# Chapter 1

## Introduction

Optimal transportation dates back to the work by Monge in 1781 [88]. The modern formulation has then been introduced in 1942 by Kantorovich [66] as one of the first problems in linear programming. Kantorovich's formulation of optimal transport can be derived as follows.

Given a certain amount of mass  $m > 0$ , we want to move it from position  $x \in X$  to  $y \in Y$  at a certain cost per unit of mass  $c(x, y)$ , where  $X$  and  $Y$  are suitable sets. This gives the total cost of  $mc(x, y)$  to transport all of it, and it is also the optimal cost since there is just one way to move the mass: everything goes from  $x$  to  $y$ . What if the mass is not located at one point but rather distributed on a set of points and to be transported to a set of points? Mathematically, this is modeled by (positive) measures  $\rho \in \mathcal{M}(X)$ ,  $\nu \in \mathcal{M}(Y)$  where the initial mass  $\rho(X)$  should be equal to the target mass  $\nu(Y)$ , so  $\rho(X) = \nu(Y) = m$ . Now, the way Kantorovich modeled the transportation of mass between the two measures is to consider a measure on the product space  $\gamma \in \mathcal{M}(X \times Y)$  which has suitable marginals, i.e.  $\gamma(\cdot \times Y) = \rho$  and  $\gamma(X \times \cdot) = \nu$ . We write  $\gamma \in \Pi(\rho, \nu)$ . This means that for two sets  $A \subset X$ ,  $B \subset Y$  the quantity  $\gamma(A \times B)$  encodes how much mass is transported from  $A$  to  $B$ . Or, if one is thinking more in probabilistic terms, for  $m = 1$ , it gives us a coupling between two random variables distributed according to  $\rho$  and  $\nu$ . In order to choose a coupling which is optimal, we are interested in minimizing the total (or in probabilistic terms average w.r.t.  $\gamma$ ) cost. This yields the optimal transportation (OT) problem

$$W_c(\rho, \nu) := \inf \left\{ \int_{X \times Y} c(x, y) d\gamma(x, y) : \gamma \in \Pi(\rho, \nu) \right\}. \quad (1.0.1)$$

The OT problem gives a measure of discrepancy between the two measures  $\rho$  and  $\nu$ , which translates well the relationship between elements in the underlying spaces given by the cost function  $c$  in the following sense. If we naturally embed two points and their total mass into the space of measures by identifying them with their weighted Dirac masses and define the transport cost between two measures  $\rho$  and  $\nu$

$$\bar{W}_c(\rho, \nu) := \begin{cases} mc(x, y) & \text{if } \rho = m\delta_x, \nu = m\delta_y, \\ +\infty & \text{else,} \end{cases} \quad (1.0.2)$$

then (under very mild assumptions on the spaces) (1.0.1) is the lower semicontinuous convex envelope of (1.0.2), i.e. the somehow closest convex problem on the space of measures. This has been shown recently in [106]. Hopefully, this serves as a mathematical intuition that

the OT problem translates geometrical or topological properties of the underlying spaces, encoded in the cost function  $c$ , to the spaces of measures equipped with the corresponding OT cost.

As such it has become a popular in fields like economics [33, 35, 57], data science [70, 75, 87, 96], physics [17, 22, 41] and several other areas.

Let us now take  $m = 1$  from now on, as the exact total mass does not matter for our purposes. Then, OT can be seen as matching two probability distributions in an optimal way as to minimize the average cost. This has been extended in [33] to matching of several probability measures. One formulation of the multi-matching problem in [33] is given as the following variational problem over several OT functionals.

$$\inf \left\{ \sum_{i=1}^N W_{c_i}(\rho, \nu_i) : \rho \in \mathcal{P}(Y) \right\}. \quad (1.0.3)$$

The goal of this thesis is to study certain variants of this problem.

Suppose that the cost functions  $c_i$  are given such that (1.0.3) becomes the minimization problem of a convex combination of OT functionals depending on the same cost  $c$

$$\inf \left\{ \sum_{i=1}^N p_i W_c(\rho, \nu_i) : \rho \in \mathcal{P}(Y) \right\},$$

which equivalently means minimizing the expectation w.r.t. the probability measure  $P = \sum_{i=1}^N p_i \delta_{\nu_i}$  on the space of probability measures

$$\inf \{ \mathbb{E}_{\nu \sim P} [W_c(\rho, \nu)] : \rho \in \mathcal{P}(Y) \}. \quad (1.0.4)$$

The probabilistic interpretation of this variational problem dates back to Fréchet [56], where he was interested in generalizing probabilistic notions established for (number valued) random variables to more general random objects, which do not necessarily have values in a vector space. Motivated by the observation that a *typical element* (in French *élément typique*), like the median or mean, of a real-valued random variable solves a variational problem, he defines the following generalizations. As soon as we are given a metric space  $(\mathcal{E}, d)$  and a random variable  $U$  with values in  $\mathcal{E}$ , a solution of

$$\inf \{ \mathbb{E} [d(a, U)] : a \in \mathcal{E} \} \quad (1.0.5)$$

can be seen as *median* or *equiprobable position* (in French *position équiprobable*) of  $U$ , and a solution of

$$\inf \{ \mathbb{E} [d(a, U)^2] : a \in \mathcal{E} \} \quad (1.0.6)$$

is the (non-linear) analogue of an *expectation* or *mean position* (in French *position moyenne*).

Going back to the OT problem, if one chooses the cost function  $c$  in a way such that  $W_c$  becomes a metric distance, we can interpret a solution to (1.0.4) as a typical element of a measure valued random variable. Two of the works presented in this thesis are inspired by this observation.

The thesis is structured as follows. We give an overview of the preliminaries required in Chapter 2. Starting with a non-exhaustive overview of optimal transport theory with a focus on results needed in our work, we provide the link to the Monge-Ampère equation and highlight the case when the cost function is given by the power of a metric, making

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the optimal transport functional (up to a power) a metric as well. We then list different characterizations of the multi-matching problem (1.0.3) and give the most important properties and challenges of the Wasserstein barycenter, a special case of the multi-matching problem. Finally, we discuss the entropic regularization of optimal transport and explain the Sinkhorn algorithm from the primal and dual perspective.

The next three chapters contain our scientific contributions, each chapter corresponding to one work.

### Chapter 3: Entropically regularized Wasserstein barycenters

Chapter 3 is based on joint work with G. Carlier and A. Kroshnin [32] and studies a regularized version of the case of quadratic cost  $c_i(x, y) = |x - y|^2$  on  $\mathbb{R}^d \times \mathbb{R}^d$  in (1.0.4). The unregularized version has been introduced in [1] as a generalization of the Euclidean barycenter problem to the Wasserstein space of order 2. In the spirit of Fréchet, it can be seen as a mean in the space of probability measures as in (1.0.6) since  $W_{|\cdot|^2}$ , commonly denoted  $W_2^2$  in the literature, turns out to be the square of a metric on the space of probability measures with finite second moment  $\mathcal{P}_2(\mathbb{R}^d)$ . It has since gained a lot of popularity in image processing [101, 100, 110], statistics [91, 111, 115, 13], data analysis and machine learning [43, 45, 62, 63] and economy [33]. In order to tackle regularity issues, the following problem is considered

$$\inf_{\rho \in \mathcal{P}_2(\mathbb{R}^d)} \frac{1}{2} \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\rho, \nu) dP(\nu) + \lambda E(\rho), \quad (1.0.7)$$

where  $E$  is a penalization aiming to regularize the barycenter. This problem has been introduced in [10] for a variety of penalization terms. In Chapter 3 the relative entropy w.r.t. the Lebesgue measure is used as a penalization term  $E$ . We call any solution entropic Wasserstein barycenter. After providing existence and uniqueness under mild conditions, analytical properties are studied. Notably, some global bounds and a maximum principle are proved. Under stronger hypothesis, higher regularity of the entropic Wasserstein barycenter are provided. Then the stochastic setting is considered where the expectation with respect to  $P$  in (1.0.7) is replaced by its empirical counterpart. Namely, for  $(\nu_i)_{i \in \mathbb{N}^*} \subset \mathcal{P}_2(\mathbb{R}^d)$  with  $\nu_i \sim P$  independent and identically distributed consider

$$\inf_{\rho_n \in \mathcal{P}_2(\mathbb{R}^d)} \frac{1}{2} \sum_{i=1}^n W_2^2(\rho_n, \nu_i) + \lambda E(\rho).$$

Then with the help of stability properties of the entropic Wasserstein barycenter a law of large numbers is deduced. Finally, inspired by a general proof strategy to establish a central limit theorem (CLT) on Riemannian manifolds, a central limit theorem for the entropic Wasserstein barycenter is provided. The crucial part is to prove that the map

$$\Phi_\nu : \rho \mapsto \varphi_\rho^\nu,$$

is continuously differentiable in a suitable space. This is explained in more detail in Section 3.5.2. We then provide three explicit cases where one has enough regularity for the CLT. The case where all measures are sufficiently regular and supported on a ball (as a prototype for a smooth convex set), the case of the torus and the semi-discrete setting where we rely on the analysis of [68].

## Chapter 4: Wasserstein medians

After the success of Wasserstein barycenters in various applications, it is reasonable to study the equivalent of a median on the space of probability measures. This is done in Chapter 4 by considering (1.0.4) for the cost function  $c(x, y) = d(x, y)$  where  $d$  is a metric of an underlying suitable metric space. It based on an ongoing work with G. Carlier and E. Chenchene [29]. In this case  $W_d$ , often also denoted by  $W_1$  in the literature, defines a metric on the space of probability measures with finite first moment. In view of the observation by Fréchet (1.0.5) a solution of

$$\inf \left\{ \sum_{i=1}^N p_i W_1(\rho, \nu_i) : \rho \in \mathcal{P}_1(Y) \right\}$$

is defined to be a Wasserstein median. One of the main statistical advantages of a median object, its robustness with respect to corrupted data is discussed. This is quantified by the so-called breakdown point of a statistical estimator, which shows a better robustness of the median estimator compared to the mean. After establishing standard properties such as existence and stability of the Wasserstein median, a rigorous study of Wasserstein medians for the underlying metric space  $(\mathbb{R}, |\cdot|)$  is given. We provide a selection procedure for the possibly non-unique Wasserstein median and give some integrability estimates. In contrast to the Wasserstein barycenter, integrability properties from the given data do not seem to carry over to the Wasserstein median in more complicated spaces, such as even  $\mathbb{R}^d$ . We provide a counterexample, providing that a (linear)  $L^\infty$ -bound does not carry over. Nevertheless, various equivalent formulations of the Wasserstein median problem are given. As a convex problem, it is classical to establish its dual formulation. Furthermore, two multimarginal formulations are discussed and various properties of Wasserstein medians are deduced from it. In the end, we display the connection to the Beckmann problem and give a PDE characterization of Wasserstein medians.

## Chapter 5: Constrained Wasserstein interpolation

In Chapter 5, which is based on the preprint [20] in joint work with G. Buttazzo and G. Carlier, we still study problems of the type (1.0.3). This time it is under the slightly different motivation of finding optimal parking places. We are given two probability measures  $\mu_0$ , representing the distribution of a population, and  $\mu_1$ , representing a distribution of facilities. In order to move from their current location to the facilities, residents may either walk directly to their target location, which costs them  $c_1(x, z)$  to go from  $x$  to  $z$ , or take their car (or more environmentally friendly their bike), costing them  $c_0(x, y)$  to move from  $x$  to  $y$ , park it at a parking spot indicated by a measure  $\rho$  (the unknown to be determined) and walk the remaining way, at the cost  $c_1(y, z)$  to move from  $y$  to  $z$ . Denoting the distribution of residents who choose to first take the car by  $0 \leq \nu_0 \leq \mu_0$  to go to the facilities located at  $0 \leq \nu_1 \leq \mu_1$ , the optimal parking location may be mathematically modeled as follows with optimal transport costs.

$$\inf \left\{ \underbrace{W_{c_1}(\mu_0 - \nu_0, \mu_1 - \nu_1)}_{\text{walking directly}} + \underbrace{W_{c_0}(\nu_0, \rho) + W_{c_1}(\rho, \nu_1)}_{\text{driving and walking}} : (\rho, \nu_0, \nu_1) \in \mathcal{S} \right\}, \quad (1.0.8)$$

---

where  $\mathcal{S}$  denotes the set of triplets of measures  $(\rho, \nu_0, \nu_1)$  satisfying

$$0 \leq \nu_0 \leq \mu_0, \quad 0 \leq \nu_1 \leq \mu_1, \quad \text{and} \quad \int d\nu_0 = \int d\nu_1 = \int d\rho,$$

and imposing additional constraints on  $\rho$

- location constraints, that is  $\text{spt } \rho \subset K$ , with a compact set  $K$  a priori given;
- density constraints, that is  $\rho \leq \phi$ , for a given non-negative and integrable function  $\phi$ .

To further study properties of optimal solutions, we then consider the reduced problem (with  $\nu_0$  and  $\nu_1$  fixed)

$$\inf \{W_{c_0}(\nu_0, \rho) + W_{c_1}(\rho, \nu_1) : \rho \in \mathcal{A}\}, \quad (1.0.9)$$

where  $\mathcal{A}$  is the set of probability measures satisfying one of the possible constraints imposed on  $\rho$ , listed above. For the following we restrict the analysis to compactly supported measures on  $\mathbb{R}^d$ . We start by establishing existence of minimizers and reformulations, such as the dual problem and a multimarginal formulation. In the case of density constraint, we give mild sufficient conditions for optimizers to be of bang-bang type, i.e. to be of the form  $\mathbb{1}_A \phi$  for some measurable set  $A$ . Then, special attention is given to distance-like costs, more concretely costs of the form  $c_i(x, y) \equiv |x - y|^\alpha$  for  $0 < \alpha \leq 1$ , which all satisfy the triangle inequality. It turns out that under reasonable assumptions (from the model point of view) all optimal  $\rho$  are concentrated on the boundary of the set  $K$ . Nevertheless, it is proven that in this case  $\rho$  is absolutely continuous with respect to the Hausdorff measure, given  $K$  is regular enough and one of the measures discrete and the other one absolutely continuous with respect to the Lebesgue measure. Given the degeneracy of a parking on the boundary, it is reasonable to study the density-constrained problem, which turns out to be of bang-bang type under the same hypothesis as the one for the concentration on the boundary of the location constraint. A mathematically more feasible situation is given if the costs are smooth, strong convex functions of the difference  $x - y$ . Then, we prove an  $L^\infty$ -bound for the part of  $\rho$  which is concentrated in the interior of  $K$  by its link to a Monge-Ampère type equation and an approximation argument.

Finally, we give a numerical scheme to compute solutions of (1.0.8), (1.0.9) and more generally (1.0.3) based on entropic regularization of the transport plans in the formulation of OT. This yields an extension of the celebrated Sinkhorn algorithm. We deduce it from the dual perspective of the entropically regularized formulation.



# Chapter 2

## Preliminaries

In this chapter, we recall the known theory which is used in this thesis. This includes giving a (non-exhaustive) overview of the theory of optimal transport, introducing the variational formulation of the multi-matching problem, discussing the special case of barycenters in the Wasserstein space, explaining the entropically regularized transport problem and giving the link to the celebrated Sinkhorn algorithm.

### 2.1 Optimal transport in a nutshell

We start by reviewing the fundamental properties of optimal transportation theory. For a detailed introduction to the subject we refer to [104, 112, 113], which the following presentation is mainly based on but we also recommend [7, 5].

The optimal transport problem has been introduced by Monge in the 18th century in *Mémoire sur la théorie des déblais et des remblais* [88]. It can be stated as follows.

**Definition 2.1.1.** *Let  $X, Y$  be two Polish spaces. Given  $\rho \in \mathcal{P}(X)$ ,  $\nu \in \mathcal{P}(Y)$  and a Borel measurable cost function  $c : X \times Y \rightarrow \mathbb{R}_+$  the Monge formulation of the optimal transport (OT) problem is given by*

$$\inf \left\{ \int_X c(x, T(x)) d\rho(x) : T \text{ Borel-measurable s.t. } T_{\#}\rho = \nu \right\}, \quad (2.1.1)$$

where  $T_{\#}\rho$  is the push-forward defined just below. In the context of optimal transport a feasible map for (2.1.1) is called a transport map and an optimal solution to (2.1.1) is referred to as an optimal transport (OT) map.

**Definition 2.1.2** (Push-forward). *Let  $X, Y$  be two Polish spaces,  $\rho \in \mathcal{P}(X)$ . We define for  $T : X \rightarrow Y$  Borel measurable the push-forward of  $\rho$  under  $T$ ,  $T_{\#}\rho$  by*

$$T_{\#}\rho(A) = \rho(T^{-1}(A)),$$

for all  $A \subset Y$  Borel measurable.

In the language of OT we call  $T$  a transport map from  $\rho$  to  $\nu := T_{\#}\rho$ .

As it stands the problem turns out to be quite difficult to solve directly due to the non-linear push-forward condition.

A milestone has been made when Kantorovich introduced a relaxation of the Monge problem in 1942 [66]. The Kantorovich formulation of the classical optimal transport problem can be formulated as follows.

**Definition 2.1.3.** Let  $X, Y$  be two Polish spaces. Given  $\rho \in \mathcal{P}(X)$ ,  $\nu \in \mathcal{P}(Y)$  and a Borel measurable cost function  $c : X \times Y \rightarrow \mathbb{R}_+$  the Kantorovich formulation of the optimal transport (OT) problem is given by

$$W_c(\rho, \nu) := \inf \left\{ \int_{X \times Y} c(x, y) d\gamma(x, y) : \gamma \in \Pi(\rho, \nu) \right\}, \quad (\text{OT})$$

where  $\Pi(\rho, \nu)$  is the set

$$\Pi(\rho, \nu) := \{ \gamma \in \mathcal{P}(X \times Y) : \pi_{1\#}\gamma = \rho, \pi_{2\#}\gamma = \nu \},$$

with  $\pi_1 : X \times Y \rightarrow X$ ,  $(x, y) \mapsto x$ ,  $\pi_2 : X \times Y \rightarrow Y$ ,  $(x, y) \mapsto y$  being the projections.

An element of  $\Pi(\rho, \nu)$  is called transport plan and a minimizer of (OT) is referred to as optimal transport plan or OT plan.

*Remark 2.1.4.* Note that a transport map  $T$  from  $\rho$  to  $\nu$  always induces a transport plan  $\gamma$  by setting  $\gamma = (\text{id}, T)_{\#}\rho$ . This implies that we always have

$$(2.1.1) \geq (\text{OT}).$$

If there is an OT plan induced by a map, then clearly (2.1.1) = (OT). More generally, in [99] Pratelli showed that if one of the measures is non-atomic and the cost function  $c$  continuous, then the values of the two problems coincide, regardless of the fact if an OT plan is induced by a map.

*Remark 2.1.5.* The OT problem can be restated in probabilistic form

$$\inf \{ \mathbb{E} [c(U, V)] : U \sim \rho, V \sim \nu \}, \quad (2.1.2)$$

where  $U \sim \rho$  means that the random variable  $U$  is distributed according to the probability measure  $\rho$ .

If we assume  $X = Y = \mathbb{R}^d$  equipped with the Euclidean norm  $|\cdot|$  and take as a cost function  $c(x, y) = |x - y|^2$ , then by developing the squares, the OT problem amounts to maximizing the covariance among all couplings of random variables with given marginal laws. From this, one can expect that an optimal plan (if it exists) should be *deterministic* if possible, in the sense that for a given map  $T : X \rightarrow Y$  one would hope for  $V = T(U)$  for an optimal coupling of (2.1.2) or in other terminology the optimal transport plan of (OT) should be of the form  $(\text{id}, T)_{\#}\rho$ .

We will see in the following that this is true under some regularity assumptions on the measure  $\rho$  and the cost function  $c$ .

The Kantorovich formulation of the OT problem is a (infinite dimensional) linear programming problem. As such, under mild hypothesis one can guarantee existence of a minimizer.

**Theorem 2.1.6.** Let  $X, Y$  be Polish spaces,  $\rho \in \mathcal{P}(X)$ ,  $\nu \in \mathcal{P}(Y)$  and  $c : X \times Y \rightarrow \mathbb{R}_+$  lower semicontinuous. Then (OT) admits an optimal solution.

*Proof.* The proof is by now a standard argument called direct method in calculus of variations. It is based on the fact that the set of transport plans  $\Pi(\rho, \nu)$  is compact in the

narrow topology, that is the weak topology  $\sigma(\mathcal{P}(X \times Y), C_b(X \times Y))$  in duality with continuous and bounded functions. This guarantees existence of an accumulation point of any minimizing sequence. To guarantee optimality of this accumulation point, it sufficient that

$$\gamma \mapsto \int_{X \times Y} c(x, y) d\gamma(x, y)$$

is lower semicontinuous w.r.t. the narrow topology. The latter is obvious if  $c$  is continuous and bounded and can be extended to lower semicontinuous  $c$  by approximation from below. We refer to Chapter 1.1 in [104].  $\square$

Note that under the hypothesis of Theorem 2.1.6 the optimal value of (OT) may be  $+\infty$ . Then (trivially) every plan is “optimal”.

For convex optimization problems, it is natural to consider their dual formulation.

**Theorem 2.1.7** (Kantorovich duality, Theorem 5.10 (i) [113]). *Let  $X, Y$  be Polish spaces,  $\rho \in \mathcal{P}(X)$ ,  $\nu \in \mathcal{P}(Y)$  and  $c : X \times Y \rightarrow \mathbb{R}_+$  lower semicontinuous. Then the OT problem (OT) admits the following dual formulation*

$$\begin{aligned} & \sup_{(\varphi, \psi) \in L^1(X, \rho) \times L^1(Y, \nu)} \left\{ \int_X \varphi(x) d\rho(x) + \int_Y \psi(y) d\nu(y) : \varphi(x) + \psi(y) \leq c(x, y) \right\} \\ = & \sup_{(\varphi, \psi) \in C_b(X) \times C_b(Y)} \left\{ \int_X \varphi(x) d\rho(x) + \int_Y \psi(y) d\nu(y) : \varphi(x) + \psi(y) \leq c(x, y) \right\}, \end{aligned} \quad (\text{OT}^*)$$

in the sense that strong duality holds

$$(\text{OT}) = (\text{OT}^*).$$

Note, that we have *weak duality* immediately by definition of the problems, i.e.

$$(\text{OT}) \geq (\text{OT}^*).$$

The proof of the equality in Theorem 2.1.7 can be done in several ways. A proof based on Fenchel-Rockafellar duality is given in the proof of Theorem 1.3 [112]. We sketch a proof employing  $c$ -cyclical monotonicity from the proof of Theorem 5.10 [113].

**Definition 2.1.8** (Cyclical monotonicity). *Let  $X, Y$  be two sets,  $c : X \times Y \rightarrow \mathbb{R}_+$ . A set  $\Gamma \subset X \times Y$  is called  $c$ -cyclically monotone if for all  $N \in \mathbb{N}^*$ ,  $\{(x_i, y_i)\}_{i=1}^N \subset \Gamma$  and permutations  $\sigma$  of  $\{1, \dots, N\}$*

$$\sum_{i=1}^N c(x_i, y_i) \leq \sum_{i=1}^N c(x_i, y_{\sigma(i)}).$$

For continuous cost functions it is quite straightforward to show that an OT plan  $\gamma$  is  $c$ -cyclically monotone. A lemma from convex analysis stated first by Rockafellar (for the cost function  $c(x, y) = -x \cdot y$ ) characterizes  $c$ -cyclically monotone sets to be contained in the  $c$ -superdifferential of a  $c$ -concave function, see the following definition.

**Definition 2.1.9.** *Let  $X, Y$  be Polish spaces,  $c : X \times Y \rightarrow \mathbb{R}_+$ . For the functions  $f : X \rightarrow \mathbb{R} \cup \{-\infty, +\infty\} =: \bar{\mathbb{R}}$ ,  $g : Y \rightarrow \bar{\mathbb{R}}$  define the following.*

The  $c$ -transform of  $f$  is a function  $f^c : Y \rightarrow \bar{\mathbb{R}}$  defined as

$$f^c(y) := \inf_{x \in X} \{c(x, y) - f(x)\}. \quad (2.1.3)$$

If there exists  $f : X \rightarrow \bar{\mathbb{R}}$  such that  $g = f^c$  and  $g$  is not identically  $-\infty$ , then  $g$  is called  $c$ -concave.

Similarly, the  $c$ -transform of  $g$  is given by

$$g^c(x) := \inf_{y \in Y} \{c(x, y) - g(y)\}. \quad (2.1.4)$$

The function  $f$  is called  $c$ -concave if there is  $g : Y \rightarrow \bar{\mathbb{R}}$  such that  $f = g^c$  and it is not identically  $-\infty$ .

Finally, the  $c$ -superdifferential of  $f$  at a point  $x \in X$  is given by

$$\partial_c f(x) := \{y \in Y : f(x) + f^c(y) = c(x, y)\},$$

and the  $c$ -superdifferential of  $f$  is

$$\partial_c f = \{(x, y) \in X \times Y : f(x) + f^c(y) = c(x, y)\}.$$

*Remark 2.1.10.* We slightly abuse notation here because we call a priori two different  $c$ -transforms by the same letter. As in most of our arguments in this thesis the cost function  $c$  is symmetric and we do not need this distinction explicitly, this should however not cause any problems.

Assuming the cost function  $c$  is bounded, we can apply the lemma from convex analysis first stated by Rockafeller, whose generalized version can be found in e.g. Theorem 1.37 [104]. Together with Theorem 1.38 [104], which justifies that the support of an OT plan for continuous cost functions is  $c$ -cyclically monotone, we obtain the existence of a proper (i.e. not identically equal to  $\pm\infty$ )  $c$ -concave function  $\varphi : X \rightarrow \bar{\mathbb{R}}$  such that

$$\text{spt}(\gamma) \subset \partial_c \varphi. \quad (2.1.5)$$

Set  $\psi = \varphi^c$ . If additionally  $c$  is bounded, one can check with (2.1.3), (2.1.4) that both  $\varphi$  and  $\psi$  are bounded, hence feasible for (OT\*). This finally leads to the important relation of the optimal plan  $\gamma$  and the constructed  $\varphi, \psi$

$$\begin{aligned} \int_{X \times Y} c(x, y) \, d\gamma(x, y) &= \int_{X \times Y} \varphi(x) + \psi(y) \, d\gamma(x, y) \\ &= \int_X \varphi(x) \, d\rho(x) + \int_Y \psi(y) \, d\nu(y). \end{aligned}$$

Duality for the general case can then be concluded by approximation. We refer to the proof of Theorem 5.10 [113] or Section 1.6.2 [104] for the details of the proof.

*Remark 2.1.11* (Primal-dual optimality conditions). As soon as strong duality holds, we have the following powerful relation. The plan  $\gamma \in \Pi(\rho, \nu)$  is an OT plan (a minimizer of (OT)) and  $(\varphi, \psi) \in L^1(X, \rho) \times L^1(Y, \nu)$  is a solution for the dual problem (OT\*) if and only if

$$\begin{aligned} \varphi(x) + \psi(y) &\leq c(x, y) \text{ for every } (x, y) \in X \times Y, \\ \varphi(x) + \psi(y) &= c(x, y) \text{ for } \gamma\text{-a.e. } (x, y). \end{aligned} \quad (2.1.6)$$

We see in the following how we can deduce geometric properties of the OT plan from (2.1.6) under some regularity assumptions.

*Remark 2.1.12* (Restriction to  $c$ -concave functions). A standard trick is to observe that one can always replace a feasible pair  $(\varphi, \psi) \in C_b(X) \times C_b(Y)$  of  $(\text{OT}^*)$  by the  $c$ -concave pair  $(\varphi^{cc}, \varphi^c)$  since by definition of the  $c$ -transforms (Definition 2.1.9) this pair satisfies

$$c(x, y) \geq \varphi^{cc}(x) + \varphi^c(y)$$

and a straightforward computation yields

$$\varphi^{cc}(x) \geq \varphi(x) \text{ and } \varphi^c(y) \geq \psi(y).$$

This implies that  $(\varphi^{cc}, \varphi^c)$  is both feasible and does not decrease the value of the objective function of  $(\text{OT}^*)$ . This means that

$$(\text{OT}^*) = \sup \left\{ \int_X \varphi(x) d\rho(x) + \int_Y \varphi^c(y) d\nu(y) : \varphi \in C_b(X) \text{ } c\text{-concave} \right\}, \quad (2.1.7)$$

which we have already used in the proof sketch for Kantorovich duality (Theorem 2.1.7).

While strong duality holds in a quite general framework, as announced in Theorem 2.1.7, one needs to impose additional assumptions on the cost function to obtain existence of solutions of the dual problem. We give two sufficient conditions in the following theorem, the first one already used in the proof sketch of Theorem 2.1.7.

**Theorem 2.1.13** (Theorem 1.39 [104], Theorem 5.10 (iii) [113]). *Let  $X, Y$  be Polish spaces,  $\rho \in \mathcal{P}(X)$ ,  $\nu \in \mathcal{P}(Y)$  and  $c : X \times Y \rightarrow \mathbb{R}_+$  be lower semicontinuous. Then,*

- *If  $c$  is in addition bounded and uniformly continuous, then  $(\text{OT}^*)$  admits a solution  $(\varphi, \psi) \in C_b(X) \times C_b(Y)$ .*
- *If there are  $(c_X, c_Y) \in L^1(X, \rho) \times L^1(Y, \nu)$  s.t.*

$$c(x, y) \leq c_X(x) + c_Y(y),$$

*then  $(\text{OT}^*)$  admits a solution  $(\varphi, \psi) \in L^1(X, \rho) \times L^1(Y, \nu)$ .*

*Optimal solutions are called Kantorovich potentials.*

*Remark 2.1.14* (Non-uniqueness of Kantorovich potentials). Clearly, if  $(\varphi, \psi)$  are Kantorovich potentials, then the pair  $(\varphi + k, \psi - k)$  for any  $k \in \mathbb{R}$  is optimal as well. Even up to this translation, uniqueness cannot be guaranteed. We state sufficient conditions for uniqueness in Remark 2.1.20.

With this at hand one can prove sparsity of the optimal transport plans, in the sense that they are induced by a map, i.e. an optimal  $\gamma$  is of the form  $\gamma = (\text{id}, T)_\# \rho$  for a (Borel) measurable map  $T : X \rightarrow Y$ . In this case  $T$  is an optimal solution to Monge's original problem formulation (2.1.1), see also Remark 2.1.4. The first proof of this geometrical property of optimal transport plans has been established by Brenier [18] and further been generalized by Gangbo and McCann [59]. A quite general sufficient condition for the existence of a Monge map is given in Theorem 5.30 [113], which essentially requires the  $c$ -superdifferential of a  $c$ -concave function at  $x \in X$  to have only one element  $\rho$ -a.e.

We present a special case of this assumption, assuming regularity of  $c$  ensuring this condition, similar to the arguments introduced in [59]. The proof relies on the differential structure of the underlying space and the so-called *twist condition* of the underlying cost function  $c$ . We state it on  $\mathbb{R}^d$ .

**Definition 2.1.15.** *The function  $c : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$  satisfies the so-called twist condition if  $x \mapsto c(x, y)$  is differentiable for all  $(x, y) \in \mathbb{R}^d \times \mathbb{R}^d$  and for  $x \in \mathbb{R}^d$  fixed*

$$y \mapsto \nabla_x c(x, y) \tag{2.1.8}$$

is injective.

With this condition at hand we can give sufficient conditions for existence of maps. In the interest of readability, we formulate the theorem for the special case that the cost function  $c(x, y) = h(x - y)$  for a nice convex function  $h$  as this is what we need in this thesis. This has been first proved by Gangbo and McCann in Theorem 1.2 [59]. More general sufficient conditions are given in Theorem 10.28 [113]. We state here a slightly weaker version than the original one from Gangbo and McCann.

**Theorem 2.1.16.** *Let  $X = Y = \mathbb{R}^d$ . Suppose that  $c(x, y) = h(x - y)$  for a strictly convex function  $h \in C^1(\mathbb{R}^d, \mathbb{R})$  satisfying in addition*

- $h(x)/|x| \rightarrow +\infty$  as  $|x| \rightarrow \infty$ ,
- For  $r \in \mathbb{R}_+$ ,  $\theta \in (0, \pi)$  whenever  $p \in \mathbb{R}^d$  is far enough from the origin, there exists a cone

$$K(r, \theta, z, p) := \left\{ x \in \mathbb{R}^d : |x - p||z| \cos\left(\frac{1}{2}\theta\right) \leq z \cdot (x - p) \leq r|z| \right\},$$

with  $z \in \mathbb{R}^d \setminus \{0\}$ , such that  $h$  attains its maximum over  $K(r, \theta, z, p)$  at  $p$ .

Then any solution  $\gamma$  to the OT problem (OT) is induced by a map, i.e. there exists  $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$  (Borel) measurable such that

$$\gamma = (\text{id}, T)_{\#}\rho,$$

and the map is unique  $\rho$ -a.e. The explicit form of  $T$  is given by

$$T(x) = (\nabla h)^{-1}(\nabla \varphi(x)),$$

where  $\varphi$  is a  $c$ -concave function whose  $c$ -superdifferential contains the support of an OT plan. If there exist Kantorovich potentials, then  $\varphi$  coincides with a Kantorovich potential  $\rho$ -a.e.

*Proof comment.* The hypothesis give sufficient conditions to be able to differentiate the optimality conditions from Remark 2.1.11 (where if no Kantorovich potentials exist we take the  $c$ -concave function as in (2.1.5) and its  $c$ -transform) as it is shown in [59]. Then we obtain for an OT plan  $\gamma$

$$\nabla \varphi(x) = \nabla_x c(x, y) = \nabla h(x - y) \text{ for } \gamma\text{-a.e. } (x, y).$$

The solvability for  $y$  corresponds to the twist condition (2.1.8) for  $c$ , which is satisfied here thanks to strict convexity of  $h$ . □

*Remark 2.1.17.* Let us mention that convex functions satisfying the conditions of Theorem 2.1.16 include in particular quadratic polynomials and radial functions.

If we restrict ourselves to the compact case, we can give a more general statement without needing to go into technical details “at infinity”.

**Theorem 2.1.18.** *Let  $X \subset \mathbb{R}^d$  be the closure of an open bounded set,  $\mathcal{L}^d(\partial X) = 0$  and  $Y \subset \mathbb{R}^d$  compact. Suppose that  $c : X \times Y \rightarrow \mathbb{R}_+$  satisfies the twist condition (2.1.8) and that it is Lipschitz continuous on  $X \times Y$ . Assume further that  $\rho$  is absolutely continuous.*

*Then any solution  $\gamma$  to the OT problem (OT) is induced by a map, i.e. there exists  $T : X \rightarrow Y$  (Borel) measurable such that*

$$\gamma = (\text{id}, T)_{\#}\rho,$$

*and the map is unique  $\rho$ -a.e. The explicit form of  $T$  is given by*

$$T(x) = (\nabla_x c)^{-1}(\nabla \varphi(x)),$$

*where by  $(\nabla_x c)^{-1}$  we mean the left inverse of (2.1.8) (parametrized by  $x$ ) and  $\varphi$  is a  $c$ -concave Kantorovich potential.*

*Proof comment.* This is a special case of Theorem 10.28 [113] in combination with Remark 10.33 [113].  $\square$

*Remark 2.1.19 (Uniqueness of optimal transport plans).* If every optimal plan  $\gamma$  is given by a map, i.e.  $\gamma = (\text{id}, T)_{\#}\rho$ , then it is the unique optimal plan. This follows directly by convexity of (OT), as stated in Remark 1.19 [104]. Indeed, suppose that there are two optimal plans  $\gamma = (\text{id}, T)_{\#}\rho$ ,  $\tilde{\gamma} = (\text{id}, \tilde{T})_{\#}\rho$  for  $T, \tilde{T}$  (Borel) measurable maps. Then by convexity  $\frac{1}{2}\gamma + \frac{1}{2}\tilde{\gamma}$  must be an optimal plan as well which can only be induced by a map if  $T = \tilde{T}$   $\rho$ -a.e.

*Remark 2.1.20 (Uniqueness of Kantorovich potentials).* As mentioned in Remark 2.1.14 we can only expect uniqueness of Kantorovich potentials up to a constant, in the sense that for two pairs of Kantorovich potentials  $(\varphi_i, \psi_i)_{i=1,2}$  we have

$$\begin{aligned} \varphi_1 - \varphi_2 &= k \mathcal{L}^d\text{-a.e. on } \text{spt } \rho = X \\ \psi_1 - \psi_2 &= -k \nu\text{-a.e.} \end{aligned}$$

for a constant  $k \in \mathbb{R}$ . This condition seems slightly off, but as soon as  $\rho \ll \mathcal{L}^d$  we can replace the first condition by  $\rho$ -a.e. The reason we emphasize that uniqueness of one of the potentials holds  $\mathcal{L}^d$ -a.e. on the support is that later when taking variations of the optimal transport functional in one of the arguments, we need uniqueness of the potentials to hold for these variations, see also the comment after Proposition 7.18 [104].

Uniqueness of the Kantorovich potentials up to a constant is guaranteed if  $X \subset \mathbb{R}^d$  is the closure of a connected open subset,  $\mathcal{L}^d(\partial X) = 0$ ,  $\text{spt } \rho = X$  and sufficient conditions for differentiability of  $c$  and the Kantorovich potentials associated to  $\rho$  are given. Similar to Theorem 2.1.16 or Theorem 2.1.18 two examples for sufficient conditions for differentiability are

- $Y = \mathbb{R}^d$   $c(x, y) = h(x - y)$  for a strictly convex function  $h \in C^1(\mathbb{R}^d, \mathbb{R})$  satisfying the technical conditions as in Theorem 2.1.16, or
- $Y \subset \mathbb{R}^d$  compact, and  $c$  is Lipschitz continuous on  $X \times Y$ .

The proof is a slight generalization of Proposition 7.18 [104]. We sketch it for convenience.

Under the assumptions above, let  $(\varphi_i, \psi_i)$  ( $i = 1, 2$ ) be two pairs of Kantorovich potentials. By strong duality (Remark 2.1.11), we have for an OT plan  $\gamma$  for  $i = 1, 2$

$$\begin{aligned}\varphi_i(x) + \psi_i(y) &\leq c(x, y) \text{ on } X \times Y, \\ \varphi_i(x) + \psi_i(y) &= c(x, y) \text{ on } \text{spt } \gamma.\end{aligned}$$

This implies that  $\varphi_i$  coincides with a  $c$ -concave function on  $\text{spt } \rho = X$ . With the assumptions above it is differentiable  $\mathcal{L}^d$ -a.e. We get

$$\nabla\varphi_1(x) = \nabla_x c(x, y) = \nabla\varphi_2(x)$$

for  $\mathcal{L}^d$ -a.e.  $x \in X$  and  $(x, y) \in \text{spt } \gamma$ . Since  $X$  is connected, this implies that  $\varphi_1 - \varphi_2$  is constant  $\mathcal{L}^d$ -a.e. on  $\text{spt } \rho$ . Now note that  $\psi_i$  coincides with the  $c$ -transform of  $\varphi_i$  ( $i = 1, 2$ )  $\nu$ -a.e., which implies uniqueness up to a constant for it as well  $\nu$ -a.e.

*Remark 2.1.21* (The case of quadratic cost). Let  $X = Y = \mathbb{R}^d$  equipped with the Euclidean norm  $|\cdot|$  and  $\rho$  and  $\nu$  have finite second moments. The case  $c(x, y) = \frac{1}{2}|x - y|^2$  is somewhat special as already pointed out in Remark 2.1.5. By developing the square and putting the second moments to the other side, the strong duality of between (OT) and (OT\*) becomes

$$\sup_{\gamma \in \Pi(\rho, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} x \cdot y \, d\gamma(x, y) = \inf_{(\varphi, \psi) \in L^1(\rho) \times L^1(\nu)} \int_{\mathbb{R}^d} \frac{|x|^2}{2} - \varphi(x) \, d\rho(x) + \int_{\mathbb{R}^d} \frac{|y|^2}{2} - \varphi(y) \, d\nu(y)$$

By Theorem 2.1.13, there are Kantorovich potentials  $\varphi \in L^1(\rho)$ ,  $\psi \in L^1(\nu)$ . So choosing  $u(x) := \frac{|x|^2}{2} - \varphi(x)$  and  $v(y) := \frac{|y|^2}{2} - \varphi(y)$ , the  $c$ -transforms become the classical Legendre transform

$$u^*(y) := \sup_{x \in \mathbb{R}^d} \{x \cdot y - u(x)\}.$$

Hence  $u$  and  $v$  coincide with a convex function on the support of an OT plan. The literature on convex functions and their regularity is vast, see for instance [27], [50] or [102].

Now, assuming that  $\rho$  is absolutely continuous, Theorem 2.1.16 becomes existence of an OT map  $T$ , given by  $T(x) = \nabla u(x)$  for  $\rho$ -a.e.  $x$ , which is the gradient of a convex function. This recovers the initial statement by Brenier [18]. In the literature one often refers to  $u$  as *Brenier potential*.

*Remark 2.1.22.* Under the hypothesis of Theorem 2.1.16 or Theorem 2.1.18, suppose that we have a (Borel) measurable map  $T$  such that  $T_{\#}\rho = \nu$  and for a proper  $c$ -concave function  $\varphi : X \rightarrow \bar{\mathbb{R}}$

$$\varphi(x) + \varphi^c(T(x)) = c(x, T(x)) \quad \rho\text{-a.e.}$$

which equivalently means by considering Definition 2.1.9 that for  $\rho$ -a.e.  $x$  we have  $(x, T(x)) \in \partial_c \varphi$ . Then  $T$  is an OT map, the detailed argument is a slight extension of part of the proof of Theorem 2.12 [112].

While this condition may not be easy to verify for general cost functions, it becomes particularly handy when considering the quadratic case  $c(x, y) = |x - y|^2$ . The fact that  $(x, T(x)) \in \partial_c \varphi$  for  $\rho$ -a.e.  $x$  becomes  $T$  coincides  $\rho$ -a.e. with the gradient of a convex function by Remark 2.1.21.

### 2.1.1 Link with Monge-Ampère equation

We begin by a formal discussion. In the case that the (unique) optimal plan for (OT) is given by  $\gamma = (\text{id}, T)_\# \rho$  for a (Borel) measurable map  $T$ , we have  $T_\# \rho = \nu$ . The functional characterization of this pushforward condition is that for all test functions  $f$  (e.g.  $f \in C_b(Y)$ )

$$\int_{\text{spt } \nu} f(y) \, d\nu(y) = \int_{\text{spt } \rho} f(T(x)) \, d\rho(x).$$

Suppose now that  $X = Y = \mathbb{R}^d$  and both  $\rho$  and  $\nu$  are absolutely continuous w.r.t. the Lebesgue measure  $\mathcal{L}^d$  on  $\mathbb{R}^d$ . By abuse of notation we identify their densities with the same letter. By applying the standard change of variables “ $y = T(x)$ ” we obtain

$$\int_{T^{-1}(\text{spt } \nu)} f(T(x)) \nu(T(x)) |\det(DT(x))| \, dx = \int_{\text{spt } \rho} f(T(x)) \rho(x) \, dx.$$

Since this is true for any test function  $f$  this yields at least formally (with the fundamental lemma of calculus of variations) the Jacobian equation subject to a non-linear “boundary condition”

$$\begin{aligned} \nu(T) |\det(DT)| &= \rho, \text{ on } \text{int}(\text{spt } \rho), \\ \overline{T(\text{spt } \rho)} &= \text{spt } \nu. \end{aligned} \tag{2.1.9}$$

In particular, if we consider the quadratic cost function  $c(x, y) = |x - y|^2$ ,  $\rho, \nu \in \mathcal{P}_2(\mathbb{R}^d)$  with  $\rho$  and  $\nu$  absolutely continuous, we are in the setting of Theorem 2.1.16, so that the optimal plan  $\gamma = (\text{id}, T)_\# \rho$  for a (Borel) measurable map  $T$ . Furthermore, by Remark 2.1.21 we have  $T = \nabla u$   $\rho$ -a.e. for a convex function  $u$ . Plugging this into (2.1.9) we obtain that  $u$  solves the Monge-Ampère equation

$$\begin{aligned} \nu(\nabla u) \det(D^2 u) &= \rho, \text{ on } \text{int}(\text{spt } \rho), \\ \overline{\nabla u(\text{spt } \rho)} &= \text{spt } \nu. \end{aligned} \tag{2.1.10}$$

The above relation can be made somewhat rigorous by employing regularity of convex functions. In that way both  $\nabla u$  and  $D^2 u$  can be defined  $\mathcal{L}^d$ -almost everywhere, see for instance Theorem 4.8 [112] for the case of the quadratic cost function and more generally Theorem 2.1.25 below.

It is natural to ask the question whether higher regularity of the convex function  $u$  can be guaranteed given some hypothesis on the the measures  $\rho$  and  $\nu$ , ensuring even validity of (2.1.10) in the classical sense. A breakthrough has been made with the work by Caffarelli [24, 23, 25]. His results can be summarized as follows

**Theorem 2.1.23** (Theorem 3.3 [44]). *Let  $X, Y \subset \mathbb{R}^d$  be the closure of open bounded sets,  $\rho \in \mathcal{P}_{\text{ac}}(X)$ ,  $\nu \in \mathcal{P}_{\text{ac}}(Y)$ . Suppose that their densities are bounded away from zero and infinity on  $X$ , respectively  $Y$ . Denote by  $T = \nabla u : \text{int } X \rightarrow \text{int } Y$  the optimal transport map for the quadratic cost function  $c(x, y) = |x - y|^2$ . Assume further that  $Y$  is convex. Then,*

- $T \in C_{\text{loc}}^{0, \alpha}(\text{int } X) \cap W_{\text{loc}}^{1, 1 + \varepsilon}(X)$  for some  $\alpha \in (0, 1)$  and some  $\varepsilon > 0$ .
- If in addition  $\rho \in C_{\text{loc}}^{k, \beta}(\text{int } X)$ ,  $\nu \in C_{\text{loc}}^{k, \beta}(\text{int } Y)$  for some  $k \in \mathbb{N}$ ,  $\beta \in (0, 1)$ , then  $T \in C_{\text{loc}}^{k+1, \beta}(\text{int } X)$ .

- If  $X, Y$  are smooth and uniformly convex,  $\rho \in C^{k,\beta}(X)$ ,  $\nu \in C^{k,\beta}(Y)$  for some  $k \in \mathbb{N}$ ,  $\beta \in (0, 1)$ , then  $T : X \rightarrow Y$  is a global diffeomorphism of class  $C^{k+1,\beta}$ .

*Remark 2.1.24.* The convexity of the support of the target measure  $Y$  is crucial. In [24] Caffarelli gave the following counterexample for non-convex support of the target measure.

On  $\mathbb{R}^2$  consider  $\rho$  to be the uniform measure on  $X = \overline{B_1(0)}$  and  $\nu$  the uniform measure on  $Y = (B_1^+ + (1, 0)^T) \cup (B_1^- - (1, 0)^T)$ , where  $B_1^+$  and  $B_1^-$  denote the right and left half discs

$$B_1^+ = \overline{B_1(0)} \cap \{x_1 \geq 0\}, \quad B_1^- = \overline{B_1(0)} \cap \{x_1 \leq 0\}.$$

Then the OT map from  $\rho$  to  $\nu$  is given by  $T(x_1, x_2) = (x_1 + \operatorname{sgn} x_1, x_2)$  since  $T_{\#}\rho = \nu$  and in view of Remark 2.1.22 it suffices to note that it is  $\rho$ -a.e. the gradient of the convex function  $\varphi(x) = |x_1| + \frac{1}{2}|x|^2$ . Clearly  $T$  is not continuous.

If we modify the support of the target measure to be connected by adding a small horizontal strip  $S_\varepsilon := \{|x_2| \leq \varepsilon, |x_1| \leq 1\}$  for  $\varepsilon > 0$  and take  $\nu_\varepsilon$  to be the uniform measure on  $Y_\varepsilon := Y \cup S_\varepsilon$ , then one can show that for  $\varepsilon$  small enough the optimal maps remain discontinuous by stability of the Kantorovich potentials, see [24] for details.

A survey of the regularity theory for the Monge-Ampère equation can be found in [44], where the statement of Theorem 2.1.23 is from. A more detailed introduction to this subject is [54].

Let us mention that for more general convex cost functions Cordero-Erausquin has showed that the derivation of the Jacobian equation can be made rigorous.

**Theorem 2.1.25** (Theorem 4.8 [39]). *Let  $X, Y \subset \mathbb{R}^d$  be the closure of open bounded sets,  $\rho \in \mathcal{P}_{\text{ac}}(X)$ ,  $\nu \in \mathcal{P}_{\text{ac}}(Y)$ . Suppose that the cost function satisfies  $c(x, y) = h(x - y)$  with  $h$  convex and  $h, h^* \in C^2(\mathbb{R}^d)$ . Let  $\varphi$  be a Kantorovich potential associated to  $\rho$ , i.e. an optimal solution to (OT\*), then the optimal transport map  $T$  satisfies  $T(x) = x - \nabla h^*(\nabla \varphi(x))$  a.e. and there is a measurable set  $K \subset X$  with  $\rho(K) = 1$  such that the following equation is well-defined and holds true for all  $x \in K$*

$$\rho(x) = \nu(T(x)) \det (Id - D^2 h^*(\nabla \varphi(x)) D^2 \varphi(x)).$$

### 2.1.2 Wasserstein spaces

If one chooses cost functions depending on the distance of the underlying Polish space, many topological and geometric properties are transferred to the space of probability measures equipped with a distance given by the optimal transport problem (OT), as justified below.

In this section, we take  $X = Y$  a Polish space with metric  $d$  and define the Wasserstein distance as special instance of the optimal transport problem (OT).

**Definition 2.1.26.** *Let  $1 \leq p < \infty$ . The Wasserstein distance of order  $p$  between the measures  $\rho, \nu \in \mathcal{P}_p(X) := \{\rho \in \mathcal{P}(X) : \int_X d^p(x_0, x) d\rho(x) < \infty, x_0 \in X\}$  is defined by*

$$W_p(\rho, \nu) := \inf \left\{ \int_{X \times Y} d^p(x, y) d\gamma(x, y) : \gamma \in \Pi(\rho, \nu) \right\}^{\frac{1}{p}}.$$

The term distance is justified by the following proposition which also characterizes the topology of  $\mathcal{P}_p(X)$  equipped with  $W_p$  as distance.

**Proposition 2.1.27.** *Let  $1 \leq p < \infty$ . The Wasserstein distance of order  $p$  is a metric on  $\mathcal{P}_p(X)$ . Moreover, as soon as  $(X, d)$  is a Polish space, then  $(\mathcal{P}_p(X), W_p)$  is Polish as well. In particular for  $(\rho_n)_{n \in \mathbb{N}} \subset \mathcal{P}_p(X)^{\mathbb{N}}$  and  $\rho \in \mathcal{P}_p(X)$  the following statements are equivalent*

- $\lim_{n \rightarrow \infty} W_p(\rho_n, \rho) = 0$ ,
- $\rho_n$  converges narrowly to  $\rho$  (i.e. in  $\sigma(\mathcal{P}(X), C_b(X))$ ) and for  $x_0 \in X$

$$\lim_{n \rightarrow \infty} \int_X d(x_0, x) d\rho_n(x) = \int_X d(x_0, x) d\rho(x).$$

We call  $(\mathcal{P}_p(X), W_p)$  the Wasserstein space of order  $p$ .

*Proof sketch.* The proof of the triangular inequality relies on the gluing lemma see for instance Lemma 5.4 and 5.5 [104]. The fact that this makes  $(\mathcal{P}_p(X), W_p)$  a Polish space with its characterization for converging sequences is included in Proposition 7.1.5 and Remark 7.1.11 [7].  $\square$

*Remark 2.1.28.* Note that local compactness from  $X$  does not carry over to  $(\mathcal{P}_p(X), W_p)$ . It is actually a necessary condition that  $X$  is compact for local compactness of  $(\mathcal{P}_p(X), W_p)$ , see Remark 7.1.9 [7]. But if  $X$  is compact then  $(\mathcal{P}_p(X), W_p)$  is compact as well. Indeed, by compactness of  $X$  any subset of  $\mathcal{P}(X) = \mathcal{P}_p(X)$  is precompact in the narrow topology by Prokhorov's theorem and the convergence of moments of a converging sequence in  $\mathcal{P}(X)$  follows since the moment is just a bounded continuous function in this case.

Even though not needed in this thesis, we mention for completeness that the dynamic formulation in  $(\mathcal{P}_2(X), W_2)$ .

**Theorem 2.1.29** (Theorem 8.1 [112]). *Let  $X \subset \mathbb{R}^d$  compact,  $\rho, \nu \in \mathcal{P}_{2,ac}(X)$ . Then*

$$W_2^2(\rho, \nu) = \inf \left\{ \int_0^1 \int_X \mu_t(x) |v_t(x)|^2 dx dt : (\mu_t, v_t)_{0 \leq t \leq 1} \in V(\rho, \nu) \right\}$$

where  $V(\rho, \nu)$  is the set of  $(\mu_t, v_t)_{0 \leq t \leq 1}$  satisfying

- $\mu \in C([0, 1], (\mathcal{P}_{ac}(X), \sigma(\mathcal{P}_{ac}(X), C(X))))$ ,
- $v \in L^2(\mu_t \otimes \mathcal{L}_{|[0,1]}^1)$ ,
- $\partial_t \mu_t + \operatorname{div}(v_t v_t) = 0$  in the weak sense,
- $\mu_0 = \rho, \mu_1 = \nu$ .

*Remark 2.1.30.* As observed by Otto [90] the dynamic formulation allows to formally view the Wasserstein space of order 2 as Riemannian manifold. This is further studied and made rigorous in Chapter 8 [7]. We do not go into details here because we only use this interpretation to compare our proof strategy for the CLT of regularized Wasserstein barycenters to the strategy employed on Riemannian manifolds, see Section 5.6.3. Very loosely speaking, in the notation of Theorem 2.1.29 given an optimal solution  $(\mu_t, v_t)_{0 \leq t \leq 1}$ ,  $(\mu_t)_{0 \leq t \leq 1}$  becomes a geodesic between  $\rho$  and  $\nu$  with tangent vector  $v_t$  at the point  $\mu_t$ . The relationship to an optimal Kantorovich potential  $\varphi$  associated to  $\rho$  (i.e. solution to (2.1.7)) is given by  $v_0 = -\nabla \varphi$ , see Proposition 8.5.2 [7]. Hence by fixing the constant of the Kantorovich potential (assuming uniqueness up to a constant) the Kantorovich potentials are isomorphic to the tangent vectors.

A special case of equivalent formulation arises for  $p = 1$ . In order to see that, recall that by Remark 2.1.12 a formulation of the dual problem is given by

$$(\text{OT}) = \sup \left\{ \int_X \varphi(x) d\rho(x) + \int_X \varphi^c(y) d\nu(y) : \varphi \in C(X) \text{ } c\text{-concave} \right\}$$

For simplicity we take  $X \subset \mathbb{R}^d$  a convex set. Then this corresponds to  $c(x, y) = |x - y|$ , which is special since  $c$ -concave functions have a specific characterization.

**Proposition 2.1.31** (Proposition 3.1 [104]). *Let  $X \subset \mathbb{R}^d$  be a convex set,  $c(x, y) = |x - y|$ . Then the set of  $c$ -concave functions on  $X$  coincide with the set 1-Lipschitz functions. Furthermore, for every 1-Lipschitz function  $f$  on  $X$ , we have  $f^c(x) = -f(x)$  for all  $x \in X$ .*

In particular, for  $X \subset \mathbb{R}^d$  a compact convex set with non-empty interior, Lipschitz functions on  $X$  can be identified with the Sobolev space  $W^{1,\infty}(X)$  (see for instance Proposition 2.13 [6]). Taking into account Proposition 2.1.31 and Remark 2.1.12 the Kantorovich duality from Theorem 2.1.7 then becomes

$$(\text{OT}) = \sup \left\{ \int_X \varphi d(\rho - \nu) : \varphi \in W^{1,\infty}(X), |\nabla\varphi| \leq 1 \right\}.$$

Then at least formally the dual is given by the following problem, which represents another equivalent formulation of (OT) in this case.

**Definition 2.1.32** (Beckmann problem). *Suppose that  $X \subset \mathbb{R}^d$  is a compact convex set with non-empty interior,  $\rho, \nu \in \mathcal{P}(X)$ . Then the Beckmann problem is given by*

$$\inf \left\{ \|\sigma\|_{\text{TV}} : \sigma \in \mathcal{M}_{\text{div}}(X, \mathbb{R}^d), \nabla \cdot \sigma = \rho - \nu \right\}, \quad (2.1.11)$$

where  $\mathcal{M}_{\text{div}}(X, \mathbb{R}^d)$  is the space of vector-valued finite Radon measures whose weak divergence is a scalar Radon measure,  $\|\cdot\|_{\text{TV}}$  is the total variation norm

$$\|\sigma\|_{\text{TV}} = \sup_{f \in C(X, \mathbb{R}^d)} \left\{ \int_X f d\sigma : \|f\|_{L^\infty(X, \mathbb{R}^d)} \leq 1 \right\},$$

and the divergence constraint  $\nabla \cdot \sigma = \rho - \nu$  is to be understood weakly with Neumann boundary conditions, i.e. for all  $f \in C^1(X, \mathbb{R})$

$$- \int_X \nabla f d\sigma = \int_X f d(\rho - \nu).$$

The relation to the OT problem is given in the following proposition.

**Proposition 2.1.33** (Theorem 4.6 [104]). *Let  $X \subset \mathbb{R}^d$  be a compact convex set with non-empty interior,  $\rho, \nu \in \mathcal{P}(X)$ . Then the Beckmann problem (2.1.11) and the OT problem (OT) have equal minimal values*

$$(\text{OT}) = (2.1.11).$$

Moreover, given an OT plan  $\gamma$  a solution  $\sigma$  to (2.1.11) is given by  $\sigma$  defined as

$$\int_X f d\sigma := \int_{X \times X} \int_0^1 f((1-t)x + ty) \cdot (x - y) dt d\gamma(x, y),$$

for every  $f \in C(X, \mathbb{R}^d)$ .

## 2.2 The matching for teams problem

The prototype for the problems considered in this thesis has been introduced in Carlier and Ekeland in their paper *Matching for teams* [33] as the following multi-matching problem.

**Definition 2.2.1** (Definition 1 [33]). *Given  $X_1, \dots, X_N, Z$  compact metric spaces, cost functions  $c_i \in C(Z \times X_i)$  and  $\nu_i \in \mathcal{P}(X_i)$  for  $i = 1, \dots, N$ . The family  $\varphi_i \in C(Z)$ ,  $\gamma_i \in \mathcal{P}(Z \times X_i)$  for  $i = 1, \dots, N$  and  $\rho \in \mathcal{P}(Z)$  is called matching equilibrium if*

- for all  $z \in Z$

$$\sum_{i=1}^N \varphi_i(z) = 0,$$

- $\gamma_i \in \Pi(\rho, \nu_i)$  for all  $i = 1, \dots, N$ ,
- for all  $i = 1, \dots, N$

$$\varphi_i(z) + \varphi_i^{c_i}(x_i) = c_i(z, x_i) \quad \text{for } \gamma_i\text{-a.e. } (z, x_i).$$

In their paper they have related the conditions of being a matching equilibrium to a convex optimization problem involving sums of optimal transport functionals and its dual formulation. Indeed, the above mentioned conditions turn out to be the primal-dual optimality conditions.

**Theorem 2.2.2** (Theorem 4 [33]). *In the setting of Definition 2.2.1 consider the coupling  $((\varphi_i)_{i=1}^N, (\gamma_i)_{i=1}^N, \rho) \in C(Z)^N \times \mathcal{P}(Z \times X_1) \times \dots \times \mathcal{P}(Z \times X_N) \times \mathcal{P}(Z)$ . It is a matching equilibrium if and only if*

- $\rho$  solves the convex optimization problem

$$\inf \left\{ \sum_{i=1}^N W_{c_i}(\rho, \nu_i) : \rho \in \mathcal{P}(Z) \right\}, \quad (2.2.1)$$

- $(\varphi_i)_{i=1}^N$  solve its (pre-) dual formulation

$$\sup \left\{ \sum_{i=1}^N \int_{X_i} \varphi_i^{c_i}(x_i) d\nu_i(x_i) : \sum_{i=1}^N \varphi_i = 0 \right\},$$

- for each  $i = 1, \dots, N$   $\gamma_i$  is an OT plan for  $W_{c_i}(\rho, \nu_i)$ .

Finally, finding the equilibrium measure  $\rho \in \mathcal{P}(Z)$  can also be recast as a multimarginal problem by defining the cost function

$$c(x_1, \dots, x_N) := \inf_{z \in Z} \left\{ \sum_{i=1}^N c_i(z, x_i) \right\}. \quad (2.2.2)$$

**Proposition 2.2.3** (Proposition 3 [33]). *Given  $X_1, \dots, X_N, Z$  compact metric spaces, cost functions  $c_i \in C(Z \times X_i)$  and  $\nu_i \in \mathcal{P}(X_i)$  for  $i = 1, \dots, N$ . Define  $c$  as in (2.2.2) and consider*

$$\inf \left\{ \int_{X_1 \times \dots \times X_N} c(x_1, \dots, x_N) d\pi(x_1, \dots, x_N) : \pi \in \Pi(\nu_1, \dots, \nu_N) \right\}. \quad (2.2.3)$$

Then (2.2.3) admits a solution and  $\inf (2.2.3) = \inf (2.2.1)$ . Furthermore, for a solution  $\pi$  of (2.2.3) and for any measurable map  $T : X_1 \times \dots \times X_N \rightarrow Z$  satisfying

$$T(x_1, \dots, x_N) \in \arg \min_{z \in Z} \left\{ \sum_{i=1}^N c_i(x_i, z) \right\},$$

the measure  $\rho := T_{\#}\pi$  is a solution to (2.2.1).

## 2.3 Barycenters in the Wasserstein space

In [1] Agueh and Carlier have introduced and analyzed thoroughly an important special case of the multi-matching problem by taking all costs  $c_i$  to be equal to the quadratic cost function. In analogy to the Euclidean barycenter problem, they define the Wasserstein barycenter.

**Definition 2.3.1** (Wasserstein barycenter). *Let  $\nu_i \in \mathcal{P}_2(\mathbb{R}^d)$  for  $i = 1, \dots, N$  and  $p \in \mathbb{R}_+^N$  such that  $\sum_{i=1}^N p_i = 1$ . A Wasserstein barycenter is a solution to the following variational problem*

$$\inf \left\{ \frac{1}{2} \sum_{i=1}^N p_i W_2^2(\rho, \nu_i) : \rho \in \mathcal{P}(\mathbb{R}^d) \right\}. \quad (\text{B})$$

Several remarks are in place at this stage.

*Remark 2.3.2.* Their terminology comes from the fact that the Wasserstein barycenter is a natural generalization of the (generalized) Euclidean barycenter problem

$$\inf_{x \in \mathbb{R}^d} \left\{ \frac{1}{2} \sum_{i=1}^N p_i |x - x_i|^2 \right\},$$

to the Wasserstein space of order 2. Here  $x_i \in \mathbb{R}^d$ ,  $p_i \in \mathbb{R}_+$   $i = 1, \dots, N$  (with  $\sum_{i=1}^N p_i = 1$ ) are given.

The case  $N = 2$  is a special case of a well-known object in OT introduced by McCann [86].

*Remark 2.3.3.* The Wasserstein barycenter for  $N = 2$  coincides with McCann's displacement interpolation, introduced in [86]. More precisely, given two measures  $\nu_0, \nu_1 \in \mathcal{P}_2(\mathbb{R}^d)$  with  $\nu_0$  absolutely continuous, let  $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$  be the optimal transport map for  $W_2^2(\nu_0, \nu_1)$  (existence is guaranteed by Theorem 2.1.16), McCann's displacement interpolation is defined to be for  $t \in (0, 1)$

$$\nu_t := ((1-t)Id + tT)_{\#}\nu_0.$$

As it turns out  $(\nu_t)_{t \in [0,1]}$  is a constant-speed geodesic in the space  $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ , i.e. for  $0 \leq s \leq t \leq 1$

$$W_2(\nu_s, \nu_t) = (t-s)W_2(\nu_0, \nu_1).$$

Moreover, for  $t \in [0, 1]$ ,  $\nu_t$  is the unique Wasserstein barycenter for

$$\inf \left\{ (1-t)W_2^2(\nu_0, \rho) + tW_2^2(\nu_1, \rho) : \rho \in \mathcal{P}_2(\mathbb{R}^d) \right\}.$$

There are at least three ways to see this. One by employing the triangular inequality, another one is to consider the multimarginal formulation (2.2.3) and a third one by duality as displayed in 6.2 [1].

In their paper [1], Agueh and Carlier have furthermore generalized Theorem 2.2.2 and Theorem 2.2.3 to the whole space in the quadratic setting. In Section 4 [1], they show that the multimarginal formulation of (B) coincides with the problem considered by Gangbo and Swiech [60] as the cost function (2.2.2) in the quadratic case

$$c(x_1, \dots, x_N) = \inf_{x \in \mathbb{R}^d} \left\{ \sum_{i=1}^N \frac{p_i}{2} |x - x_i|^2 \right\},$$

has a unique minimizer  $S(x_1, \dots, x_N) = \sum_{i=1}^N p_i x_i$ , which gives a nice explicit expression for  $c$ .

Even though the Wasserstein barycenter is the most well-studied case of the multi-matching problem, it is still an open problem to establish higher regularity properties. This is due to the optimality conditions which characterize the Wasserstein barycenter (see Proposition 3.8 [1]). Namely, in the setting of Definition 2.3.1 if in addition  $\nu_i$  is absolutely continuous for all  $i = 1, \dots, N$ , then  $\rho \in \mathcal{P}_2(\mathbb{R}^d)$  is a Wasserstein barycenter if and only if there exist Brenier potentials  $u_i$  such that  $\nabla u_i$  is the OT map from  $\nu_i$  to  $\rho$  and a constant  $C$  such that

$$\sum_{i=1}^N p_i u_i^*(x) \leq C + \frac{|x|^2}{2} \quad \text{for all } x \in \mathbb{R}^d \text{ with equality } \rho\text{-a.e.}$$

Recall that the potentials are (a priori formally) coupled with  $\nu_i$  and  $\rho$  through the Monge-Ampère equation (2.1.10)

$$\begin{aligned} \nu_i(\nabla u_i^*) \det(D^2 u_i^*) &= \rho, \\ \overline{\nabla u_i^*(\text{spt } \rho)} &= \text{spt } \nu_i. \end{aligned}$$

This makes the Wasserstein barycenter a free boundary problem coupled to a Monge-Ampère equation, whose regularity depends highly on the support of the target measure (recall Remark 2.1.24) which is unknown. Even worse, there exist counterexamples showing that even if the supports of the given measure  $\nu_i$  are all convex, the support of the Wasserstein barycenter may not be, see [105] for a counterexample for  $N = 2$  by using Remark 2.3.3.

In Chapter 3 we will circumvent this problem by introducing a regularizing term in (B).

Nevertheless, Agueh and Carlier managed to prove with the PDE characterization above at least a maximum principle for the Wasserstein barycenter.

**Theorem 2.3.4** (Theorem 5.1 [1]). *Let  $\nu_i \in \mathcal{P}_{2,\text{ac}}(\mathbb{R}^d)$  for  $i = 1, \dots, N$  and  $p \in \mathbb{R}_+^N$  such that  $\sum_{i=1}^N p_i = 1$ . Assume that  $\nu_1 \in L^\infty(\mathbb{R}^d)$  (by abuse of notation we denote the density with the same letter). Let  $\rho$  be the unique Wasserstein barycenter. Then  $\rho \in L^\infty(\mathbb{R}^d)$  and more precisely*

$$\|\rho\|_{L^\infty(\mathbb{R}^d)} \leq \frac{1}{p_1^d} \|\nu_1\|_{L^\infty(\mathbb{R}^d)}.$$

Finally let us mention the probabilistic interpretation of barycenters, which motivates our work displayed in Chapter 3.

*Remark 2.3.5* (Interpretation as mean). The Wasserstein barycenter can also be seen as a natural generalization of the mean to the metric space  $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ . This idea dates back to Fréchet [56].

Indeed, in a Hilbert space  $(H, \|\cdot\|)$  consider any random variable  $Z$  distributed according to  $P \in \mathcal{P}(H)$  with  $\mathbb{E}[\|Z\|^2] < \infty$ . Then its mean  $\mathbb{E}[Z]$  is well-defined and satisfies the following variational principle. It is the unique solution of

$$\inf_{c \in H} \mathbb{E}_{Z \sim P}[\|Z - c\|^2], \quad \text{respectively} \quad \inf_{c \in H} \int_H \|z - c\|^2 dP(z).$$

The variational formulation has the advantage of being generalizable to a metric space  $(M, d)$  by replacing  $\|\cdot\|$  by  $d(\cdot, \cdot)$ . In [56], Fréchet calls this generalization *mean position* (in French *position moyenne*) as a generalization of the mean. This concept applied to the metric space  $(\mathcal{P}_2(\mathbb{R}^d), W_2)$  and probability distribution  $P = \sum_{i=1}^N p_i \delta_{\nu_i}$  yields the Wasserstein barycenter problem (B).

The past remark motivates the following generalization of the barycenter problem, which has been first considered by several authors [11, 67, 76, 92].

**Definition 2.3.6.** Let  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ . A (generalized) Wasserstein barycenter is a solution of the following variational problem

$$\inf_{\rho \in \mathcal{P}_2(\mathbb{R}^d)} \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\rho, \nu) dP(\nu), \quad (2.3.1)$$

or in probabilistic notation

$$\inf_{\rho \in \mathcal{P}_2(\mathbb{R}^d)} \mathbb{E}_{\nu \sim P} [W_2^2(\rho, \nu)].$$

Its probabilistic interpretation together with the fact that Wasserstein barycenters have gained popularity in image processing and data science ([91, 101, 111, 115]) arise the questions of simulating it numerically and estimating it from given data. By now many numerical algorithms have been developed, see for instance [9, 34, 43, 96] and many more. Moreover, several groups have provided a law of large numbers (LLN) for empirical Wasserstein barycenters, which, for random variables  $(\nu_i)_{i \in \mathbb{N}}$  independent and identically distributed (i.i.d.) according to  $P$ , are solutions of

$$\inf_{\rho_n \in \mathcal{P}_2(\mathbb{R}^d)} \frac{1}{n} \sum_{i=1}^n W_2^2(\rho_n, \nu_i). \quad (2.3.2)$$

Notably, in [11] Bigot and Klein prove a LLN if all measures are supported on a compact set in  $\mathbb{R}^d$ , in the sense that under suitable existence and uniqueness assumptions they prove that for  $\rho$  solution of (2.3.1) and  $\rho_n$  solution of (2.3.2) for  $n \in \mathbb{N}^*$

$$W_2(\rho_n, \rho) \rightarrow 0, \quad \text{as } n \rightarrow \infty.$$

Le Gouic and Loubes consider in [76] the barycenter on the Wasserstein of order  $p$  on suitable geodesic spaces, where they prove the following stronger consistency result. If  $(P_n)_{n \in \mathbb{N}} \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))^{\mathbb{N}}$ ,  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$  such that  $\mathcal{W}_2(P_n, P) \rightarrow 0$  as  $n \rightarrow \infty$  (here  $\mathcal{W}_2$

denotes the Wasserstein distance of order 2 on  $\mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ , then a sequence of minimizers of (2.3.2) given by  $(\rho_n)_{n \in \mathbb{N}}$  is precompact in the Wasserstein topology, and each accumulation point is a Wasserstein barycenter. One readily sees that under suitable assumptions guaranteeing uniqueness on Wasserstein barycenters that this implies the LLN. This consistency result has further been generalized in [71] by Kroshnin to an even larger class of cost functions and regularized version of (2.3.1) (which has first introduced in [10]).

Due to lack of regularity, quantifying the speed of convergence of the law of large numbers in the spirit of a central limit theorem (CLT) turns out to be quite difficult. In [2] Agueh and Carlier have provided a central limit theorem for a few specific cases. Kroshnin et al. [72] study the case of Gaussian measures in detail and provide a CLT in this case.

In order to advance this question, we consider a regularized version of the Wasserstein barycenter problem, as introduced in [10]. In Chapter 3, we prove a CLT for this version under some additional assumptions on the support of the probability measure  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ .

Let us also mention that average rates of convergence of empirical barycenters have been established in Ahidar-Coutrix et al. [3] and generalized in Le Gouic et al. [73] on a quite general class of (geodesic) metric space assuming regularity on the Brenier potentials, which in our setting translates to

$$\mathbb{E} [W_2^2(\rho_n, \rho)] \leq \frac{C}{n},$$

for  $\rho$  Wasserstein barycenter (solution of (2.3.1)) and  $\rho_n$  empirical Wasserstein barycenters (solution of (2.3.2)) for  $n \in \mathbb{N}^*$ .

Finally, in a very recent work Carlier et al. [30] have proven Hölder continuity of Wasserstein barycenters w.r.t. the Wasserstein distance of order 1 on  $\mathcal{P}(\mathcal{P}(B_R(0)))$  ( $B_R(0) \subset \mathbb{R}^d$ ,  $R > 0$ )  $\mathcal{W}_1$  between measure  $P, Q \in \mathcal{P}(\mathcal{P}(B_R(0)))$  supported on sufficiently nice measures. From this they deduce the following quantitative result (notation as before)

$$\mathbb{E} [W_2(\rho_n, \rho)] \leq C \mathbb{E} [\mathcal{W}_1(P_n, P)]^{\frac{1}{6}},$$

where  $P_n = \frac{1}{n} \sum_{i=1}^n \delta_{\nu_i}$  denotes the empirical measure.

## 2.4 Entropic regularization of optimal transport

For the numerical simulation of examples in Chapter 5 we replace the optimal transportation functionals by their entropically regularized versions. This will enable us to apply some extensions of the celebrated Sinkhorn algorithm [109] (also known as iterative proportional fitting procedure [46]), popularized in the context of optimal transport and matching by [42] and [58]. For an introduction to this rapidly developing subject and convergence results, we refer the reader to [96] and [89]. For convenience we repeat here the basic idea and adapt it to the setting we are interested in.

We only work on  $\mathbb{R}^d$  here but give refer to [89], [80] and references therein for a more general treatment.

**Definition 2.4.1.** *The relative entropy between  $P, Q \in \mathcal{M}_+(\mathbb{R}^M)$  on  $\mathbb{R}^M$  (usually  $M = 2d$ ) is defined by*

$$H(P|Q) := \begin{cases} \int_{\mathbb{R}^M} \left( \log \left( \frac{dP}{dQ} \right) - 1 \right) dP & \text{if } P \ll Q, \\ +\infty & \text{otherwise.} \end{cases} \quad (2.4.1)$$

With this we can define the entropically regularized optimal transport problem.

**Definition 2.4.2.** *The entropically regularized optimal transport cost for a (Borel) measurable cost function  $c : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}_+$ , a regularizing parameter  $\varepsilon > 0$  and a fixed reference measure  $Q \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$  is given by*

$$\inf \left\{ \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) \, d\gamma(x, y) + \varepsilon H(\gamma|Q) : \gamma \in \Pi(\nu, \rho) \right\}. \quad (\text{EOT})$$

*Remark 2.4.3.* Note that, by setting  $R = e^{-c(x,y)/\varepsilon} Q$ , we have

$$\varepsilon H(\gamma|R) = \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y) \, d\gamma(x, y) + \varepsilon H(\gamma|Q)$$

so that (EOT) amounts to minimizing  $H(\cdot|R)$  among transport plans between  $\mu_0$  and  $\mu_1$ . The relative entropy w.r.t. a reference measure  $R$  is well-known in large deviations theory to be the rate function of the empirical measure of i.i.d. random variables distributed according to  $R$ , according to Sanov's theorem. This is why minimizing the relative entropy is connected to the problem introduced by Schrödinger [108, 107] of finding the most likely evolution of particles, following a certain law, knowing their distribution at two distinct time points. For a detailed review we refer to [80] and references therein.

Hence, we continue studying the slightly more general problem for  $R \in \mathcal{M}_+(\mathbb{R}^d)$  with finite total mass

$$\inf \{ H(\gamma|R) : \gamma \in \Pi(\nu, \rho) \}, \quad (2.4.2)$$

and it should be clear how the results carry over to (EOT).

Before studying the regularized optimal transport problem (EOT), let us mention that it is indeed an approximation of (OT) in the sense that (EOT)  $\Gamma$ -converges to (OT) as  $\varepsilon \rightarrow 0$ . This has been shown for instance in [79] in a quite general framework and in [31] for the cost function  $c(x, y) = |x - y|^2$ .

Under mild hypothesis, there is existence and uniqueness of a minimizer of (EOT).

**Theorem 2.4.4** (Theorem 2.1 [89]). *Assume that there is a plan  $\gamma \in \Pi(\nu, \rho)$  such that  $H(\gamma|R) < \infty$ . Then there exists a unique minimizer  $\gamma^*$  of (2.4.2) (hence of (EOT)).*

Furthermore,

1. if  $R \sim \nu \otimes \rho$ , then there exist  $\varphi, \psi$  measurable functions such that

$$\frac{d\gamma^*}{dR} = \exp(\varphi(x) + \psi(y)) \quad R\text{-a.s.} \quad (2.4.3)$$

2. Conversely, if there is  $\bar{\gamma} \in \Pi(\nu, \rho)$  with

$$\frac{d\bar{\gamma}}{dR} = \exp(\varphi(x) + \psi(y)) \quad R\text{-a.s.}$$

for two measurable functions  $\varphi, \psi$ , then  $\bar{\gamma}$  is optimal for (2.4.2).

If in addition  $\nu \otimes \rho \ll R$  and

$$\log \frac{d(\nu \otimes \rho)}{dR} \in L^1(\nu \otimes \rho), \quad (2.4.4)$$

then  $\varphi \in L^1(\nu)$  and  $\psi \in L^1(\rho)$ .

The following duality relation holds.

**Proposition 2.4.5.** *Let  $c : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}_+$ ,  $Q \in \mathcal{M}_+(\mathbb{R}^d \times \mathbb{R}^d)$  a finite Radon measure. Set  $R = e^{-c/\varepsilon}Q$ . Suppose  $R \sim \nu \otimes \rho$  and (2.4.4). The dual of (EOT) is given by*

$$\sup_{(\psi, \varphi) \in L^1(\nu) \otimes L^1(\rho)} \left\{ \int_{\mathbb{R}^d} \varphi \, d\nu + \int_{\mathbb{R}^d} \psi \, d\rho - \int_{\mathbb{R}^{2d}} \exp(\varphi(x) + \psi(y)) \, dR(x, y) \right\}. \quad (\text{EOT}^*)$$

There exist solutions to the dual problem, they satisfy (2.4.3) and strong duality holds, i.e.

$$(\text{EOT}) = \varepsilon(\text{EOT}^*).$$

Moreover, it is also equal to

$$\sup_{(\psi, \varphi) \in C_0(\mathbb{R}^d)^2} \left\{ \int_{\mathbb{R}^d} \varphi \, d\nu + \int_{\mathbb{R}^d} \psi \, d\rho - \int_{\mathbb{R}^{2d}} \exp(\varphi(x) + \psi(y)) \, dR(x, y) \right\}.$$

*Proof comment.* The proof of this duality result in high generality is usually done by observing that weak duality holds, i.e.  $(\text{EOT}) \geq (\text{EOT}^*)$ . The fact that strong duality holds is quite technical by standard tools of convex duality as soon as the underlying spaces are not compact. Hence it can be done by showing that there exist  $L^1$ -functions which achieve equality by Theorem 2.4.4, see the proof of Theorem 3.2 [89]. The last equality to the optimization in the space of continuous functions vanishing at infinity follows by density of  $C_0(\mathbb{R}^d)^2$  in  $L^1(\nu) \otimes L^1(\rho)$ . □

This enables us to describe the basic form of Sinkhorn's algorithm in the dual perspective, where it becomes the form of an alternate gradient ascent scheme of the dual potentials. The relation between the dual and primal iterates are discussed in Remark 2.4.6.

From now on we take  $R = e^{-c(x,y)/\varepsilon} R_\nu \otimes R_\rho$  with  $c \in L^1(\nu \otimes \rho)$ ,  $R_\nu \sim \nu$  and  $R_\rho \sim \rho$ , and  $\log\left(\frac{d\nu}{dR_\nu}\right) \in L^1(\nu)$ ,  $\log\left(\frac{d\rho}{dR_\rho}\right) \in L^1(\rho)$  (in order to satisfy (2.4.4)). This the usual setting to apply Sinkhorn's algorithm as the reference measure may not necessarily coincide with the marginals (which is of significant interest if we want to compute an a priori unknown interpolation of several measures). The first order optimality conditions of (EOT\*) are given by

$$\begin{aligned} \varphi(x) &= \log \frac{d\nu}{dR_\nu}(x) - \log \int_{\mathbb{R}^d} \exp(\psi(y) - c(x, y)/\varepsilon) \, dR_\rho(y) \quad \nu\text{-a.s.} \\ \psi(y) &= \log \frac{d\rho}{dR_\rho}(y) - \log \int_{\mathbb{R}^d} \exp(\varphi(x) - c(x, y)/\varepsilon) \, dR_\nu(x) \quad \rho\text{-a.s.} \end{aligned}$$

The alternate gradient ascent hence takes the following form.

**Algorithm 1** (Sinkhorn's algorithm). Given  $\varphi_0 = 0$ . Iterate for  $i \geq 0$

$$\begin{aligned} \psi_i(y) &= \log \frac{d\rho}{dR_\rho}(y) - \log \int_{\mathbb{R}^d} \exp(\varphi_i(x) - c(x, y)/\varepsilon) \, dR_\nu(x) \\ \varphi_{i+1}(x) &= \log \frac{d\nu}{dR_\nu}(x) - \log \int_{\mathbb{R}^d} \exp(\psi_i(y) - c(x, y)/\varepsilon) \, dR_\rho(y) \end{aligned}$$

In line with Theorem 2.4.4 an approximate solution  $\gamma$  of (2.4.2) after iterate  $i$  is given by

$$\frac{d\gamma}{d(R_\nu \otimes R_\rho)}(x, y) = \exp(-c(x, y)/\varepsilon + \varphi_{i+1}(x) + \psi_i(y)). \quad (2.4.5)$$

*Remark 2.4.6.* The algorithm initially introduced by Sinkhorn [109] is also called iterative proportional fitting procedure (IPFP). In the context of entropy minimization this corresponds to iterative fitting of the marginals and takes the following form. Given  $\gamma_{-1} = R$ , iterate for  $i \geq 0$

$$\begin{aligned} \gamma_{2i} &= \arg \min \{H(\gamma|\gamma_{2i-1}) : \pi_{2\#}\gamma = \rho\} \\ \gamma_{2i+1} &= \arg \min \{H(\gamma|\gamma_{2i}) : \pi_{1\#}\gamma = \nu\} \end{aligned} \quad (2.4.6)$$

To give the link to Algorithm 1, we need to understand better the form of the iterates. We show the argument only for the first iterate (2.4.6) but it carries over by symmetry for the second iterate. The argument follows closely the one in Section 6 [89].

We disintegrate  $\gamma$  with  $\pi_{2\#}\gamma = \rho$  to  $\gamma = K \otimes \rho$  and  $\gamma_{2i-1} = K_{2i-1} \otimes \rho_{2i-1}$ , where  $\rho_{2i-1} = \pi_{2\#}\gamma_{2i-1}$  to obtain

$$H(\gamma|\gamma_{2i-1}) = H(\rho|\rho_{2i-1}) + \int_{\mathbb{R}^d} H(K|K_{2i-1}) d\rho.$$

Since  $H(\rho|\rho_{2i-1})$  is constant, the minimum in (2.4.6) is achieved by choosing  $K = K_{2i-1}$ . The minimizer is hence given by  $\gamma_{2i} = K_{2i-1} \otimes \rho$ . In order to get an explicit representation of the iterates and compare it to (2.4.5) we compute the density

$$\frac{d\gamma_{2i}}{d(R_\nu \otimes R_\rho)}.$$

For this we want a representation of  $\frac{dK_{2i-1}}{dR_\nu}$ . This is nothing but the conditional density of  $\gamma_{2i-1}$  with respect to  $R_\nu \otimes R_\rho$  given  $y$  which is the quotient of  $\frac{d\gamma_{2i-1}}{d(R_\nu \otimes R_\rho)}$  and the marginal  $\int_{\mathbb{R}^d} \frac{d\gamma_{2i-1}}{d(R_\nu \otimes R_\rho)}(x, y) d\nu(x)$ .

If we now assume that

$$\frac{d\gamma_{2i-1}}{d(R_\nu \otimes R_\rho)}(x, y) = \exp(-c(x, y)/\varepsilon + \varphi_i(x) + \psi_{i-1}(y)),$$

(which is the case for  $\gamma_{-1} = R$  with  $\varphi_0 = 0$ ,  $\psi_{-1} = 0$ ) then

$$\begin{aligned} \frac{dK_{2i-1}}{dR_\nu}(x, y) &= \frac{\exp(-c(x, y)/\varepsilon + \varphi_i(x) + \psi_{i-1}(y))}{\int_{\mathbb{R}^d} \exp(-c(x, y)/\varepsilon + \varphi_i(x) + \psi_{i-1}(y)) dR_\nu(x)} \\ &= \frac{\exp(-c(x, y)/\varepsilon + \varphi_i(x))}{\int_{\mathbb{R}^d} \exp(-c(x, y)/\varepsilon + \varphi_i(x)) dR_\nu(x)}. \end{aligned}$$

In total we have

$$\begin{aligned} \frac{d\gamma_{2i}}{d(R_\nu \otimes R_\rho)}(x, y) &= \frac{dK_{2i-1}}{dR_\nu}(x, y) \frac{d\rho}{dR_\rho}(y) \\ &= \frac{d\rho}{dR_\rho}(y) \frac{\exp(-c(x, y) + \varphi_i(x))}{\int_{\mathbb{R}^d} \exp(-c(x, y) + \varphi_i(x)) dR_\nu(x)}, \end{aligned}$$

which, choosing  $\psi_i(y) = \log \frac{d\rho}{dR_\rho}(y) - \log \int_{\mathbb{R}^d} \exp(-c(x, y) + \varphi_i(x)) d\nu(x)$  as in Algorithm 1 yields

$$\frac{d\gamma_{2i}}{d(R_\nu \otimes R_\rho)}(x, y) = \exp(-c(x, y) + \varphi_i(x) + \psi_i(y)).$$

Observe that in the dual perspective of the Sinkhorn algorithm (Algorithm 1) the iterations correspond to

$$\begin{aligned} \psi_i &= \arg \max_{\psi} J(\varphi_i, \psi) \\ \varphi_{i+1} &= \arg \max_{\varphi} J(\varphi, \psi_i) \end{aligned}$$

for each  $i \geq 0$ , where

$$J(\varphi, \psi) = \int_{\mathbb{R}^d} \varphi d\nu + \int_{\mathbb{R}^d} \psi d\rho - \int_{\mathbb{R}^{2d}} \exp(\varphi(x) + \psi(y)) dR(x, y),$$

is the objective functional of (EOT\*). By strict concavity of  $J$  each iteration hence strictly increases the value function and by weak duality  $J$  is bounded from above. From this we get that  $(J(\varphi_i, \psi_i))_{i \in \mathbb{N}}$  converges and we can hope for convergence of the potentials as well. A proof has been given for example in [103] in the continuous setting. A very general treatment is considered in [36].



## Chapter 3

# Entropically regularized Wasserstein barycenters

This chapter is based on the published article [32]. We decided to adapt the presentation of the central limit theorem compared to the paper in order to illustrate the basic idea and detail a few more cases where the central limit theorem is valid.

The Wasserstein barycenter can be interpreted as generalization of the mean in the Wasserstein space of order two. This naturally arises several questions studying its empirical counterpart. Several authors have established a law of large numbers (LLN) for it (see e.g. [11, 76, 71]). Having this law of large numbers in mind, it is natural to look for error estimates and asymptotic normality of the error between population Wasserstein barycenters and their empirical counterpart. However, establishing a central limit theorem (CLT) for Wasserstein barycenters and, more generally, for Fréchet means over a non-negatively curved metric space seems to be a delicate task (see [3]) except in very particular cases (dimension one or the case of Gaussians, see [2], [72]). The difficulty is not only due to the fact that the problem is infinite-dimensional but also (and in fact more importantly) to the fact that Wasserstein barycenters are related to an obstacle problem for a system of Monge-Ampère equations (see Section 2.3). The support of the Wasserstein barycenter is indeed an unknown of the problem and very little is known about its regularity. The free-boundary aspect of Wasserstein barycenters actually makes the dependence of the barycenter possibly non-smooth on the sample and thus prevents one from using a delta method.

Bigot, Cazelles and Papadakis in [10] observed that when one discretizes continuous measures, the corresponding (discrete) barycenters exhibit strong oscillations and proposed to add an entropic penalization to the Wasserstein variance functional to rule out such discretization artefacts. Such regularizations were also considered in a more general setting by Kroshnin in [71]. Once one adds an entropic term, the free-boundary aspect of the unregularized Wasserstein problem, as discussed in Section 2.3, disappears and one can expect regularity and quite strong estimates by PDE arguments. The objective of this work is precisely to investigate the regularizing effect of the entropic penalty term. Starting from the optimality condition which consists in an elliptic system of Monge-Ampère equations, we will prove various bounds (on the Fisher information, by a maximum principle, or higher regularity based on the regularity theory for Monge-Ampère). We will then consider the stochastic setting of entropic Wasserstein barycenters of random i.i.d. measures. As a

consequence of our estimates, we will obtain a strengthened form of the law of large numbers (that is, not only for a.s. convergence in Wasserstein distance, but also for Sobolev norms) and more importantly, under suitable additional assumptions, we will obtain a CLT.

The remainder of the chapter is organized as follows. In Section 3.1, we introduce the setting and prove existence and uniqueness of the entropic Wasserstein barycenter. The entropic barycenter is then characterized by a system of Monge-Ampère equations in section 3.2 where we treat the Gaussian case as a simple application. Section 3.3 is devoted to further properties: global moment and Sobolev bounds, strong stability and a maximum principle. Higher regularity is considered in Section 3.4 first in the bounded case and then on  $\mathbb{R}^d$  for log-concave measures. Section 3.5 deals with asymptotic results for entropic barycenters of empirical measures with a law of large numbers and a CLT. Section 3.6, 3.7 and 3.8 contain some material related to the linearization of Monge-Ampère equations, to a discrete version of the Monge-Ampère equation and to the situation on the torus. Finally, the appendix gathers auxiliary probability results which are used in the proof of our CLT.

### 3.1 Setting

Motivated by the interpretation of barycenters as mean from Remark 2.3.5, we give ourselves a Borel (with respect to the Wasserstein metric) probability measure on the Wasserstein space  $(\mathcal{P}_2(\mathbb{R}^d), W_2)$  (see Definition 2.1.26 and Proposition 2.1.27) with finite second moment, i.e.  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ . In view of Definition 2.1.26, this means that

$$\int_{\mathcal{P}_2(\mathbb{R}^d)} m_2(\nu) dP(\nu) < +\infty, \quad (3.1.1)$$

where  $m_2(\nu)$  denotes the second moment of  $\nu$  i.e.

$$m_2(\nu) := W_2^2(\nu, \delta_0) = \int_{\mathbb{R}^d} |x|^2 d\nu(x), \quad \forall \nu \in \mathcal{P}_2(\mathbb{R}^d).$$

Given a regularization parameter  $\lambda > 0$  and  $\Omega$  a non-empty open connected subset of  $\mathbb{R}^d$  with a Lebesgue negligible boundary (of particular interest is the case where  $\Omega = \mathbb{R}^d$  or  $\Omega$  is convex), we are interested in the following problem (which was introduced in [10] as an entropic regularization of the Wasserstein barycenter problem):

$$\inf_{\rho \in \mathcal{P}_2(\mathbb{R}^d)} V_{P,\lambda,\Omega}(\rho) := \frac{1}{2} \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\rho, \nu) dP(\nu) + \lambda \text{Ent}_\Omega(\rho), \quad (\text{EB})$$

where  $\text{Ent}_\Omega$  is the relative entropy with respect to  $\mathcal{L}_\Omega^d$ , the Lebesgue measure restricted to  $\Omega$ , restricted to probability measures, as defined in (2.4.1)

$$\text{Ent}_\Omega(\rho) := H(\rho | \mathcal{L}_\Omega^d) = \begin{cases} \int_\Omega \rho \log \rho, & \text{if } \mu = \rho dx \text{ and } \int_\Omega \rho = 1, \\ +\infty & \text{otherwise.} \end{cases}$$

If  $\Omega = \mathbb{R}^d$  we simply denote  $\text{Ent}_{\mathbb{R}^d} = \text{Ent}$  and  $V_{P,\lambda,\mathbb{R}^d} = V_{P,\lambda}$ .

*Example 3.1.1.* If  $\Omega = \mathbb{R}^d$  and  $P = \sum_{i=1}^I p_i \delta_{x_i}$  is concentrated on Dirac masses, (EB) can be reformulated as

$$\inf_{\rho \in \mathcal{P}_2(\mathbb{R}^d)} \frac{1}{2} \int_{\mathbb{R}^d} \left| x - \sum_{i=1}^I p_i x_i \right|^2 d\rho(x) + \lambda \text{Ent}(\rho)$$

whose solution is the Gaussian

$$\rho(x) := \frac{1}{(2\pi\lambda)^{\frac{d}{2}}} \exp\left(-\frac{1}{2\lambda}\left|x - \sum_{i=1}^I p_i x_i\right|^2\right)$$

whereas the (unregularized) Wasserstein barycenter of  $P$  is just  $\delta_{\sum_{i=1}^I p_i x_i}$ .

By the direct method of the calculus of variations, one easily obtains

**Proposition 3.1.2.** *Assume  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ , then (EB) admits a unique solution.*

*Proof.* Let  $(\rho_n)_{n \in \mathbb{N}}$  be a minimizing sequence for (EB) (necessarily 0 outside  $\bar{\Omega}$ ). In what follows  $C$  will denote a constant which may vary from one line to the other. Observing that

$$\frac{1}{2}W_2^2(\rho_n, \nu) \geq \frac{1}{4}m_2(\rho_n) - m_2(\nu),$$

we deduce from the fact that  $V_{P,\lambda,\Omega}(\rho_n)$  is bounded from above and (3.1.1) that we have

$$\frac{1}{4}m_2(\rho_n) + \lambda \text{Ent}_\Omega(\rho_n) \leq C. \quad (3.1.2)$$

It now follows from [65] ((14) in the proof of Proposition 4.1) that for  $\alpha \in (\frac{d}{d+2}, 1)$ , one can bound from below the entropy by

$$\text{Ent}_\Omega(\rho) \geq -C(1 + m_2(\rho))^\alpha. \quad (3.1.3)$$

Together with (3.1.2) this shows that  $(m_2(\rho_n))_{n \in \mathbb{N}}$  is bounded so that  $(\rho_n)_{n \in \mathbb{N}}$  is tight by Markov's inequality. One may therefore assume, taking a subsequence if necessary (not relabeled) that  $(\rho_n)_{n \in \mathbb{N}}$  converges narrowly to some  $\bar{\rho}$ . Of course  $\bar{\rho} \in \mathcal{P}_2(\mathbb{R}^d)$  (with  $m_2(\bar{\rho}) \leq \liminf_{n \rightarrow \infty} m_2(\rho_n)$ ) and  $\bar{\rho}$  vanishes outside  $\bar{\Omega}$ . Now since  $(m_2(\rho_n))_{n \in \mathbb{N}}$  is bounded and  $(\rho_n)_{n \in \mathbb{N}}$  converges narrowly to  $\bar{\rho}$  we have (by e.g. Corollary A.4 [31])

$$\text{Ent}_\Omega(\bar{\rho}) \leq \liminf_{n \rightarrow \infty} \text{Ent}_\Omega(\rho_n). \quad (3.1.4)$$

and  $\text{Ent}_\Omega(\bar{\rho}) > -\infty$  thanks to (3.1.3). We also have for every  $\nu \in \mathcal{P}_2(\mathbb{R}^d)$

$$W_2^2(\bar{\rho}, \nu) \leq \liminf_{n \rightarrow \infty} W_2^2(\rho_n, \nu).$$

Hence, by Fatou's Lemma:

$$\int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\bar{\rho}, \nu) dP(\nu) \leq \liminf_{n \rightarrow \infty} \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\rho_n, \nu) dP(\nu),$$

which, together with (3.1.4) enables us to conclude that  $\bar{\rho}$  solves (EB). The uniqueness of the minimizer directly follows from the strict convexity of the entropy and the convexity of the Wasserstein term.  $\square$

Entropic-Wasserstein barycenters can therefore be defined as follows.

**Definition 3.1.3.** *The unique solution  $\bar{\rho}$  of (EB) is called the entropic-Wasserstein barycenter of  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$  with respect to  $\lambda$  and  $\Omega$  and denoted  $\text{bar}_{\lambda,\Omega}(P)$  and simply  $\text{bar}_\lambda(P)$  if  $\Omega = \mathbb{R}^d$ .*

*Remark 3.1.4.* Theorem 4.4 in [10] states under the additional assumption that  $\Omega$  is convex and compact (note that taking the closure of  $\Omega$  does not change the entropic-Wasserstein barycenter) and  $\text{supp } \nu \subset \Omega$  for  $P$ -a.e.  $\nu$ , that

$$W_2(\text{bar}_{\lambda,\Omega}(P), \text{bar}_{0,\Omega}(P)) \rightarrow 0 \quad \text{as } \lambda \rightarrow 0,$$

provided  $\text{bar}_{0,\Omega}(P)$  is unique. By inspecting their proof, one can actually see that the compactness assumption on  $\Omega$  can be relaxed by the same argument as in Proposition 3.1.2. The assumption on the inclusion of the support can also be omitted if one understands  $\text{bar}_{0,\Omega}(P)$  as the Wasserstein barycenter of  $P$  constrained to have support in  $\Omega$ .

Since  $\text{bar}_{\lambda,\Omega}(P)$  is absolutely continuous with respect to the Lebesgue measure, we shall slightly abuse notations and use the same notation for its density.

We can immediately state some basic invariance properties of entropic-Wasserstein barycenters in the case  $\Omega = \mathbb{R}^d$ . For instance, if we shift all measures  $\nu$  by some vector  $s \in \mathbb{R}^d$  and rotate by some orthogonal matrix  $Q \in O(d)$ , then entropic-Wasserstein barycenters will be also shifted and rotated by the same vector and matrix (clearly, the same result holds for any subgroup of translations and orthogonal transformations that  $\Omega$  is invariant to). The next proposition shows that translations can actually be “factored out” from the barycenter.

**Proposition 3.1.5.** *Let  $\Omega = \mathbb{R}^d$ ,  $\lambda > 0$ ,  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ , and  $\bar{\rho} = \text{bar}_{\lambda}(P)$ . Fix a measurable map  $\mathbf{s} \in L^2(P; \mathbb{R}^d)$  and define a measure  $P_{\mathbf{s}} := (\nu \mapsto \nu \oplus \mathbf{s}(\nu))_{\#} P$ , where  $\nu \oplus \mathbf{s} := (x \mapsto s + x)_{\#} \nu$  for all  $\nu \in \mathcal{P}_2(\mathbb{R}^d)$  and  $s \in \mathbb{R}^d$ . Then  $\text{bar}_{\lambda}(P_{\mathbf{s}}) = \bar{\rho} \oplus \bar{\mathbf{s}}$ , with  $\bar{\mathbf{s}} := \int_{\mathcal{P}_2(\mathbb{R}^d)} \mathbf{s}(\nu) dP(\nu)$ .*

*Proof.* Note that it is enough to consider the case  $\mathbb{E}_{\nu}[X] = 0$  for  $P$ -a.e.  $\nu$ , where the term  $\mathbb{E}_{\nu}[X] = \int_{\mathbb{R}^d} x d\nu(x)$  is the average of  $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ . Recall that due to the bias-variance decomposition

$$W_2^2(\mu, \nu) = W_2^2(\mu \ominus \mathbb{E}_{\mu}[X], \nu \ominus \mathbb{E}_{\nu}[X]) + |\mathbb{E}_{\mu}[X] - \mathbb{E}_{\nu}[X]|^2, \quad \mu, \nu \in \mathcal{P}_2(\mathbb{R}^d).$$

Since entropy is invariant to shifts, we get for any  $\rho \in \mathcal{P}_2(\mathbb{R}^d)$  and  $a \in \mathbb{R}^d$

$$\begin{aligned} V_{P_{\mathbf{s}}, \lambda}(\rho \oplus a) &= \frac{1}{2} \int_{\mathcal{P}_2(\mathbb{R}^d)} [W_2^2(\rho \ominus \mathbb{E}_{\rho}[X], \nu) + |\mathbb{E}_{\rho}[X] + a - \mathbf{s}(\nu)|^2] dP(\nu) \\ &\quad + \lambda \text{Ent}(\rho) \\ &= V_{P, \lambda}(\rho) - \frac{1}{2} |\mathbb{E}_{\rho}[X]|^2 + \frac{1}{2} |a + \mathbb{E}_{\rho}[X] - \bar{\mathbf{s}}|^2 + C. \end{aligned}$$

In particular, taking  $\mathbf{s} \equiv 0$ ,  $\rho = \bar{\rho}$ , and using that the minimum with respect to  $a$  is attained at 0, we get that  $\mathbb{E}_{\bar{\rho}}[X] = 0$ . Now, we can first minimize  $V_{P, \lambda}(\rho)$  over  $\rho$ 's with zero mean:  $\mathbb{E}_{\rho}[X] = 0$ , and then minimize the third term with respect to  $a$ , hence  $\text{bar}_{\lambda}(P_{\mathbf{s}}) = \bar{\rho} \oplus a$ ,  $a = \bar{\mathbf{s}}$ . The claim follows.  $\square$

*Remark 3.1.6.* Note that, when  $\Omega = \mathbb{R}^d$ , a useful corollary of Proposition 3.1.5 is that the average of entropic-Wasserstein barycenter is the expectation of averages:

$$\mathbb{E}_{\bar{\rho}}[X] = \int_{\mathcal{P}_2(\mathbb{R}^d)} \mathbb{E}_{\nu}[X] dP(\nu).$$

## 3.2 Characterization

The entropic term forces the regularized barycenter to be everywhere positive. Indeed, arguing in a similar way as in Lemma 8.6 from [104], we arrive at:

**Lemma 3.2.1.** *Let  $\bar{\rho} := \text{bar}_{\lambda, \Omega}(P)$  then  $\bar{\rho} > 0$  a.e. on  $\Omega$  and  $\log(\bar{\rho}) \in L^1_{\text{loc}}(\Omega)$ .*

*Proof.* Let  $g$  be a Gaussian density, scaled so as to give mass 1 to  $\Omega$ . For  $t \in (0, 1)$ , set  $\rho_t := (1-t)\bar{\rho} + tg$ . The convexity of  $\rho \mapsto W_2^2(\rho, \nu)$  together with the optimality of  $\bar{\rho}$ , give

$$\lambda(\text{Ent}_{\Omega}(\rho_t) - \text{Ent}_{\Omega}(\bar{\rho})) \geq \frac{t}{2} \int_{\mathcal{P}_2(\mathbb{R}^d)} [W_2^2(\bar{\rho}, \nu) - W_2^2(g, \nu)] dP(\nu),$$

so that for some  $C$ , we have for every  $t \in (0, 1)$ ,

$$\frac{1}{t}(\text{Ent}_{\Omega}(\rho_t) - \text{Ent}_{\Omega}(\bar{\rho})) \geq C. \quad (3.2.1)$$

Now, observe that

$$\begin{aligned} \frac{1}{t}(\text{Ent}_{\Omega}(\rho_t) - \text{Ent}_{\Omega}(\bar{\rho})) &= \int_{\{\bar{\rho}=0\}} g \log(tg) + \int_{\{\bar{\rho}>0\}} \frac{1}{t}(\rho_t \log(\rho_t) - \bar{\rho} \log(\bar{\rho})) \\ &\leq \int_{\{\bar{\rho}=0\}} g \log(tg) + \int_{\{\bar{\rho}>0\}} (g \log(g) - \bar{\rho} \log(\bar{\rho})) \\ &\leq \log(t) \int_{\{\bar{\rho}=0\}} g + \text{Ent}_{\Omega}(g) - \text{Ent}_{\Omega}(\bar{\rho}), \end{aligned}$$

where in the second line we have used the convexity of  $s \mapsto s \log(s)$ . Combining this inequality with (3.2.1) and letting  $t \rightarrow 0^+$ , we immediately see that  $\mathcal{L}^d(\{\bar{\rho} = 0\}) = 0$ .

Let us now show that  $\log(\bar{\rho}) \in L^1_{\text{loc}}(\Omega)$ . Since  $\max(0, \log(\bar{\rho})) \leq \bar{\rho}$  we have to show that  $\int_K \log(\bar{\rho}) > -\infty$  for every compact subset (of positive Lebesgue measure)  $K$  of  $\Omega$ . Calling  $\mu$  the uniform probability measure on  $K$ , setting  $\nu_t := \bar{\rho} + t(\mu - \bar{\rho})$  for  $t \in (0, 1)$  and arguing as above, we have

$$\frac{1}{t}(\text{Ent}_{\Omega}(\nu_t) - \text{Ent}_{\Omega}(\bar{\rho})) \geq C,$$

moreover  $\frac{1}{t}(\nu_t \log(\nu_t) - \bar{\rho} \log(\bar{\rho})) \leq \mu \log(\mu) - \bar{\rho} \log(\bar{\rho}) \in L^1(\Omega)$ , Fatou's Lemma and the previous inequality thus give

$$\begin{aligned} C &\leq \limsup_{t \rightarrow 0^+} \frac{1}{t}(\text{Ent}_{\Omega}(\nu_t) - \text{Ent}_{\Omega}(\bar{\rho})) \\ &\leq \int_{\Omega} \limsup_{t \rightarrow 0^+} (\nu_t \log(\nu_t) - \bar{\rho} \log(\bar{\rho})) = \int_{\Omega} \log(\bar{\rho})(\mu - \bar{\rho}) \end{aligned}$$

and since  $\text{Ent}_{\Omega}(\bar{\rho})$  is finite, this gives  $\int_K \log(\bar{\rho}) > -\infty$ .  $\square$

The fact that the regularized barycenter is everywhere positive guarantees uniqueness (up to a constant) of the Kantorovich potential between  $\bar{\rho}$  and  $\nu \in \mathcal{P}_2(\mathbb{R}^d)$  by Remark 2.1.20. This uniqueness is well-known to be very useful in terms of differentiability of  $\mu \mapsto W_2^2(\mu, \nu)$  at  $\mu = \bar{\rho}$  as expressed in Lemma 3.2.4 below (which is slight generalization of Proposition 7.17 in [104]). The following inequality will be useful to justify the differentiability of  $\mu \mapsto \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\mu, \nu) dP(\nu)$  at  $\mu = \bar{\rho}$ :

**Lemma 3.2.2.** *Let  $\rho \in L^1(\Omega)$  and  $\rho > 0$  a.e. on  $\Omega$ . Then for any compact set  $K \subset \Omega$  and any convex function  $u: \Omega \rightarrow \mathbb{R}$  one has*

$$\operatorname{osc}_K u := \max_K u - \min_K u \leq \frac{\operatorname{diam}(K) + r}{\inf_{x \in K_{r/2}} \rho(B_{r/2}(x))} \int_{\Omega} |\nabla u| \rho, \quad (3.2.2)$$

where  $0 < r \leq d(K, \partial\Omega)$  and  $K_\sigma = \bigcup_{x \in K} \bar{B}_\sigma(x)$  for any  $\sigma > 0$ . Moreover, the Lipschitz constant of  $u$  on  $K$ ,  $\operatorname{Lip}(u|_K)$ , can be estimated as

$$\operatorname{Lip}(u|_K) \leq \frac{2 \operatorname{diam}(K) + 3r}{r \inf_{x \in K_{3r/4}} \rho(B_{r/4}(x))} \int_{\Omega} |\nabla u| \rho. \quad (3.2.3)$$

*Remark 3.2.3.* Notice that  $\Omega$  is not necessary convex, thus we say a function  $u$  on  $\Omega$  is convex if it can be extended to a convex function on  $\mathbb{R}^d$  (possibly taking value  $+\infty$ ), see [54].

*Proof.* Let  $x_1 \in \arg \max_K u$ ,  $x_0 \in \arg \min_K u$ , and  $w \in \partial u(x_1)$ . Then for any  $x \in \Omega$  and  $z \in \partial u(x)$  one has

$$u(x_0) + z \cdot (x - x_0) \geq u(x) \geq u(x_1) + w \cdot (x - x_1),$$

and thus the Cauchy–Schwarz inequality yields

$$|z| \geq \frac{\operatorname{osc}_K u + w \cdot (x - x_1)}{|x - x_0|}.$$

Since  $u$  is a.e. differentiable, we have

$$\begin{aligned} \int_{\Omega} |\nabla u| \rho &\geq \int_{W_r(x_1, w)} |\nabla u| \rho \geq \operatorname{osc}_K u \int_{W_r(x_1, w)} \frac{1}{|x - x_0|} \rho(x) \, dx \\ &\geq \operatorname{osc}_K u \int_{W_r(x_1, w)} \frac{1}{|x - x_1| + |x_1 - x_0|} \rho(x) \, dx \\ &\geq \operatorname{osc}_K u \frac{\rho\left(B_{r/2}\left(x + \frac{rw}{2|w|}\right)\right)}{\operatorname{diam}(K) + r}, \end{aligned}$$

where we have set  $W_r(x, w) := \{y \in B_r(x) : w \cdot (y - x) \geq 0\}$  and used the fact that  $B_{r/2}\left(x + \frac{rw}{2|w|}\right) \subset W_r(x, w)$  and  $x + \frac{rw}{2|w|} \in K_{r/2}$ . Finally, the positivity of  $\rho$  together with the compactness of  $K$  implies that

$$\inf \left\{ \rho(W_r(x, w)) : x \in K, w \in \mathbb{R}^d \right\} \geq \inf_{x \in K_{r/2}} \rho(B_{r/2}(x)) > 0.$$

The first claim follows.

To prove (3.2.3) we apply (3.2.2) to  $K_{r/2}$ , which yields

$$\begin{aligned} \operatorname{osc}_{K_{r/2}} u &\leq \frac{\operatorname{diam}(K_{r/2}) + r/2}{\inf_{x \in K_{3r/4}} \rho(B_{r/4}(x))} \int_{\Omega} |\nabla u| \rho \\ &\leq \frac{\operatorname{diam}(K) + 3r/2}{\inf_{x \in K_{3r/4}} \rho(B_{r/4}(x))} \int_{\Omega} |\nabla u| \rho. \end{aligned}$$

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Note that for any  $x \in K$  and  $w \in \partial u(x)$  one has  $B_{r/2}(x) \subset K_{r/2}$ , hence

$$\operatorname{osc}_{K_{r/2}} u \geq \operatorname{osc}_{B_{r/2}(x)} u \geq \frac{r}{2}|w|.$$

Therefore,

$$|w| \leq \frac{2}{r} \operatorname{osc}_{K_{r/2}} u \leq \frac{2 \operatorname{diam}(K) + 3r}{r \inf_{x \in K_{3r/4}} \rho(B_{r/4}(x))} \int_{\Omega} |\nabla u| \rho,$$

thus we obtain the desired bound on  $\operatorname{Lip}(u|_K)$ .  $\square$

**Lemma 3.2.4.** *For  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ , let  $\bar{\rho} := \operatorname{bar}_{\lambda, \Omega}(P)$  and given  $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ , let  $\varphi_{\bar{\rho}}^{\nu}$  be the (unique on  $\Omega$ , up to an additive constant) Kantorovich potential between  $\bar{\rho}$  and  $\nu$  (for cost function  $\frac{1}{2}|x - y|$ ). Let  $\mu \in L^1(\Omega)$  be a probability density such that  $\mu - \bar{\rho}$  has compact support in  $\Omega$ , defining  $\rho_{\varepsilon} := \bar{\rho} + \varepsilon(\mu - \bar{\rho})$  for  $\varepsilon \in (0, \frac{1}{2})$ , we have*

$$\lim_{\varepsilon \rightarrow 0^+} \frac{1}{2\varepsilon} [W_2^2(\rho_{\varepsilon}, \nu) - W_2^2(\bar{\rho}, \nu)] = \int_{\Omega} \varphi_{\bar{\rho}}^{\nu} d(\mu - \bar{\rho}),$$

and

$$\lim_{\varepsilon \rightarrow 0^+} \frac{1}{2\varepsilon} \int_{\mathcal{P}_2(\mathbb{R}^d)} [W_2^2(\rho_{\varepsilon}, \nu) - W_2^2(\bar{\rho}, \nu)] dP(\nu) = \int_{\mathcal{P}_2(\mathbb{R}^d)} \left( \int_{\Omega} \varphi_{\bar{\rho}}^{\nu} d(\mu - \bar{\rho}) \right) dP(\nu).$$

*Proof.* Let us shorten notations by defining

$$\varphi := \varphi_{\bar{\rho}}^{\nu}, \quad u := u_{\bar{\rho}}^{\nu} = \frac{1}{2}|\cdot|^2 - \varphi_{\bar{\rho}}^{\nu},$$

and let  $\varphi_{\varepsilon}$  be a Kantorovich potential between  $\rho_{\varepsilon}$  and  $\nu$  and  $u_{\varepsilon} := \frac{1}{2}|\cdot|^2 - \varphi_{\varepsilon}$ . Let  $K$  be a compact subset of  $\Omega$  supporting  $\mu - \bar{\rho}$  and normalize the potentials  $u$  and  $u_{\varepsilon}$  in such a way that their minimum on  $K$  is 0. It immediately follows from the Kantorovich duality formula that

$$\int_K \varphi_{\varepsilon} d(\mu - \bar{\rho}) \geq \frac{1}{2\varepsilon} [W_2^2(\rho_{\varepsilon}, \nu) - W_2^2(\bar{\rho}, \nu)] \geq \int_K \varphi d(\mu - \bar{\rho}). \quad (3.2.4)$$

Now observe that since  $(\nabla u_{\varepsilon})_{\#} \rho_{\varepsilon} = \nu$ , we have

$$m_2(\nu) = \int_{\Omega} |\nabla u_{\varepsilon}|^2 \rho_{\varepsilon} \geq (1 - \varepsilon) \int_{\Omega} |\nabla u_{\varepsilon}|^2 \bar{\rho}. \quad (3.2.5)$$

We then deduce from Jensen's inequality a bound on  $\int_{\Omega} |\nabla u_{\varepsilon}| \bar{\rho}$  which does not depend on  $\varepsilon$ . Thanks to Lemma 3.2.2, we obtain local uniform bounds on  $u_{\varepsilon}$  and therefore can deduce that for some vanishing sequence of  $(\varepsilon_n)_{n \in \mathbb{N}}$ ,  $(u_{\varepsilon_n})_{n \in \mathbb{N}}$  converges locally uniformly on  $\Omega$  to some convex  $v$  whose minimum is 0 on  $K$  and that  $(\nabla u_{\varepsilon_n})_{n \in \mathbb{N}}$  converges  $\bar{\rho}$ -a.e. to  $\nabla v$ . Using continuous bounded test-functions and Lebesgue's dominated convergence theorem, we can pass to the limit in  $\nabla u_{\varepsilon_n \#} \rho_{\varepsilon_n} = \nu$  to deduce that  $\nabla v_{\#} \bar{\rho} = \nu$ , which, with our normalization and the uniqueness of Brenier's map implies that  $u = v$  and also full uniform convergence on  $K$  of  $\varphi_{\varepsilon}$  to  $\varphi$ . Passing to the limit in (3.2.4) gives the first claim of the lemma.

To prove the second claim, set

$$\theta_\varepsilon(\nu) := \frac{1}{2\varepsilon} [W_2^2(\rho_\varepsilon, \nu) - W_2^2(\bar{\rho}, \nu)],$$

and observe that it follows from (3.2.4)-(3.2.5) and Lemma 3.2.2 that  $\theta_\varepsilon(\nu)$  can be bounded from above and from below by two affine functions of  $m_2(\nu)$ , the desired result therefore follows from (3.1.1), Lebesgue's dominated convergence theorem and the first claim.  $\square$

We are now in position to characterize the regularized barycenter.

**Proposition 3.2.5.** *For  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$ , let  $\bar{\rho} \in \mathcal{P}_2(\mathbb{R}^d)$ , then  $\bar{\rho} = \text{bar}_{\lambda, \Omega}(P)$  if and only if, denoting by  $\nabla u_{\bar{\rho}}^\nu$  Brenier's map between  $\bar{\rho}$  and  $\nu$ , there are normalizing constants for  $u_{\bar{\rho}}^\nu$  such that  $\bar{\rho}$  has a continuous density given by*

$$\bar{\rho}(x) := \exp\left(-\frac{1}{2\lambda}|x|^2 + \frac{1}{\lambda} \int_{\mathcal{P}_2(\mathbb{R}^d)} u_{\bar{\rho}}^\nu(x) dP(\nu)\right) \quad (3.2.6)$$

for every  $x \in \Omega$ . Moreover,  $\log(\bar{\rho})$  is semi-convex hence differentiable a.e. and for a.e.  $x \in \Omega$ , one has

$$x + \lambda \nabla \log(\bar{\rho})(x) = \int_{\mathcal{P}_2(\mathbb{R}^d)} \nabla u_{\bar{\rho}}^\nu(x) dP(\nu). \quad (3.2.7)$$

*Proof.* For necessity fix a compact with non-empty interior subset  $K$  of  $\Omega$  and normalize  $\varphi_{\bar{\rho}}^\nu = \frac{1}{2}|\cdot|^2 - u_{\bar{\rho}}^\nu$  such that it has minimum 0 on  $K$ , then, arguing as in the proof of Lemma 3.2.4, there is a constant  $C_K$  such that  $\|\varphi_{\bar{\rho}}^\nu\|_{L^\infty(K)} \leq C_K(1 + m_2(\nu))$  so that the (semi-concave) potential

$$x \mapsto U(x) := \int_{\mathcal{P}_2(\mathbb{R}^d)} \varphi_{\bar{\rho}}^\nu(x) dP(\nu),$$

is bounded on  $K$ . Now we claim that  $V := \lambda \log(\bar{\rho}) + U$  (which is integrable on  $K$  thanks to Lemma 3.2.1) coincides Lebesgue a.e. with a constant on  $K$  (which taking an exhaustive sequence of compact subsets of  $\Omega$  will enable to find normalizing constants for  $u_{\bar{\rho}}^\nu$  that do not depend on  $K$  and therefore prove (3.2.6)). Assume, by contradiction, that  $V$  does not coincide Lebesgue a.e. with a constant on  $K$ , then we could find two measurable subsets  $K_1$  and  $K_2$  of  $K$ , both of positive Lebesgue measure and  $\alpha \in \mathbb{R}$  and  $\delta > 0$  such that

$$V \geq \alpha + \delta \text{ a.e. on } K_1, \quad V \leq \alpha - \delta \text{ a.e. on } K_2. \quad (3.2.8)$$

In particular  $\bar{\rho}(K_1) > 0$  and  $\bar{\rho}(K_2) > 0$ , now set  $\beta := \frac{\bar{\rho}(K_1)}{2\bar{\rho}(K_2)}$  and define the probability density  $\mu \in L^1(\Omega)$  by

$$\mu(x) := \begin{cases} \frac{1}{2}\bar{\rho}(x) & \text{if } x \in K_1, \\ (1 + \beta)\bar{\rho}(x) & \text{if } x \in K_2, \\ \bar{\rho}(x) & \text{otherwise,} \end{cases}$$

and  $\rho_\varepsilon := \bar{\rho} + \varepsilon(\mu - \bar{\rho})$ . It is straightforward to check that

$$\lim_{\varepsilon \rightarrow 0^+} \frac{1}{\varepsilon} (\text{Ent}(\rho_\varepsilon) - \text{Ent}(\bar{\rho})) = \int_K \log(\bar{\rho})(\mu - \bar{\rho}).$$

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With Lemma 3.2.4, the construction of  $\mu$  and (3.2.8), this yields

$$\begin{aligned} & \lim_{\varepsilon \rightarrow 0^+} \frac{1}{\varepsilon} [V_{P,\lambda,\Omega}(\rho_\varepsilon) - V_{P,\lambda,\Omega}(\bar{\rho})] \\ &= \int_K V(\mu - \bar{\rho}) = -\frac{1}{2} \int_{K_1} V\bar{\rho} + \beta \int_{K_2} V\bar{\rho} \leq -\delta\bar{\rho}(K_1) < 0 \end{aligned}$$

contradicting the fact by optimality of  $\bar{\rho}$ ,  $V_{P,\lambda,\Omega}(\rho_\varepsilon) \geq V_{P,\lambda,\Omega}(\bar{\rho})$ .

Now assume that  $\bar{\rho} \in \mathcal{P}_2(\mathbb{R}^d)$  satisfies (3.2.6), and let  $\mu \in \mathcal{P}_2(\mathbb{R}^d)$  be supported on  $\bar{\Omega}$  and such that  $\text{Ent}_\Omega(\mu) < \infty$ . Using the convexity of the entropy firstly gives

$$\lambda \text{Ent}_\Omega(\mu) \geq \lambda \text{Ent}_\Omega(\bar{\rho}) + \lambda \int_\Omega \log(\bar{\rho})(\mu - \bar{\rho}). \quad (3.2.9)$$

Secondly, by Kantorovich duality formula and using the fact that  $\varphi_\rho^\nu$  is a Kantorovich potential between  $\bar{\rho}$  and  $\nu$ , we get

$$\begin{aligned} \frac{1}{2} \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\mu, \nu) dP(\nu) &\geq \frac{1}{2} \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\bar{\rho}, \nu) dP(\nu) \\ &+ \int_{\mathcal{P}_2(\mathbb{R}^d)} \left( \int_\Omega \varphi_\rho^\nu d(\mu - \bar{\rho}) \right) dP(\nu). \end{aligned}$$

Adding (3.2.9), observing that (3.2.6) means that  $\lambda \log \bar{\rho} + \int_{\mathcal{P}_2(\mathbb{R}^d)} \varphi_\rho^\nu dP(\nu) = 0$  and using Fubini's theorem, we thus get

$$V_{P,\lambda,\Omega}(\mu) \geq V_{P,\lambda,\Omega}(\bar{\rho}),$$

so that  $\bar{\rho} = \text{bar}_{\lambda,\Omega}(P)$ .

Let us now prove (3.2.7). Since

$$\Phi := \int_{\mathcal{P}_2(\mathbb{R}^d)} u_\rho^\nu dP(\nu)$$

is convex,  $\log \bar{\rho}$  is semi-convex. It is therefore differentiable a.e. Now we claim that if  $x \in \Omega$  is a differentiability point of  $\Phi$  it also has to be a differentiability point of  $u_\rho^\nu$  for  $P$ -almost every  $\nu$ . Indeed, assume that  $\Phi$  is differentiable at  $x \in \Omega$ . For  $n \in \mathbb{N}^*$ , let  $A_n$  denote the set of  $\nu \in \mathcal{P}_2(\mathbb{R}^d)$  for which there exist  $p_\nu$  and  $q_\nu$  in  $\partial u_\rho^\nu(x)$  such that  $|p_\nu - q_\nu| \geq 1/n$ . The desired claim will be established if we prove that  $P(A_n) = 0$  for every  $n \in \mathbb{N}^*$ . Let then  $(q_\nu, p_\nu) \in \partial u_\rho^\nu(x)^2$  be chosen (in a measurable way) so that  $|p_\nu - q_\nu| \geq 1/n$  when  $\nu \in A_n$ , then, for every  $h \in \Omega - x$ , one has

$$u_\rho^\nu(x+h) - u_\rho^\nu(x) - \frac{1}{2}(p_\nu + q_\nu) \cdot h \geq \frac{1}{2}|(p_\nu - q_\nu) \cdot h|,$$

so that, by integration  $s := \int_{\mathcal{P}_2(\mathbb{R}^d)} \frac{p_\nu + q_\nu}{2} dP(\nu) \in \partial\Phi(x) = \{\nabla\Phi(x)\}$  and then

$$\Phi(x+h) - \Phi(x) - s \cdot h = o(h) \geq \frac{1}{2} \int_{A_n} |(p_\nu - q_\nu) \cdot h| dP(\nu).$$

By homogeneity, we thus have  $\int_{A_n} |(p_\nu - q_\nu) \cdot h| dP(\nu) = 0$  for every  $h$ . This implies  $\int_{A_n} |p_\nu - q_\nu| dP(\nu) = 0 \geq P(A_n)/n$  and therefore  $P(A_n) = 0$ . Hence, if  $\Phi$  is differentiable at  $x$ , for every  $h \in \mathbb{R}^d$ , we have

$$\frac{u_\rho^\nu(x+th) - u_\rho^\nu(x)}{t} \rightarrow \nabla u_\rho^\nu(x) \cdot h \text{ as } t \rightarrow 0^+, \text{ for } P\text{-a.e. } \nu.$$

Moreover, the left-hand side above is controlled in absolute value by the Lipschitz constant of  $u_{\bar{\rho}}^{\nu}$  in a compact neighbourhood of  $x$  which, thanks to Lemma 3.2.2, in turn, is controlled by

$$\int_{\Omega} |\nabla u_{\bar{\rho}}^{\nu}| \bar{\rho} = \int_{\mathbb{R}^d} |y| d\nu(y) \leq \sqrt{m_2(\nu)}.$$

Thanks to (3.1.1) and Lebesgue's dominated convergence theorem, we thus get

$$\nabla \Phi(x) = \int_{\mathcal{P}_2(\mathbb{R}^d)} \nabla u_{\bar{\rho}}^{\nu}(x) dP(\nu),$$

which shows (3.2.7). □

*Remark 3.2.6* (A first regularizing effect). One immediately deduces from (3.2.6) and the convexity of  $u_{\bar{\rho}}^{\nu}$ , further regularity properties of the regularized barycenter:

$$\log(\bar{\rho}) \in L_{\text{loc}}^{\infty}(\Omega), \bar{\rho} \in W_{\text{loc}}^{1,\infty}(\Omega), \text{ and } \nabla \bar{\rho} \in \text{BV}_{\text{loc}}(\Omega, \mathbb{R}^d).$$

*Example 3.2.7* (Gaussian case). Suppose now that  $P$  is concentrated on Gaussian measures and  $\Omega = \mathbb{R}^d$ ; then the regularized barycenter is Gaussian as well. In order to prove this we can assume thanks to Proposition 3.1.5 that  $P$ -a.e.  $\nu = \mathcal{N}(0, S_{\nu})$ , where  $S_{\nu}$  are positive semi-definite matrices with  $\mathbb{E}_P[S_{\nu}] \leq \sigma^2 I$ ,  $\sigma > 0$ . We want to prove that there is a positive definite symmetric matrix  $\bar{S}$  such that

$$\text{bar}_{\lambda}(P) = \mathcal{N}(0, \bar{S}).$$

In order to see that, recall that the optimal transport  $T_{\rho}^{\nu}$  from  $\rho = \mathcal{N}(0, S)$  to  $\nu = \mathcal{N}(0, S_{\nu})$  is given by (see e.g. [47])

$$T_{\rho}^{\nu}(x) := \underbrace{S^{-1/2} \left( S^{1/2} S_{\nu} S^{1/2} \right)^{1/2} S^{-1/2}}_{=: T_S^{S_{\nu}}} x.$$

Thus  $u_{\rho}^{\nu} = \frac{1}{2} x \cdot T_S^{S_{\nu}} x + C$ , and the optimality condition (3.2.6) can be rewritten as

$$-\frac{\lambda}{2} x \cdot \bar{S}^{-1} x = -\frac{|x|^2}{2} + \frac{1}{2} \mathbb{E}_P \left[ x \cdot T_S^{S_{\nu}} x \right] + C,$$

i.e.

$$I = \lambda \bar{S}^{-1} + \bar{S}^{-1/2} \mathbb{E}_P \left[ \left( \bar{S}^{1/2} S_{\nu} \bar{S}^{1/2} \right)^{1/2} \right] \bar{S}^{-1/2}.$$

Thus  $\bar{S}$  has to be a solution of the following fixed-point equation

$$S = \Phi(S) := \lambda I + \mathbb{E}_P \left[ \left( S^{1/2} S_{\nu} S^{1/2} \right)^{1/2} \right].$$

This has a solution by Brouwer's fixed-point theorem. Indeed, denote by  $\alpha_{\nu}$  the largest eigenvalue of  $S_{\nu}$ . Then, by assumption

$$\mathbb{E}_P[\alpha_{\nu}] \leq \text{tr} \mathbb{E}_P[S_{\nu}] \leq d\sigma^2.$$

Define

$$\alpha := 2\lambda + d\sigma^2,$$

then for any  $\lambda I \leq S \leq \alpha I$  it holds that

$$\begin{aligned} \Phi(S) &\leq \left( \lambda + \mathbb{E}_P \left[ (\alpha_\nu \alpha)^{1/2} \right] \right) I \leq \left( \lambda + \frac{\alpha}{2} + \frac{\mathbb{E}_P[\alpha_\nu]}{2} \right) I \\ &\leq \left( \lambda + \frac{\alpha}{2} + \frac{d\sigma^2}{2} \right) I = \alpha I. \end{aligned}$$

So,  $\Phi(\cdot)$  maps the convex set  $\{\lambda I \leq S \leq \alpha I\}$  to itself, and it is clearly continuous. The existence of  $\bar{S}$  such that  $\bar{S} = \Phi(\bar{S})$  therefore follows from Brouwer's fixed-point theorem.

*Example 3.2.8* (Discrete case). Consider now the case where  $\Omega = \mathbb{R}^d$  and  $P$  is a discrete measure supported on discrete measures

$$P = \sum_{i \in I} p_i \delta_{\nu_i} \text{ with } \nu_i := \sum_{j \in J_i} \nu_i^j \delta_{x_i^j},$$

where  $I$  and each  $J_i$  are finite and for every  $i \in I$ , the points  $(x_i^j)_{j \in J_i}$  are pairwise distinct and the weights  $\nu_i^j$  are positive. Then, it follows from Proposition 3.2.5 that  $\bar{\rho} = \text{bar}_\lambda(P)$  has the form

$$\bar{\rho}(x) = \exp\left(-\frac{1}{2\lambda}|x|^2 + \frac{1}{\lambda} \sum_{i \in I} p_i u_i(x)\right),$$

where  $\nabla u_i$  is the optimal transport between  $\bar{\rho}$  and  $\nu_i$  so that  $u_i$  takes the form

$$u_i(x) = \max_{j \in J_i} \{x \cdot x_i^j - v_i^j\} := u_{v_i}(x),$$

where the  $v_i = (v_i^j)_{j \in J_i}$  should match the mass conservation condition, i.e. be such that

$$\nu_i^j = \bar{\rho}(\partial u_{v_i}^*(x_i^j)), \quad \forall i \in I, \quad \forall j \in J_i. \quad (3.2.10)$$

In the semi-discrete optimal terminology,  $\partial u_{v_i}^*(x_i^j)$  is the so-called Laguerre cell where  $u_{v_i}$  coincides with  $x \mapsto x \cdot x_i^j - v_i^j$ . Computing  $\bar{\rho} = \text{bar}_\lambda(P)$  therefore amounts to finding  $\{v_i^j, i \in I, j \in J_i\}$  such that (3.2.10) holds for  $\bar{\rho}$  depending on the  $v_i^j$  as well:

$$\bar{\rho}(x) = \exp\left(-\frac{1}{2\lambda}|x|^2 + \frac{1}{\lambda} \sum_{i \in I} p_i \max_{j \in J_i} \{x \cdot x_i^j - v_i^j\}\right). \quad (3.2.11)$$

Using results from [68] concerning the differentiability of the Kantorovich functional in the semi-discrete case, it is easy to see that the non-linear system (3.2.10)–(3.2.11) is the system of Euler–Lagrange equations for the finite-dimensional concave maximization problem

$$\sup_{v_i^j} \left[ - \sum_{i \in I} p_i \sum_{j \in J_i} v_i^j \nu_i^j - \lambda \int_{\mathbb{R}^d} \exp\left(-\frac{1}{2\lambda}|x|^2 + \frac{1}{\lambda} \sum_{i \in I} p_i \max_{j \in J_i} \{x \cdot x_i^j - v_i^j\}\right) dx \right],$$

which is the dual of the entropic barycenter problem in this semi-discrete setting.

### 3.3 Properties of the entropic barycenter

#### 3.3.1 Global bounds

The aim of this paragraph is to emphasize some global bounds on the entropic barycenter which hold in the case where  $\Omega$  may be unbounded, in particular it covers the case of the whole space.

**Lemma 3.3.1.** *The entropic Wasserstein barycenter  $\bar{\rho}$  of  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$  enjoys the following bound on the Fisher information:*

$$\int_{\Omega} |\nabla \log(\bar{\rho})|^2 \bar{\rho} \leq \frac{1}{\lambda^2} \int_{\mathcal{P}_2(\mathbb{R}^d)} W^2(\bar{\rho}, \nu) dP(\nu).$$

In particular,  $\sqrt{\bar{\rho}} \in H^1(\Omega)$ , hence in case  $\Omega = \mathbb{R}^d$  it holds that  $\bar{\rho} \in L^\infty(\mathbb{R}) \cap C^{0,1/2}(\mathbb{R})$  if  $d = 1$ ,  $\bar{\rho} \in L^q(\mathbb{R}^2)$  for every  $q \in [1, +\infty)$  if  $d = 2$  and  $\bar{\rho} \in L^{\frac{d}{d-2}}(\mathbb{R}^d)$  if  $d \geq 3$ . Finally,  $(1 + |x|) \nabla \bar{\rho} \in L^1(\mathbb{R}^d)$ .

*Proof.* According to Proposition 3.2.5

$$\nabla \log(\bar{\rho}(x)) = \frac{1}{\lambda} \int_{\mathcal{P}_2(\mathbb{R}^d)} (\nabla u_{\bar{\rho}}^\nu(x) - x) dP(\nu) = -\frac{1}{\lambda} \int_{\mathcal{P}_2(\mathbb{R}^d)} \nabla \varphi_{\bar{\rho}}^\nu(x) dP(\nu),$$

thus

$$\int_{\Omega} \frac{|\nabla \bar{\rho}|^2}{\bar{\rho}} = \int_{\Omega} |\nabla \log(\bar{\rho})|^2 \bar{\rho} \leq \frac{1}{\lambda^2} \int_{\Omega} \bar{\rho}(x) \int_{\mathcal{P}_2(\mathbb{R}^d)} |\nabla \varphi_{\bar{\rho}}^\nu(x)|^2 dP(\nu) dx,$$

and using Fubini's Theorem, we get that

$$\int_{\Omega} \frac{|\nabla \bar{\rho}|^2}{\bar{\rho}} \leq \frac{1}{\lambda^2} \int_{\mathcal{P}_2(\mathbb{R}^d)} \left[ \int_{\Omega} |\nabla \varphi_{\bar{\rho}}^\nu|^2 \bar{\rho} \right] dP(\nu) = \frac{1}{\lambda^2} \int_{\mathcal{P}_2(\mathbb{R}^d)} W_2^2(\bar{\rho}, \nu) dP(\nu).$$

Finally,  $(1 + |x|) \nabla \bar{\rho} = 2(1 + |x|) \sqrt{\bar{\rho}} \nabla \sqrt{\bar{\rho}}$  belongs to  $L^1(\mathbb{R}^d)$  since both  $(1 + |x|) \sqrt{\bar{\rho}}$  and  $\nabla \sqrt{\bar{\rho}}$  are in  $L^2(\mathbb{R}^d)$ .  $\square$

**Proposition 3.3.2.** *Let  $p \geq 1$ , and assume that*

$$\int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) dP(\nu) < +\infty \quad (3.3.1)$$

(where  $m_p(\nu) := \int_{\mathbb{R}^d} |x|^p d\nu(x)$ ). Then the entropic-Wasserstein barycenter  $\bar{\rho}$  of  $P$  satisfies  $m_p(\bar{\rho}) < +\infty$ , and more precisely, for any  $r > 0$  it holds that

$$m_p(\bar{\rho}) \leq \frac{6^p}{2} \left( r^p + \int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) dP(\nu) \right) + \frac{\mathcal{L}^d(B_1(0)) \Gamma\left(\frac{d+p}{2}\right)}{2\mathcal{L}^d(\Omega \cap B_r(0))} (96\lambda)^{(d+p)/2}. \quad (3.3.2)$$

In particular, if  $\Omega = \mathbb{R}^d$ , then

$$m_p(\bar{\rho}) \leq \frac{6^p}{2} \int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) dP(\nu) + (3456\lambda)^{p/2} \Gamma\left(\frac{d+p}{2}\right). \quad (3.3.3)$$

### 3.3. PROPERTIES OF THE ENTROPIC BARYCENTER

*Proof.* Fix  $r > 0$  s.t.  $\mathcal{L}^d(\Omega \cap B_r(0)) > 0$  and denote  $S := \Omega \cap B_r(0)$ . Now let us take  $R > 0$  and consider the set

$$Q_R := \{x \in B_R(0) \setminus B_{R/2}(0) : |x| \geq 3(\mathbb{E}|T_{\bar{\rho}}^\nu(x)| + r)\}. \quad (3.3.4)$$

Here and after, expectations are taken w.r.t.  $\nu \sim P$ . Assume  $\bar{\rho}(Q_R) > 0$  and define

$$\rho_t := \bar{\rho} + t \left( \frac{\bar{\rho}(Q_R)}{\mathcal{L}^d(S)} \mathbb{1}_S - \bar{\rho} \mathbb{1}_{Q_R} \right) \in \mathcal{P}_2(\Omega), \quad 0 \leq t \leq 1.$$

Then

$$\begin{aligned} \left. \frac{d}{dt} \text{Ent}_\Omega(\rho_t) \right|_{t=0^+} &= \frac{\bar{\rho}(Q_R)}{\mathcal{L}^d(S)} \int_S \log \bar{\rho} - \int_{Q_R} \bar{\rho} \log \bar{\rho} \\ &\leq \bar{\rho}(Q_R) \log \left( \frac{\bar{\rho}(S)}{\mathcal{L}^d(S)} \right) - \bar{\rho}(Q_R) \log \left( \frac{\bar{\rho}(Q_R)}{\mathcal{L}^d(Q_R)} \right) \\ &\leq \bar{\rho}(Q_R) \log \left( \frac{\mathcal{L}^d(Q_R) \bar{\rho}(S)}{\bar{\rho}(Q_R) \mathcal{L}^d(S)} \right) \\ &\leq \bar{\rho}(Q_R) \log \left( \frac{\mathcal{L}^d(B_R(0))}{\bar{\rho}(Q_R) \mathcal{L}^d(S)} \right) \\ &= \bar{\rho}(Q_R) \log \left( \frac{V_d R^d}{\bar{\rho}(Q_R) \mathcal{L}^d(S)} \right), \end{aligned}$$

where  $V_d := \mathcal{L}^d(B_1(0))$  is the volume of the unit ball in  $\mathbb{R}^d$ . Furthermore, for any  $\nu$  we can estimate  $W_2^2(\rho_1, \nu)$  using the transport plan

$$\gamma := (\text{id}, T_{\bar{\rho}}^\nu)_\# \left( \bar{\rho} \mathbb{1}_{\mathbb{R}^d \setminus Q_R} \right) + \frac{1}{\mathcal{L}^d(S)} \mathbb{1}_S \otimes (T_{\bar{\rho}}^\nu)_\# \left( \bar{\rho} \mathbb{1}_{Q_R} \right) \in \Pi(\rho_1, \nu),$$

which gives us

$$\begin{aligned} W_2^2(\rho_1, \nu) &\leq \int_{\mathbb{R}^d \setminus Q_R} |T_{\bar{\rho}}^\nu(x) - x|^2 \bar{\rho} + \int_S \left[ \int_{Q_R} |T_{\bar{\rho}}^\nu(x) - y|^2 \bar{\rho}(x) \right] dy \\ &\leq W_2^2(\rho_0, \nu) + \int_{Q_R} \left[ (r + |T_{\bar{\rho}}^\nu(x)|)^2 - |T_{\bar{\rho}}^\nu(x) - x|^2 \right] \bar{\rho} \\ &\leq W_2^2(\rho_0, \nu) + \int_{Q_R} [r^2 + 2r|T_{\bar{\rho}}^\nu(x)| - |x|^2 + 2|T_{\bar{\rho}}^\nu(x)||x|] \bar{\rho}. \end{aligned}$$

Then it is easy to see that, due to convexity of  $W_2^2(\cdot, \cdot)$ ,

$$\begin{aligned} \left. \frac{d}{dt} \mathbb{E} W_2^2(\rho_t, \nu) \right|_{t=0^+} &\leq \mathbb{E} W_2^2(\rho_1, \nu) - \mathbb{E} W_2^2(\rho_0, \nu) \\ &\leq \int_{Q_R} [r^2 + 2(r + |x|) \mathbb{E}|T_{\bar{\rho}}^\nu(x)| - |x|^2] \bar{\rho} \\ &= \int_{Q_R} \left[ (r + \mathbb{E}|T_{\bar{\rho}}^\nu(x)|)^2 - (|x| - \mathbb{E}|T_{\bar{\rho}}^\nu(x)|)^2 \right] \bar{\rho} \\ &\leq -\frac{1}{3} \int_{Q_R} |x|^2 \bar{\rho} \leq -\frac{\bar{\rho}(Q_R) R^2}{12}. \end{aligned}$$

Therefore,

$$\left. \frac{d}{dt} V_{P,\lambda,\Omega}(\rho_t) \right|_{t=0+} \leq \lambda \bar{\rho}(Q_R) \left( \log \left( \frac{V_d R^d}{\bar{\rho}(Q_R) \mathcal{L}^d(S)} \right) - \frac{R^2}{24\lambda} \right).$$

On the other hand, by optimality this derivative should be non-negative, thus

$$\bar{\rho}(Q_R) \leq \frac{V_d R^d}{\mathcal{L}^d(S)} \exp \left( -\frac{R^2}{24\lambda} \right). \quad (3.3.5)$$

Now we set  $R_n = 2^n$  and define  $q_n := \bar{\rho}(Q_{R_n})$ ,  $n \in \mathbb{Z}$ . Note that by the definition (3.3.4) of  $Q_R$ , if  $x \in \Omega \setminus \bigcup_{n \in \mathbb{Z}} Q_{R_n}$ , then  $|x| < 3 \left( \mathbb{E} |T_{\bar{\rho}}^\nu(x)| + r \right)$ . Consequently,

$$m_p(\bar{\rho}) = \int_{\Omega} |x|^p \bar{\rho} \leq \int_{\Omega \setminus \bigcup_{n \in \mathbb{Z}} Q_{R_n}} 3^p \left( \mathbb{E} |T_{\bar{\rho}}^\nu| + r \right)^p \bar{\rho} + \sum_{n \in \mathbb{Z}} R_n^p q_n.$$

Using the fact that  $(a+b)^p \leq 2^{p-1}(a^p + b^p)$ ,  $\left( T_{\bar{\rho}}^\nu \right)_{\#} \bar{\rho} = \nu$ , and Jensen's inequality, one can bound the first term on the r.h.s. as follows:

$$\int_{\Omega \setminus \bigcup_{n \in \mathbb{Z}} Q_{2^n}} 3^p \left( \mathbb{E} |T_{\bar{\rho}}^\nu(x)| + r \right)^p \bar{\rho} \leq \frac{6^p}{2} \left( r^p + \mathbb{E} \int_{\Omega} |T_{\bar{\rho}}^\nu|^p \bar{\rho} \right) = \frac{6^p}{2} (r^p + \mathbb{E} m_p(\nu)).$$

Now let us bound the second term: due to (3.3.5) we get

$$\begin{aligned} \sum_{n \in \mathbb{Z}} R_n^p q_n &\leq \frac{V_d}{\mathcal{L}^d(S)} \sum_{n \in \mathbb{Z}} R_n^{d+p} \exp \left( -\frac{R_n^2}{24\lambda} \right) \\ &\leq \frac{V_d}{\mathcal{L}^d(S)} \sum_{n \in \mathbb{Z}} \int_{2^n}^{2^{n+1}} x^{d+p-1} \exp \left( -\frac{x^2}{96\lambda} \right) dx \\ &= \frac{V_d}{\mathcal{L}^d(S)} \int_0^{+\infty} x^{d+p-1} \exp \left( -\frac{x^2}{96\lambda} \right) dx \\ &= \frac{V_d (96\lambda)^{(d+p)/2}}{2\mathcal{L}^d(S)} \Gamma \left( \frac{d+p}{2} \right). \end{aligned}$$

Combining the above bounds together we obtain

$$m_p(\bar{\rho}) \leq \frac{6^p}{2} (r^p + \mathbb{E} m_p(\nu)) + \frac{V_d (96\lambda)^{(d+p)/2}}{2\mathcal{L}^d(S)} \Gamma \left( \frac{d+p}{2} \right),$$

thus the first claim follows.

Finally, in case  $\Omega = \mathbb{R}^d$ , we can take  $r = \frac{\sqrt{96\lambda}}{6^{p/(p+d)}}$ , then using  $\mathcal{L}^d(S) = V_d r^d$  one obtains

$$\begin{aligned} m_p(\bar{\rho}) &\leq \frac{6^p}{2} \mathbb{E} m_p(\nu) + \left( 6^{d/(p+d)} \sqrt{96\lambda} \right)^p \frac{1 + \Gamma \left( \frac{d+p}{2} \right)}{2} \\ &\leq \frac{6^p}{2} \mathbb{E} m_p(\nu) + (3456\lambda)^{p/2} \Gamma \left( \frac{d+p}{2} \right). \end{aligned}$$

□

*Remark 3.3.3.* Note that (3.3.3) (and thus, in some sense, (3.3.2)) is an interpolation between two bounds. On the one hand, if  $\lambda = 0$ , then  $\bar{\rho}$  is a standard Wasserstein barycenter and, due to convexity of  $m_p(\cdot)$  along generalized geodesics, one gets the bound

$$m_p(\bar{\rho}) \leq \int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) dP(\nu).$$

On the other hand, if  $P$  is concentrated at the measure  $\delta_0$ , then  $\bar{\rho} = \mathcal{N}(0, \lambda I)$  by Proposition 3.2.5. In this case,

$$m_p(\bar{\rho}) = \frac{(2\lambda)^{p/2} \Gamma\left(\frac{p+d}{2}\right)}{\Gamma\left(\frac{d}{2}\right)},$$

which coincides with the second term in the r.h.s. of (3.3.3) up to a constant factor to the power  $p$  and a factor depending on the dimension.

*Remark 3.3.4.* Let us indicate now a more elementary approach to obtain moment bounds when  $\Omega$  is convex. Let  $V: \mathbb{R}^d \rightarrow \mathbb{R}_+$  be a convex potential such that

$$\int_{\mathcal{P}_2(\mathbb{R}^d)} m_V(\nu) dP(\nu) < +\infty, \text{ where } m_V(\nu) := \int_{\mathbb{R}^d} V(x) d\nu(x).$$

On the one hand, thanks to (3.2.7), the convexity of  $V$  and the fact that  $\nabla u_{\bar{\rho}\#}^\nu \bar{\rho} = \nu$ , we have

$$\int_{\Omega} V(\lambda \nabla \log \bar{\rho}(x) + x) \bar{\rho}(x) dx \leq \int_{\mathcal{P}_2(\mathbb{R}^d)} m_V(\nu) dP(\nu).$$

On the other hand, again by convexity

$$V(\lambda \nabla \log \bar{\rho}(x) + x) \bar{\rho}(x) \geq V(x) \bar{\rho}(x) + \lambda \nabla V(x) \cdot \nabla \bar{\rho}(x).$$

Integrating by parts (which can be justified if  $V$  is  $C^{1,1}$  and using Lemma 3.3.1), denoting by  $\eta$  the outward normal to  $\Omega$  on  $\partial\Omega$ , we thus get

$$\int_{\Omega} (V - \lambda \Delta V) \bar{\rho} \leq \int_{\mathcal{P}_2(\mathbb{R}^d)} m_V(\nu) dP(\nu) - \lambda \int_{\partial\Omega} \partial_\eta V \bar{\rho}. \quad (3.3.6)$$

Assuming (3.3.1) and choosing  $V(x) = |x - x_0|^p$  (actually, some suitable  $C^{1,1}$  approximations of  $V$ ) with  $p \geq 2$  in (3.3.6) with  $x_0 \in \Omega$ , observing that  $\partial_\eta V \geq 0$  on  $\partial\Omega$  since  $\Omega$  is convex, we obtain the bound

$$\int_{\Omega} \left( |x - x_0|^p - \lambda p(p+d-2) |x - x_0|^{p-2} \right) \bar{\rho}(x) dx \leq \int_{\Omega} \int_{\mathbb{R}^d} |x - x_0|^p d\nu(x) dP(\nu).$$

In particular, when  $\Omega = \mathbb{R}^d$  or, more generally, when  $\Omega$  is convex and contains 0, we have

$$m_2(\bar{\rho}) \leq 2\lambda d + \int_{\mathcal{P}_2(\mathbb{R}^d)} m_2(\nu) dP(\nu),$$

and for higher moments

$$m_p(\bar{\rho}) \leq \lambda p(p+d-2) m_{p-2}(\bar{\rho}) + \int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) dP(\nu).$$

Note finally that when choosing  $V$  linear, the two convexity inequalities we used above are equalities, yielding

$$\int_{\Omega} x \bar{\rho}(x) dx + \lambda \int_{\partial\Omega} \eta \bar{\rho} = \int_{\mathcal{P}_2(\mathbb{R}^d)} \int_{\mathbb{R}^d} x d\nu(x) dP(\nu).$$

**Corollary 3.3.5.** *Under assumptions of Proposition 3.3.2 it holds that  $\bar{\rho}^{1/p} \in W^{1,p}(\Omega)$ . In particular, if  $p > d$ , then  $\bar{\rho} \in L^\infty(\Omega) \cap C^{0,1-d/p}(\Omega)$ .*

*Proof.* Once we have a bound on  $m_p(\bar{\rho})$ , the fact that  $\bar{\rho}^{1/p}$  is  $W^{1,p}$  can be proved as for Lemma 3.3.1. Indeed, by the same arguments together with the crude bound

$$|\nabla u_{\bar{\rho}}^\nu(x) - x|^p \leq 2^{p-1} (|\nabla u_{\bar{\rho}}^\nu(x)|^p + |x|^p),$$

we arrive at

$$p^p \left| \nabla \bar{\rho}^{1/p} \right|_{L^p(\Omega)}^p = \int_{\Omega} \frac{|\nabla \bar{\rho}|^p}{\bar{\rho}^{p-1}} \leq \frac{2^{p-1}}{\lambda^p} \left( \int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) dP(\nu) + m_p(\bar{\rho}) \right).$$

□

### 3.3.2 Stability

Following [76], let us define the  $p$ -Wasserstein metric between measures on  $\mathcal{P}_p(\mathbb{R}^d)$

$$\mathcal{W}_p^p(P, Q) := \inf_{\Gamma \in \Pi(P, Q)} \int_{\mathcal{P}_p(\mathbb{R}^d) \times \mathcal{P}_p(\mathbb{R}^d)} W_p^p(\mu, \nu) d\Gamma(\mu, \nu).$$

**Lemma 3.3.6** (Stability). *Take  $p \geq 2$  and let  $\{P_n\}_{n \geq 1} \subset \mathcal{P}_p(\mathcal{P}_p(\mathbb{R}^d))$ ,  $P \in \mathcal{P}_p(\mathcal{P}_p(\mathbb{R}^d))$  be s.t.  $\mathcal{W}_p(P_n, P) \rightarrow 0$ . Then for  $\bar{\rho}_n = \text{bar}_{\lambda, \Omega}(P_n)$  and  $\bar{\rho} = \text{bar}_{\lambda, \Omega}(P)$  it holds that*

$$W_p(\bar{\rho}_n, \bar{\rho}) \rightarrow 0, \quad (3.3.7)$$

$$\bar{\rho}_n^{1/p} \xrightarrow{W^{1,p}(\Omega)} \bar{\rho}^{1/p}, \quad (3.3.8)$$

$$\log \bar{\rho}_n \xrightarrow{W_{\text{loc}}^{1,q}(\Omega)} \log \bar{\rho}, \quad \forall 1 \leq q < \infty. \quad (3.3.9)$$

*Proof. Proof of (3.3.7).* Note that since  $W_2(\cdot, \cdot) \leq W_p(\cdot, \cdot)$  and  $\mathcal{W}_2(\cdot, \cdot) \leq \mathcal{W}_p(\cdot, \cdot)$ , one has  $\mathcal{W}_2(P_n, P) \rightarrow 0$ . According to the proof of Proposition 3.1.2,  $m_2(\bar{\rho}_n)$  ( $m_2(\bar{\rho})$ ) are uniformly bounded, thus by (3.1.3)  $\text{Ent}_{\Omega}(\bar{\rho}_n)$  ( $\text{Ent}_{\Omega}(\bar{\rho})$ ) are bounded from below. Moreover, replacement of  $\Omega$  with its closure  $\bar{\Omega}$  does not change an entropic-Wasserstein barycenter. Then Theorem 5.5 from [71] that  $W_2(\bar{\rho}_n, \bar{\rho}) \rightarrow 0$ .

Arguing in the same way as in the proof of Proposition 3.3.2, one can show that for any  $R > 0$

$$\int_{\{|x| \geq R\}} |x|^p \bar{\rho}_n \leq C \left[ \int_{\mathcal{P}_p(\mathbb{R}^d)} \int_{\{|x| \geq R\}} \left( 1 + |\nabla u_{\bar{\rho}_n}^\nu|^p \right) \bar{\rho}_n dP_n(\nu) + \int_R^{+\infty} x^{d+p-1} \exp\left(-\frac{x^2}{96\lambda}\right) dx \right], \quad (3.3.10)$$

where the constant  $C$  depends solely on  $\Omega$ ,  $\lambda$ ,  $p$ , and  $d$ .

To prove that  $W_p(\bar{\rho}_n, \bar{\rho}) \rightarrow 0$ , we also need the following result on continuity of optimal transport plans: once  $W_2(\rho_n, \rho) \rightarrow 0$ ,  $W_p(\nu_n, \nu) \rightarrow 0$ , and there exists a unique optimal transport plan  $\gamma_\rho^\nu$  from  $\rho$  to  $\nu$  for the quadratic cost function, one has

$$J(\gamma_{\rho_n}^{\nu_n}, \gamma_\rho^\nu) \rightarrow 0,$$

where  $J(\cdot, \cdot)$  is the optimal transport cost for the cost function

$$c((x_1, y_1), (x_2, y_2)) = |x_1 - x_2|^2 + |y_1 - y_2|^p, \quad x_i, y_i \in \mathbb{R}^d,$$

and  $\gamma_{\rho_n}^{\nu_n}$  is any optimal transport plan from  $\rho_n$  to  $\nu_n$  for the quadratic cost function. Indeed,

$$\int |x - y|^2 d\gamma_{\rho_n}^{\nu_n} = W_2^2(\rho_n, \nu_n) \rightarrow W_2^2(\rho, \nu) = \int |x - y|^2 d\gamma_{\rho}^{\nu},$$

then  $\gamma_{\rho_n}^{\nu_n} \rightarrow \gamma_{\rho}^{\nu}$  due to Prokhorov's theorem and uniqueness of the optimal transport plan. Moreover,

$$\begin{aligned} \int_{\mathbb{R}^d \times \mathbb{R}^d} (|x|^2 + |y|^p) d\gamma_{\rho_n}^{\nu_n}(x, y) &= m_2(\rho_n) + m_p(\nu_n) \\ &\rightarrow m_2(\rho) + m_p(\nu) = \int_{\mathbb{R}^d \times \mathbb{R}^d} (|x|^2 + |y|^p) d\gamma_{\rho}^{\nu}(x, y), \end{aligned}$$

thus the convergence follows from Theorem 3.7 [71]. Further, using Theorem 3.7 [71] again, it is easy to see that for any closed set  $G \subset \mathbb{R}^d$  the function

$$(\rho, \nu) \mapsto \int_G (1 + |\nabla u_{\rho}^{\nu}|^p) \rho = \int_{G \times \mathbb{R}^d} (1 + |y|^p) d\gamma_{\rho}^{\nu}(x, y)$$

is upper-semicontinuous w.r.t. convergence in  $W_2$  distance (for  $\rho$ ) and  $W_p$  distance (for  $\nu$ ), as well as its average w.r.t. a measure on  $\mathcal{P}_p(\mathbb{R}^d)$

$$(\rho, P) \mapsto \int_{\mathcal{P}_p(\mathbb{R}^d)} \int_G (1 + |\nabla u_{\rho}^{\nu}|^p) \rho dP(\nu).$$

Hence for all  $R > 0$  one obtains

$$\limsup_{n \rightarrow \infty} \int_{\mathcal{P}_p(\mathbb{R}^d)} \int_{\{|x| \geq R\}} (1 + |\nabla u_{\bar{\rho}_n}^{\nu}|^p) \bar{\rho}_n dP_n(\nu) \leq \int_{\mathcal{P}_p(\mathbb{R}^d)} \int_{\{|x| \geq R\}} (1 + |\nabla u_{\bar{\rho}}^{\nu}|^p) \bar{\rho} dP(\nu).$$

Using this together with (3.3.10), we get that

$$\begin{aligned} \limsup_{n \rightarrow \infty} \int_{\{|x| \geq R\}} |x|^p \bar{\rho}_n &\leq C \left[ \int_{\{|x| \geq R\}} \left( \int_{\mathcal{P}_p(\mathbb{R}^d)} (1 + |\nabla u_{\bar{\rho}}^{\nu}|^p) dP(\nu) \right) \bar{\rho} \right. \\ &\quad \left. + \int_R^{+\infty} x^{d+p-1} \exp\left(-\frac{x^2}{96\lambda}\right) dx \right] \rightarrow 0 \text{ as } R \rightarrow 0. \end{aligned}$$

Thus the measures  $(|\cdot|^p \bar{\rho}_n)_{n \in \mathbb{N}}$  are uniformly integrable, and by the criterion of convergence in a Wasserstein space (see e.g. Theorem 6.9 [113]), we deduce that  $W_p(\bar{\rho}_n, \bar{\rho}) \rightarrow 0$  as  $n \rightarrow \infty$ .

**Proof of (3.3.8) and (3.3.9).** Fix an arbitrary open set  $U \subset \subset \Omega$ . By Lemma 3.2.2

$$\begin{aligned} \text{Lip}\left(u_{\bar{\rho}_n}^{\nu} \Big|_U\right) &\leq \frac{C}{\inf_{x \in U_{3r/4}} \bar{\rho}_n(B_{r/4}(x))} \left( \int_{\Omega} |\nabla u_{\bar{\rho}_n}^{\nu}|^2 \bar{\rho}_n \right)^{1/2} \\ &= \frac{C}{\inf_{x \in U_{3r/4}} \bar{\rho}_n(B_{r/4}(x))} \sqrt{m_2(\nu)}, \end{aligned}$$

where  $r = d(U, \partial\Omega)$ . Since  $\bar{\rho}_n \rightarrow \bar{\rho}$  and  $\bar{\rho} > 0$  on  $\Omega$ , we have  $\inf_{x \in U_{3r/4}} \bar{\rho}_n(B_{r/4}(x)) \geq c > 0$  for any  $n$ . Therefore, the functions

$$\bar{u}_n = \lambda \log \bar{\rho}_n + \frac{|\cdot|^2}{2} = \int_{\mathcal{P}_2(\mathbb{R}^d)} u_{\bar{\rho}_n}^\nu \, dP_n(\nu)$$

are uniformly Lipschitz continuous on  $U$  for all  $n$  since  $\int_{\mathcal{P}_2(\mathbb{R}^d)} m_2(\nu) \, dP_n(\nu)$  are uniformly bounded. Furthermore, as  $\bar{\rho}_n \rightarrow \bar{\rho} > 0$ ,  $\bar{u}_n$  are also uniformly bounded on  $U$ . Then, by the Arzelà–Ascoli theorem,  $\bar{u}_n \xrightarrow{C(U)} \bar{u}$ , and we deduce from weak convergence that  $\bar{u} = \lambda \log \bar{\rho} + \frac{|\cdot|^2}{2}$ . Moreover, every  $\bar{u}_n$  is convex, thus  $\nabla \bar{u}_n \rightarrow \nabla \bar{u}$  a.e. on  $U$ . Hence, by Lebesgue’s dominated convergence theorem, we get  $\bar{u}_n \xrightarrow{W^{1,q}(U)} \bar{u}$  for any  $1 \leq q < \infty$  and thus (3.3.9).

Further, using (3.2.7), we get

$$\int_{\Omega \setminus U} \left| \nabla \bar{\rho}_n^{1/p} \right|^p = \frac{1}{p^p} \int_{\Omega \setminus U} |\nabla \log \bar{\rho}_n|^p \bar{\rho}_n \leq \frac{2^{p-1}}{(p\lambda)^p} \int_{\Omega \setminus U} (|\nabla \bar{u}_n|^p + |x|^p) \bar{\rho}_n.$$

Since the functions  $\rho \mapsto \int_{\Omega \setminus U} |x|^p \rho$  and  $(\rho, P) \mapsto \int_{\mathcal{P}_2(\mathbb{R}^d)} \int_{\Omega \setminus U} |\nabla u_\rho^\nu|^p \rho \, dP(\nu)$  are u.s.c., we obtain that

$$\limsup \int_{\Omega \setminus U} \left| \nabla \bar{\rho}_n^{1/p} \right|^p \rightarrow 0 \quad \text{as } U \rightarrow \Omega$$

(e.g. in a sense that  $\bar{\rho}(\Omega \setminus U) \rightarrow 0$ ). Finally, this together with (3.3.9) yields that  $\bar{\rho}_n^{1/p} \xrightarrow{W^{1,p}(\Omega)} \bar{\rho}^{1/p}$ .  $\square$

In particular, the previous lemma shows that one can approximate the barycenter  $\bar{\rho}$  by approximating  $P$  with discrete measures supported on some dense set of measures, e.g. discrete or having smooth densities. As another corollary of Lemma 3.3.6, in Section 3.5 we will obtain a law of large numbers for entropic-Wasserstein barycenters.

### 3.3.3 A maximum principle

**Proposition 3.3.7.** *Assume that  $\Omega$  is convex and  $P(\{\nu \in \mathcal{P}_2(\mathbb{R}^d) : \nu(\Omega) = 1\}) = 1$ , and let  $\bar{\rho} := \text{bar}_{\lambda, \Omega}(P)$  be its entropic Wasserstein barycenter. Then*

$$\|\bar{\rho}\|_{L^\infty(\mathbb{R}^d)} \leq \left( \int_{\mathcal{P}_2(\mathbb{R}^d)} \|\nu\|_{L^\infty(\mathbb{R}^d)}^{-1/d} \, dP(\nu) \right)^{-d}.$$

*Proof.* We first prove the result in the simple case where  $P$  is supported by finitely many measures and then proceed by approximation thanks to the stability Lemma 3.3.6 (more precisely, its corollary Theorem 3.5.1).

#### Step 1: the case of finitely many measures.

Fix a compact convex set  $K \subset \Omega$  with non-empty interior. Assume that  $P = \sum_{i=1}^N p_i \delta_{\nu_i}$ , where each  $\nu_i$  is supported in  $K$  and has a  $C^{0,\alpha}$ , bounded away from 0 density on  $K$ . Since  $K$  is bounded, all  $u_{\bar{\rho}}^{\nu_i}$  are Lipschitz, so we can take the continuous version of  $\bar{\rho}$  on  $\bar{\Omega}$ . Now fix an arbitrary  $x \in \bar{\Omega} \setminus K$ . Since  $\bar{\rho} > 0$  on  $\Omega$  and  $\left( \nabla u_{\bar{\rho}}^{\nu_i} \right)_{\#} \bar{\rho} = \nu_i$  for all  $i$ , there

are subgradients  $\nabla u_{\bar{\rho}}^{\nu_i}(x) \in K$ . Let  $y = \sum_{i=1}^N p_i \nabla u_{\bar{\rho}}^{\nu_i}(x) \in K$ ,  $v = \frac{y-x}{|y-x|}$ , then thanks to (3.2.6)

$$\partial_v \log \bar{\rho}(x) \geq \frac{1}{\lambda} \langle y - x, v \rangle = \frac{1}{\lambda} |y - x| > 0,$$

therefore  $x$  cannot be a maximum point of  $\bar{\rho}$ , and  $\bar{\rho}$  actually attains its maximum on  $K$ .

Further, since  $\log(\bar{\rho}) \in W_{\text{loc}}^{1,\infty}(\Omega)$ , the regularity result of Cordero-Erausquin and Figalli [40] yields that  $u_{\bar{\rho}}^{\nu_i}$  is in fact  $C_{\text{loc}}^{2,\alpha}$ . Then at its maximum point  $x \in \Omega$  we should have, on the one hand

$$\sum_{i=1}^N p_i D^2 u_{\bar{\rho}}^{\nu_i}(x) \leq I.$$

On the other hand, using the Monge-Ampère equation  $\bar{\rho} = \det \left( D^2 u_{\bar{\rho}}^{\nu_i} \right) \nu_i \left( \nabla u_{\bar{\rho}}^{\nu_i} \right)$  (see also (3.4.3)), we get

$$\bar{\rho}(x) \leq \|\nu_i\|_{L^\infty(\mathbb{R}^d)} \det \left( D^2 u_{\bar{\rho}}^{\nu_i}(x) \right), \quad i = 1, \dots, N.$$

So, using the concavity of  $\det(\cdot)^{1/d}$  over symmetric positive semi-definite matrices, we obtain

$$\begin{aligned} \sum_{i=1}^N p_i \left( \frac{\bar{\rho}(x)}{\|\nu_i\|_{L^\infty(\mathbb{R}^d)}} \right)^{1/d} &\leq \sum_{i=1}^N p_i \det \left( D^2 u_{\bar{\rho}}^{\nu_i}(x) \right)^{1/d} \\ &\leq \det \left( \sum_{i=1}^N p_i D^2 u_{\bar{\rho}}^{\nu_i}(x) \right)^{1/d} \leq 1, \end{aligned}$$

which gives

$$\bar{\rho} \leq \left( \sum_{i=1}^N p_i \|\nu_i\|_{L^\infty(\mathbb{R}^d)}^{-1/d} \right)^{-d}.$$

Of course, the requirement that  $\nu_i$  is bounded away from 0 is just here to justify twice differentiability of  $u_{\bar{\rho}}^{\nu_i}$ , if we drop this assumption replacing  $\nu_i$  by  $\nu_i^n = (1 - \frac{1}{n})\nu_i + \frac{1}{n}\mathcal{L}^d|_K$ , using Lemma 3.3.6, we get the same conclusion by letting  $n \rightarrow \infty$ . In a similar way, Hölder regularity of the  $\nu_i$ 's can also be removed by suitably mollifying these measures and arguing by stability again. Finally, if  $P = \sum_{i=1}^N p_i \delta_{\nu_i}$  with  $m_2(\nu_i) < +\infty$ , we can find an increasing sequence of compact convex sets  $K_n \subset \Omega$ , such that for every  $n \in \mathbb{N}$

$$\max_{i=1,\dots,N} \int_{\mathbb{R}^d \setminus K_n} (1 + |x|^2) d\nu_i(x) \leq \frac{1}{n}.$$

Set

$$\nu_i^n := \frac{\nu_i \mathbb{1}_{K_n}}{\nu_i(K_n)} \leq \frac{n}{n-1} \nu_i, \quad P_n := \sum_{i=1}^N p_i \delta_{\nu_i^n},$$

then  $\bar{\rho}_n := \text{bar}_{\lambda,\Omega}(P_n)$  is bounded with

$$\bar{\rho}_n \leq \frac{n}{n-1} \left( \sum_{i=1}^N p_i \|\nu_i\|_{L^\infty(\mathbb{R}^d)}^{-1/d} \right)^{-d}.$$

Since  $W_2(\nu_i^n, \nu_i) \rightarrow 0$  for all  $1 \leq i \leq N$ , we have  $W_2^2(P_n, P) \rightarrow 0$ , thus stability enables us to conclude that

$$\bar{\rho} \leq \left( \sum_{i=1}^N p_i \|\nu_i\|_{L^\infty(\mathbb{R}^d)}^{-1/d} \right)^{-d}.$$

**Step 2: the general case.**

We now consider the case of a general Borel probability  $P \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d))$  and concentrated on measures giving full mass to  $\Omega$ . Let  $\nu_1, \nu_2, \dots$  be i.i.d. random measures drawn from  $P$ . Then, by Theorem 3.5.1, the empirical barycenters  $\bar{\rho}_n := \text{bar}_{\lambda, \Omega}(P_n)$ , where  $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{\nu_i}$  is the empirical measure, a.s. converge to  $\bar{\rho}$  in the 2-Wasserstein distance. Since

$$\frac{1}{n} \sum_{i=1}^n \|\nu_i\|_{L^\infty(\mathbb{R}^d)}^{-1/d} \rightarrow \int_{\mathcal{P}_2(\mathbb{R}^d)} \|\nu\|_{L^\infty(\mathbb{R}^d)}^{-1/d} dP(\nu) \quad \text{a.s.}$$

by the strong law of large numbers, we conclude by lower semicontinuity of the  $L^\infty$ -norm w.r.t.  $W_2$ -convergence using Step 1.  $\square$

*Remark 3.3.8.* If, under the assumptions of the above proposition,

$$P\left(\{\nu \in L^\infty(\mathbb{R}^d), \nu \leq C\}\right) = \alpha > 0,$$

then it gives

$$\|\bar{\rho}\|_{L^\infty(\mathbb{R}^d)} \leq \frac{C}{\alpha^d}.$$

The same bound was obtained in Theorem 6.1 from [67] for 2-Wasserstein barycenters on Riemannian manifolds.

The following simple example shows that convexity of  $\Omega$  is essential for the maximum principle (even if  $P$ -a.e. measure  $\nu$  is concentrated on  $\Omega$ ).

*Example 3.3.9.* Consider the one-dimensional case where  $\Omega = [-8, -4] \cup [-1, 1] \cup [4, 8]$ . Let  $P = \frac{1}{2}\delta_{\nu_-} + \frac{1}{2}\delta_{\nu_+}$ ,  $\nu_- = \frac{1}{4}\mathbb{1}_{(-8, -4)}$ ,  $\nu_+ = \frac{1}{4}\mathbb{1}_{(4, 8)}$ . First, we take  $\lambda = 0$ , thus  $\bar{\rho}_0 := \text{bar}_{\Omega, 0}(P)$  is an ordinary Wasserstein barycenter (constrained to be supported on  $\Omega$ ). It is easy to see that  $\bar{\rho}_0$  is actually supported on  $[-1, 1]$ , so  $\|\bar{\rho}_0\|_{L^\infty(\Omega)} \geq \frac{1}{2}$  while  $\|\nu_-\|_{L^\infty(\Omega)} = \|\nu_+\|_{L^\infty(\Omega)} = \frac{1}{4}$ . Now we consider  $\bar{\rho}_\lambda := \text{bar}_{\Omega, \lambda}(P)$  and let  $\lambda \rightarrow 0$ . By compactness, we readily get that  $\bar{\rho}_\lambda \rightharpoonup \bar{\rho}_0$ , so, for  $\lambda$  small enough, we have  $\|\bar{\rho}_\lambda\|_{L^\infty(\Omega)} > \frac{1}{4}$ . Finally, by rescaling, one can construct examples violating the maximum principle for any  $\lambda > 0$ .

## 3.4 Higher regularity

### 3.4.1 The bounded case

The theory developed so far has needed very mild assumptions on  $\Omega$ . To deduce higher regularity (up to the boundary) of the Kantorovich potentials and the barycenter we need to impose more conditions on the domain.

### 3.4. HIGHER REGULARITY

Suppose that  $P$  is concentrated on sufficiently regular probability measures supported on a closed ball of radius  $R > 0$ ,  $\bar{B} := \bar{\Omega} = \bar{B}_R(0)$ , more precisely, assume that for some  $\alpha \in (0, 1)$ ,  $k \in \mathbb{N}^*$  and  $C > 0$

$$P\left(\underbrace{\left\{\nu \in \mathcal{P}_{\text{ac}}(\mathbb{R}^d) : \nu(\bar{\Omega}) = 1, \|\nu\|_{C^{k,\alpha}(\bar{\Omega})} + \|\log \nu\|_{L^\infty(\bar{\Omega})} \leq C\right\}}_{=: \mathcal{Q}_{k,\alpha}}\right) = 1. \quad (3.4.1)$$

*Remark 3.4.1.* The following arguments are presented here for the case of a ball for simplicity but work for compact convex sets with  $C^{k+2,\alpha}$ -boundary which are strongly convex with a uniform modulus of convexity. More precisely, we require that there are  $m$ -strongly convex functions  $H_\nu, H \in C^{k+2,\alpha}(\mathbb{R}^d)$  for  $m > 0$  such that

$$\begin{aligned} \Omega &= \{x \in \mathbb{R}^d : H(x) < 0\}, \partial\Omega = \{x \in \mathbb{R}^d : H(x) = 0\}, \\ \text{supp } \nu &= \{x \in \mathbb{R}^d : H_\nu(x) \leq 0\}, \partial(\text{supp } \nu) = \{x \in \mathbb{R}^d : H_\nu(x) = 0\}, \end{aligned}$$

and there is an  $R > 0$  such that  $\Omega, \text{supp } \nu \subset B_R(0)$  for  $P$ -a.e.  $\nu$ . We add remarks at the proofs that significantly depend on the domain.

Thanks to the entropic regularization, this regularity implies regularity for the potentials and the barycenter.

**Proposition 3.4.2.** *Under assumption (3.4.1) for  $k \in \mathbb{N}^*$ , one has*

$$u_\rho^\nu \in C^{k+2,\alpha}(\bar{\Omega}) \text{ for } P\text{-a.e. } \nu \quad \text{and} \quad \bar{\rho} \in C^{k+2,\alpha}(\bar{\Omega}),$$

and there is a constant  $K > 0$  such that

$$\|u_\rho^\nu\|_{C^{k+2,\alpha}(\bar{\Omega})}, \|u_\nu^\bar{\rho}\|_{C^{k+2,\alpha}(\bar{\Omega})} \leq K \text{ for } P\text{-a.e. } \nu.$$

Furthermore, for  $P$ -a.e.  $\nu$  the transport  $\nabla u_\rho^\nu: \bar{\Omega} \rightarrow \bar{\Omega}$  is a diffeomorphism of class  $C^{k+1,\alpha}$ .

*Proof.* By (3.4.1)  $P$ -a.e.  $\nu \in C^{0,\alpha}(\bar{\Omega})$  is bounded from below and above on  $\bar{\Omega}$  by a constant only depending on  $C$ . With the representation of  $\bar{\rho}$  in (3.2.6) we obtain that  $\nabla \log \bar{\rho}$  is bounded by  $2R/\lambda$  a.e. Together with  $\int \bar{\rho} = 1$  this implies that  $\|\log \bar{\rho}\|_{C^{0,1}(\bar{\Omega})}$  is bounded by a constant only depending on  $R$  and  $\lambda$ .

This implies by Caffarelli's regularity theory for Monge-Ampère equations (see [25] for the original paper and Theorem 3.3 [44] for a concise formulation) that for any  $\nu \in \mathcal{Q}_{k,\alpha}$ ,  $u_\rho^\nu \in C^{2,\alpha}(\bar{\Omega})$  and  $\nabla u_\rho^\nu: \bar{\Omega} \rightarrow \bar{\Omega}$  is a diffeomorphism.

For the uniform estimate again by Caffarelli's regularity theory for Monge-Ampère equations (theorem on page 3 (1143) of [23]) there is an  $\alpha_1 \in (0, 1)$  and constant  $C_1$  (only depending on  $\alpha_1, C$  and  $R$ ) such that

$$\|u_\rho^\nu\|_{C^{1,\alpha_1}(\bar{\Omega})}, \|u_\nu^\bar{\rho}\|_{C^{1,\alpha_1}(\bar{\Omega})} \leq C_1 \quad \text{for every } \nu \in \mathcal{Q}_{k,\alpha}.$$

This implies in particular  $\bar{\rho} \in C^{1,\alpha_1}(\bar{\Omega})$  by (3.2.6) and we can apply Theorem 3.6.7 to see that

$$\begin{aligned} \Phi_{\bar{\rho}}: \left\{ \nu \in C^{0,\alpha_1}(\bar{\Omega}) : \nu(\bar{\Omega}) = 1, \|\log \nu\|_{L^\infty(\bar{\Omega})} < \infty \right\} &\rightarrow \mathcal{M} \\ \nu &\mapsto u_\nu^\bar{\rho} \end{aligned}$$

is continuous (where  $\mathcal{M}$  denotes the set of  $C^{2,\alpha_1}(\bar{\Omega})$  convex potentials  $u$  with zero mean such that  $|\nabla u| = R$  on  $\partial\Omega$ ). Now note that, by the compact embedding of Hölder spaces,

$\mathcal{Q}_{k,\alpha}$  is compact in  $C^{0,\alpha_1}(\bar{\Omega})$ . This implies that  $\Phi_{\bar{\rho}}(\mathcal{Q}_{k,\alpha})$  is compact in  $C^{2,\alpha_1}(\bar{\Omega})$ . Hence, there is a  $K_1 > 0$  such that

$$\|u_{\nu}^{\bar{\rho}}\|_{C^{2,\alpha_1}(\bar{\Omega})} \leq K_1 \text{ for } P\text{-a.e. } \nu.$$

Furthermore, since each  $u_{\nu}^{\bar{\rho}}$  is strongly convex thanks to compactness of  $\Phi_{\bar{\rho}}(\mathcal{Q}_{k,\alpha})$  we conclude that there is constant  $c > 0$  such that

$$D^2 u_{\nu}^{\bar{\rho}} \geq c \text{ for } P\text{-a.e. } \nu, \quad (3.4.2)$$

so that we obtain

$$\|D^2 u_{\nu}^{\bar{\rho}}\|_{L^{\infty}(\Omega)} \leq c \text{ for } P\text{-a.e. } \nu,$$

which gives  $\bar{\rho} \in C^{1,1}(\bar{\Omega})$  and then again by Caffarelli's regularity theory for Monge-Ampère equations  $u_{\bar{\rho}}^{\nu} \in C^{3,\alpha}(\bar{\Omega})$ . Differentiating now the Monge-Ampère equation (which is satisfied in the classical sense)

$$\begin{aligned} \det(D^2 u_{\bar{\rho}}^{\nu}) \nu(\nabla u_{\bar{\rho}}^{\nu}) &= \bar{\rho} & \text{in } \Omega, \\ \left| \nabla u_{\bar{\rho}}^{\nu} \right|^2 &= R^2 & \text{on } \partial\Omega, \end{aligned}$$

in direction  $e \in \mathbb{S}^{d-1}$ , we obtain by the same considerations as in the computation in Proposition 3.6.6

$$\begin{aligned} \operatorname{div}(A_{\nu} \nabla(\partial_e u_{\bar{\rho}}^{\nu})) &= \partial_e \bar{\rho} & \text{in } \Omega, \\ \nabla u_{\bar{\rho}}^{\nu} \cdot \nabla(\partial_e u_{\bar{\rho}}^{\nu}) &= 0 & \text{on } \partial\Omega, \end{aligned}$$

where  $A_{\nu} = \nu(\nabla u_{\bar{\rho}}^{\nu}) \det(D^2 u_{\bar{\rho}}^{\nu})(D^2 u_{\bar{\rho}}^{\nu})^{-1}$ . Thanks to Lemma 3.6.3 and (3.4.2) we can finally deduce by classical Schauder estimates (Theorem 6.30 in [61]) that there is constant  $K > 0$  uniform in  $\nu$  such that

$$\|\partial_e u_{\bar{\rho}}^{\nu}\|_{C^{2,\alpha}(\bar{\Omega})} \leq K \left( \|\partial_e u_{\bar{\rho}}^{\nu}\|_{C^{0,\alpha}(\bar{\Omega})} + \|\partial_e \bar{\rho}\|_{C^{0,\alpha}(\bar{\Omega})} \right).$$

This concludes the uniform estimate of  $u_{\bar{\rho}}^{\nu}$  in  $C^{3,\alpha}(\bar{\Omega})$  for  $P$ -a.e.  $\nu$ , and by again employing (3.2.6) we deduce  $\bar{\rho} \in C^{3,\alpha}(\bar{\Omega})$ . The same bound follows for  $u_{\nu}^{\bar{\rho}}$  by exchanging the role of  $\bar{\rho}$  and  $\nu$ . Higher regularity follows by standard elliptic theory.  $\square$

Note in particular that  $u_{\bar{\rho}}^{\nu}$  satisfies the Monge-Ampère equation, subject to the *second boundary* value condition, which encodes the fact that  $\nabla u_{\bar{\rho}}^{\nu}$  maps the ball into itself, in the classical sense

$$\begin{aligned} \det(D^2 u_{\bar{\rho}}^{\nu}) \nu(\nabla u_{\bar{\rho}}^{\nu}) &= \bar{\rho} \text{ in } B \\ \nabla u_{\bar{\rho}}^{\nu}(B) &\subset B, \end{aligned} \quad (3.4.3)$$

and that the second boundary value condition is equivalent (see Lemma 3.6.1) to an eikonal equation on the boundary

$$|\nabla u_{\bar{\rho}}^{\nu}(x)|^2 = R^2, \quad \forall x \in \partial B.$$

### 3.4.2 The case of log-concave measures on $\mathbb{R}^d$

Caffarelli's contraction principle [26], generalized by Kolesnikov in [69], implies global (and dimension-free) Lipschitz (or Hölder) global estimates for the optimal transport between suitable log-concave measures. In its original form, Caffarelli's Theorem says that the optimal transport between the standard Gaussian  $\gamma$  and a measure which is more log-concave (i.e. has the form  $e^{-V}\gamma$  with  $V$  convex) is 1-Lipschitz. Since the entropic barycenter is less log-concave than a Gaussian, if the measures  $\nu$  satisfy a uniform log-concavity estimate, one can deduce a  $C^{1,1}$  regularity result for  $\log(\bar{\rho})$ :

**Proposition 3.4.3.** *Assume  $\Omega = \mathbb{R}^d$  and that for  $P$ -a.e.  $\nu$  there is some  $A_\nu > 0$  such that  $\nu$  writes as  $d\nu = e^{-V_\nu}d\gamma$  with  $D^2V_\nu \geq A_\nu I$  (in the sense of distributions), such that  $\mathbb{E} \left[ \sqrt{\lambda A_\nu}^{-1} \right] < \infty$ , where the expectation is taken with respect to the random variable  $\nu$  distributed according to  $P$ . Let  $\bar{\rho} := \text{bar}_\lambda(P)$  be its entropic barycenter.*

*Then  $\log \bar{\rho} \in C^{1,1}(\mathbb{R}^d)$  and more precisely there holds*

$$-I \leq \lambda D^2 \log \bar{\rho} \leq \left( \mathbb{E} \left[ \frac{1}{\sqrt{\lambda A_\nu}} \right] - 1 \right) I. \quad (3.4.4)$$

*Proof.* It directly follows from (3.2.6) that  $\bar{\rho} = e^{-\psi}$  with  $D^2\psi \leq \frac{I}{\lambda}$ . Since for  $P$ -a.e.  $\nu$  we have  $d\nu = e^{-V_\nu}d\gamma$  with  $D^2V_\nu \geq A_\nu I$ , thanks to Caffarelli's contraction Theorem, the optimal transport map  $\nabla u_\rho^\nu$  is Lipschitz with the explicit estimate

$$0 \leq D^2 u_\rho^\nu \leq \frac{I}{\sqrt{\lambda A_\nu}} \quad P\text{-a.e.}$$

so that the convex potential  $\Phi := \mathbb{E} \left[ u_\rho^\nu \right]$  is  $C^{1,1}$  and has  $\mathbb{E} \left[ \sqrt{\lambda A}^{-1} \right] < \infty$  as an upper bound on its Hessian. Since  $\lambda \nabla \log(\bar{\rho}) + \text{id} = \nabla \Phi$ , the bound (3.4.4) directly follows.  $\square$

## 3.5 Statistical properties

### 3.5.1 Stochastic setting and law of large numbers

Now we consider the following stochastic setting [11, 71, 3]: let  $P$ , as above, be a distribution on  $\mathcal{P}_2(\Omega)$  with finite second moment, and  $\nu_1, \nu_2, \dots$  be independent random measures drawn from  $P$ . We will call the barycenter of the first  $n$  measures  $\nu_1, \dots, \nu_n$  an *empirical barycenter*:  $\bar{\rho}_n = \text{bar}_{\lambda, \Omega}(P_n)$ , where  $P_n = \frac{1}{n} \sum_{i=1}^n \delta_{\nu_i}$  is the empirical measure. Note that  $\bar{\rho}_n$  is random, and in this section we will establish its statistical properties, namely, consistency and (under additional assumptions) a central limit theorem. As already mentioned in section 3.3, a LLN follows immediately from Lemma 3.3.6.

**Theorem 3.5.1** (Law of large numbers). *Assume  $\int_{\mathcal{P}_2(\mathbb{R}^d)} m_p(\nu) dP(\nu) < +\infty$  for some  $p \geq 2$ . Let  $\bar{\rho}$  be the entropic-Wasserstein barycenter of  $P$  and  $(\bar{\rho}_n)_{n \in \mathbb{N}}$  be the empirical barycenters. Then it a.s. holds that*

$$\begin{aligned} W_p(\bar{\rho}_n, \bar{\rho}) &\longrightarrow 0, \\ \log \bar{\rho}_n &\xrightarrow{W_{\text{loc}}^{1,q}(\Omega)} \log \bar{\rho} \quad \forall 1 \leq q < \infty, \\ \bar{\rho}_n^{1/p} &\xrightarrow{W^{1,p}(\Omega)} \bar{\rho}^{1/p}. \end{aligned}$$

In particular, if  $\bar{\Omega}$  is compact and  $(\bar{\rho}_n)_{n \in \mathbb{N}}$  is uniformly bounded in  $C^{k,\alpha}(\bar{\Omega})$  for  $k \in \mathbb{N}$ , then  $\bar{\rho}_n \xrightarrow{a.s.} \bar{\rho}$  in  $C^{k,\beta}(\bar{\Omega})$  for any  $\beta \in (0, \alpha)$ .

*Proof.* It is well-known that, since the Wasserstein space is Polish, empirical measures  $P_n$  converge to  $P$  in  $\mathcal{W}_p$  metric (see e.g. Corollary 5.9 in [71]). Then the first part of the theorem follows from Lemma 3.3.6.

The last claim follows due to compact Hölder embedding and weak convergence  $\bar{\rho}_n \rightharpoonup \bar{\rho}$ .  $\square$

### 3.5.2 Central limit theorem

#### Formal idea of the CLT

For the proof of the CLT we inspire ourselves by what is known on Riemannian manifolds, see for instance Section 5.4 [94]. This idea has also been employed for the case of Gaussian measures in [72]. Let us consider the formal computations.

Given a Wasserstein barycenter  $\bar{\rho}$  of (EB) (for  $\lambda = 0$ ,  $\Omega = \mathbb{R}^d$ ) the first order optimality conditions amount to

$$\int \varphi_{\bar{\rho}}^{\nu} dP(\nu) = 0, \quad (3.5.1)$$

where  $\varphi_{\bar{\rho}}^{\nu}$  are the Kantorovich potentials, i.e. such that  $(Id - \nabla \varphi_{\bar{\rho}}^{\nu})_{\#} \bar{\rho} = \nu$ . Note that we actually only have

$$\int \varphi_{\bar{\rho}}^{\nu} dP(\nu) \geq 0 \quad \text{with equality} \quad \bar{\rho}\text{-a.e.} \quad (3.5.2)$$

But in the following formal arguments we assume that we have (3.5.1), as it would be the case for Riemannian manifolds. This condition becomes in the empirical case for an empirical barycenter  $\bar{\rho}_n$  formally

$$\frac{1}{n} \sum_{k=1}^n \varphi_{\bar{\rho}_n}^{\nu_k} = 0. \quad (3.5.3)$$

Now a natural way to obtain a CLT on a manifold is to consider the CLT on the tangent space and hope for enough regularity to be able to project back on the manifold, using a delta method. (Here we assume that the tangent spaces at two different points can be identified with each other.) What we mean is the following. Considering Remark 2.1.30, the Kantorovich potentials can be seen as vectors in the tangent space of  $\bar{\rho}$ , resp.  $\bar{\rho}_n$ . The i.i.d. potentials  $\varphi_{\bar{\rho}}^{\nu_k}$  satisfy a CLT, i.e. taking into account that  $\mathbb{E}_P \left[ \varphi_{\bar{\rho}}^{\nu_k} \right] = 0$  we have

$$\frac{1}{\sqrt{n}} \sum_{k=1}^n \varphi_{\bar{\rho}}^{\nu_k} \longrightarrow \mathcal{N}(0, \text{Var}(\varphi_{\bar{\rho}}^{\nu_k})).$$

With (3.5.3) we obtain

$$\frac{1}{\sqrt{n}} \sum_{k=1}^n \varphi_{\bar{\rho}}^{\nu_k} - \frac{1}{\sqrt{n}} \sum_{k=1}^n \varphi_{\bar{\rho}_n}^{\nu_k} \longrightarrow \mathcal{N}(0, \text{Var}(\varphi_{\bar{\rho}}^{\nu_k})).$$

Now keep in mind that the Kantorovich potentials can be seen as vectors in the tangent space of  $\bar{\rho}$ , respectively  $\bar{\rho}_n$ , and define the map

$$\bar{\Phi}_{\nu} : \rho \mapsto \varphi_{\rho}^{\nu}, \quad (3.5.4)$$

so that

$$\frac{1}{\sqrt{n}} \sum_{k=1}^n \bar{\Phi}_{\nu_k}(\bar{\rho}) - \frac{1}{\sqrt{n}} \sum_{k=1}^n \bar{\Phi}_{\nu_k}(\bar{\rho}_n) \longrightarrow \mathcal{N}(0, \text{Var}(\varphi_{\bar{\rho}}^{\nu})).$$

If the  $\bar{\Phi}_{\nu}$  are continuously differentiable, this rewrites

$$\underbrace{\int_0^1 \frac{1}{n} \sum_{k=1}^n \bar{\Phi}'_{\nu_k}(\bar{\rho}_n^t) dt}_{=: G_n} \sqrt{n}(\bar{\rho} - \bar{\rho}_n) \longrightarrow \mathcal{N}(0, \text{Var}(\varphi_{\bar{\rho}}^{\nu})),$$

where  $\bar{\rho}_n^t := t\bar{\rho} + (1-t)\bar{\rho}_n$ . So if the operators  $G_n$  converge nicely to an invertible  $G$ , we finally obtain

$$\sqrt{n}(\bar{\rho} - \bar{\rho}_n) \longrightarrow \mathcal{N}(0, G^{-1} \text{Var}(\varphi_{\bar{\rho}}^{\nu}) G^{-1}).$$

This strategy is made rigorous in the following section with the help of the entropic regularization.

### Rigorous proof of the CLT

In the following we give a CLT under the condition that  $\bar{\Phi}_{\nu}$  from (3.5.4) (more precisely  $\bar{\Phi}_{\nu} = \frac{1}{2}|\cdot|^2 - \bar{\Phi}_{\nu}$ ) is sufficiently regular followed by corollaries giving sufficient conditions for this regularity. To overcome the problem of having an obstacle problem as pointed out in (3.5.2), we use the penalizing term in the variational problem to enforce equality on a certain fixed set  $\Omega$ .

First, let us recall some notions of probability theory in Hilbert spaces. Let  $(H, \langle \cdot, \cdot \rangle)$  be a separable Hilbert space endowed with its Borel sigma-algebra. Recall that random variables  $\{X_n\}_{n \in \mathbb{N}}$  taking values in  $H$  converge in distribution to a random variable  $X$  if  $\mathbb{E}f(X_n) \rightarrow \mathbb{E}f(X)$  for any bounded continuous function  $f$  on  $H$ . We denote this convergence by

$$X_n \xrightarrow{d} X.$$

The covariance operator of a random variable  $X$  is defined as

$$\begin{aligned} \text{Var}(X) : H &\rightarrow H \\ h &\mapsto \mathbb{E}[\langle X - \mathbb{E}[X], h \rangle (X - \mathbb{E}[X])]. \end{aligned}$$

We also need to recall the notion of strong operator topology (SOT): operators  $A_n$  on  $H$  converge to  $A$  in SOT ( $A_n \xrightarrow{\text{SOT}} A$ ), if  $A_n u \rightarrow Au$  for all  $u \in H$ .

Finally, to prove a central limit theorem for barycenters we will use some technical results from probability theory postponed to Appendix 3.A.

Let us also introduce the following notation: if  $\mathcal{F}$  is a space of integrable functions on  $\bar{\Omega}$ , then

$$\mathcal{F}_{\diamond} := \left\{ f \in \mathcal{F} : \int_{\Omega} f = 0 \right\}.$$

**Theorem 3.5.2** (Central limit theorem). *Let  $\bar{\Omega}$  be the closure of an open, bounded, convex set. For  $\alpha \in (0, 1)$  and  $\nu \in \mathcal{P}(\bar{\Omega})$  define the map*

$$\begin{aligned} \Phi_{\nu} : C^{0,\alpha}(\bar{\Omega}) \cap \mathcal{P}_{\text{ac}}(\bar{\Omega}) &\rightarrow L_{\diamond}^2(\Omega) \\ \rho &\mapsto u_{\rho}^{\nu}, \end{aligned}$$

where  $u_\rho^\nu$  is the zero-mean Brenier potential between  $\rho$  and  $\nu$ .

Assume that there is a set  $\mathcal{D} \subset \mathcal{P}_2(\bar{\Omega})$  such that  $P(\mathcal{D}) = 1$  and for  $\nu \in \mathcal{D}$  the map  $\Phi_\nu$  is continuously differentiable at  $\rho$  with  $\|\log \rho\|_{L^\infty(\Omega)} < \infty$  and its derivative  $(\Phi_\nu)'$  is Hermitian and non-positive. Suppose further that  $(\Phi_\nu)'(\rho)$  are bounded in  $L_\diamond^2(\Omega)$  uniformly in  $\rho \in C^{0,\alpha}(\bar{\Omega}) \cap \mathcal{P}_{\text{ac}}(\bar{\Omega})$  and  $\nu \in \mathcal{D}$ .

Then a CLT for empirical barycenters holds in  $L_\diamond^2(\Omega)$ , i.e.

$$\sqrt{n}(\bar{\rho}_n - \bar{\rho}) \xrightarrow{d} \xi \sim \mathcal{N}(0, \Sigma),$$

with covariance operator  $\Sigma = G^{-1} \text{Var}(u_{\bar{\rho}}^\nu) G^{-1}$ , where

$$G: u \mapsto \lambda \frac{u}{\bar{\rho}} - \lambda \int_B \frac{u}{\bar{\rho}} - \mathbb{E}[(\Phi_\nu)'(\bar{\rho})].$$

*Proof.* First note that  $\bar{\rho} = \text{bar}_{\lambda, \Omega}(P) \in C^{0,1}(\bar{\Omega})$  by compactness of  $\bar{\Omega}$  and the characterization of entropic barycenters (3.2.6), by the same argument as in the beginning of the proof of Proposition 3.4.2.

**Step 1.** Let us introduce the following map  $F$

$$F: \left\{ \rho \in C^{0,\alpha}(\bar{\Omega}) : \int_B \rho = 1, \min_{\bar{\Omega}} \rho > 0 \right\} \rightarrow C_\diamond^{0,\alpha}(\bar{\Omega})$$

$$\rho \mapsto \lambda \log \rho + \frac{|\cdot|^2}{2} - \int_B \left( \lambda \log \rho(x) + \frac{|x|^2}{2} \right).$$

It is continuously differentiable and its derivative is

$$F'(\rho): h \mapsto \lambda \frac{h}{\rho} - \lambda \int_B \frac{h}{\rho}.$$

Then the first order optimality condition (3.2.6) can be rewritten as follows

$$F(\bar{\rho}) = \mathbb{E}[\Phi_\nu(\bar{\rho})].$$

Respectively, for the empirical barycenter it reads as

$$F(\bar{\rho}_n) = \frac{1}{n} \sum_{i=1}^n \Phi_{\nu_i}(\bar{\rho}_n).$$

Combining the above equations and using differentiability of  $F$  and  $\Phi_\nu$ , we obtain

$$G_n(\bar{\rho}_n - \bar{\rho}) = F(\bar{\rho}_n) - F(\bar{\rho}) - \frac{1}{n} \sum_{i=1}^n (\Phi_{\nu_i}(\bar{\rho}_n) - \Phi_{\nu_i}(\bar{\rho})) = \frac{1}{n} \sum_{i=1}^n u_i - \mathbb{E}[u], \quad (3.5.5)$$

where  $u_i = u_{\bar{\rho}}^{\nu_i}$ ,  $\mathbb{E}[u] = \mathbb{E}_{\nu \sim P}[u_\rho^\nu]$ , and the operator  $G_n$  is defined as follows

$$G_n := \int_0^1 F'(\bar{\rho}_n^t) dt - \frac{1}{n} \sum_{i=1}^n \int_0^1 (\Phi_{\nu_i})'(\bar{\rho}_n^t) dt,$$

with  $\bar{\rho}_n^t := (1-t)\bar{\rho} + t\bar{\rho}_n$ .

**Step 2.** We are going to apply a delta method to prove a CLT and to do this we need a convergence (in an appropriate space)

$$(G_n)^{-1} \xrightarrow{P} G^{-1}, \quad G := F'(\bar{\rho}) - \mathbb{E}[(\Phi_\nu)'(\bar{\rho})].$$

But first let us extend all the linear operators above to  $L_\diamond^2(\Omega)$  and prove their uniform boundedness. Denote by  $\text{Bar}_{\lambda,\Omega}(\mathcal{D})$  the set of entropic barycenters of all measures supported on  $\mathcal{D}$

$$\text{Bar}_{\lambda,\Omega}(\mathcal{D}) := \left\{ \text{bar}_{\lambda,\Omega}(Q) : Q \in \mathcal{P}_2(\mathcal{P}_2(\mathbb{R}^d)), Q(\mathcal{D}) = 1 \right\}.$$

Clearly, the operators  $F'(\rho)$  are Hermitian, bounded and positive definite for all  $\rho \in \text{Bar}_{\lambda,\Omega}(\mathcal{D})$ . Using the characterization of the entropic barycenter (3.2.6) and the boundedness of  $\bar{\Omega}$ , we conclude that these  $\rho$  are uniformly bounded away from zero, thus  $F'(\rho)$  are uniformly positive-definite. Indeed, for any  $h \in L_\diamond^2(\Omega)$

$$\langle h, F'(\rho)h \rangle_{L^2(\Omega)} = \int_\Omega \lambda \frac{h^2}{\rho} \geq \frac{\lambda}{\min_{\bar{\Omega}} \rho} \|h\|_{L^2(\Omega)}^2 \geq c_F \|h\|_{L^2(\Omega)}^2.$$

For all  $\rho \in \text{Bar}_{\lambda,\Omega}(\mathcal{D})$  and  $\nu \in \mathcal{D}$  it holds that  $-(\Phi_\nu)'(\rho)$  are Hermitian, non-negative and uniformly bounded by assumption. In particular, the operators  $G$  and all  $G_n$  are a.s. well-defined, uniformly positive definite, and thus continuously invertible in  $L_\diamond^2(\Omega)$  with

$$\|G^{-1}\|_{L_\diamond^2(\Omega)} \leq \|F'(\bar{\rho})^{-1}\|_{L_\diamond^2(\Omega)} \leq \frac{1}{c_F}, \quad \|G_n^{-1}\|_{L_\diamond^2(\Omega)} \leq \frac{1}{c_F}. \quad (3.5.6)$$

**Step 3.** Now let us prove that  $G_n^{-1} \rightarrow G^{-1}$  in SOT. First,

$$\int_0^1 F'(\bar{\rho}_n^t) dt \rightarrow F'(\bar{\rho}) \quad \text{a.s.}$$

since  $\bar{\rho}_n \xrightarrow{C^{0,\alpha}(\bar{\Omega})} \bar{\rho}$  a.s. by Theorem 3.5.1, thanks to  $(\bar{\rho}_n)_{n \in \mathbb{N}}$  being uniformly bounded in  $C^{0,1}(\bar{\Omega})$  (again by (3.2.6) and the boundedness of  $\bar{\Omega}$ ). Second, the LLN and separability of  $L_\diamond^2(\Omega)$  yield that

$$\frac{1}{n} \sum_{i=1}^n (\Phi_{\nu_i})'(\bar{\rho}) \xrightarrow{\text{SOT}} \mathbb{E}(\Phi_\nu)'(\bar{\rho}) \quad \text{a.s.}$$

It remains to show that

$$\frac{1}{n} \sum_{i=1}^n \int_0^1 (\Phi_{\nu_i})'(\bar{\rho}_n^t) dt - \frac{1}{n} \sum_{i=1}^n (\Phi_{\nu_i})'(\bar{\rho}) \xrightarrow{\text{SOT}} 0 \quad \text{a.s.} \quad (3.5.7)$$

Let  $\nu \in \mathcal{D}$  and  $\rho \xrightarrow{C^{0,\alpha}(\bar{\Omega})} \bar{\rho}$ . Thanks to continuous differentiability of  $\Phi_\nu$

$$\|(\Phi_\nu)'(\rho)u - (\Phi_\nu)'(\bar{\rho})u\|_{L^2(\Omega)} \rightarrow 0 \quad \text{for any } u \in C_\diamond^{0,\alpha}(\bar{\Omega}).$$

Hence, density of  $C_\diamond^{0,\alpha}(\bar{\Omega})$  in  $L_\diamond^2(\Omega)$  yield that  $(\Phi_\nu)'(\rho) \rightarrow (\Phi_\nu)'(\bar{\rho})$  in SOT on  $L_\diamond^2(\Omega)$ . Now we fix  $h \in L_\diamond^2(\Omega)$ , then the functions

$$f^{\nu_i}(\rho) := \left\| \int_0^1 (\Phi_{\nu_i})'(\rho^t)h dt - (\Phi_{\nu_i})'(\bar{\rho})h \right\|_{L^2(\Omega)},$$

where  $\rho^t := (1-t)\bar{\rho} + t\rho$ , are bounded, continuous, and  $f^{\nu_i}(\bar{\rho}) = 0$ . Since  $\bar{\rho}_n \xrightarrow{C^{0,\alpha}(\bar{\Omega})} \bar{\rho}$  a.s., Lemma 3.A.1 ensures that

$$\left\| \frac{1}{n} \sum_{i=1}^n \int_0^1 (\Phi_{\nu_i})'(\bar{\rho}_n^t) h dt - \frac{1}{n} \sum_{i=1}^n (\Phi_{\nu_i})'(\bar{\rho}) h \right\|_{L^2(\Omega)} \leq \frac{1}{n} \sum_{i=1}^n f^{\nu_i}(\bar{\rho}_n) \rightarrow 0 \quad \text{a.s.}$$

Taking a dense countable set  $\{h_j\}_{j \in \mathbb{N}}$  in  $L^2_\diamond(\Omega)$  and using the uniform boundedness of  $(\Phi_\nu)'$  in  $L^2_\diamond(\Omega)$ , one obtains (3.5.7). Combining the above results we conclude that  $G_n \xrightarrow{\text{SOT}} G$  a.s. Finally, for any  $u \in L^2_\diamond(\Omega)$  one has

$$G_n^{-1}h - G^{-1}h = G_n^{-1}(G - G_n)G^{-1}h \rightarrow 0,$$

since  $G_n^{-1}$  are uniformly bounded. We thus have shown  $G_n^{-1} \xrightarrow{\text{SOT}} G^{-1}$  a.s.

**Step 4.** Note that  $\|u_\rho^\nu\|_{L^2(\Omega)} \leq C\|u_\rho^\nu\|_{C(\bar{\Omega})}$ , thus  $\mathbb{E}\|u_\rho^\nu\|_{L^2(\Omega)}^2 < \infty$ , and by the standard CLT in Hilbert spaces (see e.g. [74, Theorem 10.5]) applied to  $(u_i)_{i \in \mathbb{N}}$  we obtain that

$$\frac{S_n}{\sqrt{n}} := \frac{1}{\sqrt{n}} \sum_{i=1}^n (u_i - \mathbb{E} u_\rho^\nu) \xrightarrow{d} \xi, \quad \xi \sim \mathcal{N}(0, \text{Var}(u_\rho^\nu)).$$

According to (3.5.5),

$$\sqrt{n}(\bar{\rho}_n - \bar{\rho}) = G_n^{-1} \frac{S_n}{\sqrt{n}}.$$

Since  $G_n^{-1}$  are uniformly bounded and  $G_n^{-1} \xrightarrow{\text{SOT}} G^{-1}$  a.s., Lemma 3.A.2 yields the CLT for  $\bar{\rho}_n$ :

$$\sqrt{n}(\bar{\rho}_n - \bar{\rho}) \xrightarrow{d} G^{-1}\xi \sim \mathcal{N}(0, G^{-1} \text{Var}(u_\rho^\nu) G^{-1}).$$

□

**Corollary 3.5.3** (CLT in the regular case). *Let  $\bar{\Omega} = \overline{B_R(0)}$  for  $R > 0$  and assume (3.4.1) to be true with  $k = 1$ . Then a CLT for empirical barycenters holds in  $H^2_\diamond(B)$ .*

*Proof.* First note, that by Theorem 3.6.7 and Proposition 3.4.2 the hypothesis of Theorem 3.5.2 are satisfied with  $\mathcal{D} = \mathcal{Q}_{1,\alpha}$ . Hence, the empirical barycenters satisfy a CLT in  $L^2_\diamond(\Omega)$ . To improve the CLT to hold in  $H^2_\diamond(B)$ , we use the same notation as in the proof of Theorem 3.5.2 and need to prove uniform boundedness of the operators  $G^{-1}$  and  $G_n^{-1}$  for all  $n$  in  $H^2_\diamond(B)$ .

Clearly  $F'(\rho)$  and  $(\Phi_\nu)'(\rho)$  can be continuously extended to  $H^2_\diamond(B)$  for any  $\rho \in \text{Bar}_{\lambda,B}(\mathcal{Q}_{1,\alpha})$ ,  $\nu \in \mathcal{Q}_{1,\alpha}$ .

For all  $\rho \in \text{Bar}_{\lambda,B}(\mathcal{Q}_{1,\alpha})$  and  $\nu \in \mathcal{Q}_{1,\alpha}$  the operators  $-(\Phi_\nu)'(\rho)$  are uniformly bounded in  $H^2_\diamond(B)$  since all  $\nu$  and  $D^2 u_\rho^\nu$  are uniformly bounded away from zero according to (3.4.1) and Proposition 3.4.2: namely, Theorem 3.6.7 together with the Poincaré inequality and Theorem 6.27 [77] yield that there is a constant  $C_\Phi > 0$  such that for  $h \in H^2(B)$

$$\|(\Phi_\nu)'(\rho)h\|_{H^2(B)} \leq C_\Phi \|h\|_{L^2(B)}. \quad (3.5.8)$$

Obviously,  $F'(\bar{\rho})$  and  $\int_0^1 F'(\bar{\rho}_n^t) dt$  are continuously invertible, with uniformly bounded inverses. In particular, they are Fredholm operators of index 0. Due to (3.5.8) and the Rellich–Kondrachov theorem,  $(\Phi_\nu)'(\rho)$  are compact and uniformly bounded in  $H^2_\diamond(B)$  for all

$\rho \in \text{Bar}_{\lambda, B}(\mathcal{Q}_{1, \alpha})$ ,  $\nu \in \mathcal{Q}_{1, \alpha}$ , as well as any of their average. Thus  $G := F'(\bar{\rho}) - \mathbb{E}[(\Phi_\nu)'(\bar{\rho})]$  is a Fredholm operator, and  $\text{ind } G = \text{ind } F'(\bar{\rho}) = 0$ . Since  $G$  is positive definite in  $L_\diamond^2(B)$ ,  $\ker G = \{0\}$ , therefore  $G$  is invertible in  $H_\diamond^2(B)$ . The same applies for any  $G_n$ . Let us prove that  $G_n^{-1}$  are uniformly bounded in  $H_\diamond^2(B)$ . Suppose  $G_n h = v \in H_\diamond^2(B)$ . Then

$$\begin{aligned} \left\| \left( \int_0^1 F'(\bar{\rho}_n^t) dt \right) h \right\|_{H^2(B)} &\leq \|v\|_{H^2(B)} + \frac{1}{n} \sum_{i=1}^n \int_0^1 \|(\Phi_{\nu_i})'(\bar{\rho}_n^t) h\|_{H^2(B)} dt \\ &\leq \|v\|_{H^2(B)} + C_\Phi \|h\|_{L^2(B)} \\ &\leq \|v\|_{H^2(B)} + C_\Phi \|G_n^{-1}\|_{L_\diamond^2(B)} \|v\|_{L^2(B)} \\ &\leq \left( 1 + \frac{C_\Phi}{c_F} \right) \|v\|_{H^2(B)}, \end{aligned}$$

by employing (3.5.6). On the other hand,

$$\left\| \left( \int_0^1 F'(\bar{\rho}_n^t) dt \right) h \right\|_{H^2(B)} \geq \left\| \left( \int_0^1 F'(\bar{\rho}_n^t) dt \right)^{-1} \right\|_{H_\diamond^2(B)}^{-1} \|h\|_{H^2(B)} \geq c \|h\|_{H^2(B)}.$$

Therefore,

$$\|G_n^{-1}\|_{H_\diamond^2(B)} \leq \frac{1}{c} \left( 1 + \frac{C_\Phi}{c_F} \right).$$

To deduce the CLT in the  $H_\diamond^2(B)$  note that we have  $\bar{\rho}_n^t \xrightarrow{C^2(\bar{B})} \bar{\rho}$  again thanks to Proposition 3.4.2 and Theorem 3.5.1. As a result we can repeat Step 3 and Step 4 in  $H_\diamond^2(B)$  to conclude.  $\square$

**Corollary 3.5.4** (CLT in the discrete case). *Let  $\bar{\Omega} = \overline{B_R(0)}$  for  $R > 0$ . Assume that there are  $N \in \mathbb{N}^*$ ,  $\varepsilon > 0$  such that we have  $P(\mathcal{D}_{\text{discr}}^{\varepsilon, N}) = 1$ , where  $\mathcal{D}_{\text{discr}}^{\varepsilon, N}$  is defined in (3.7.2). Then a CLT for empirical barycenters holds in  $L_\diamond^2(B)$ .*

*Proof.* The hypothesis of Theorem 3.5.2 are satisfied with  $\mathcal{D} = \mathcal{D}_{\text{discr}}^{\varepsilon, N}$  by Corollary 3.7.3.  $\square$

**Corollary 3.5.5** (CLT on the torus). *Assume  $\bar{\Omega} = \mathbb{T}^d$  and that for some  $\alpha \in (0, 1)$ ,  $C > 0$*

$$P\left(\left\{ \nu \in \mathcal{P}_{\text{ac}}(\mathbb{R}^d) : \nu(\bar{\Omega}) = 1, \|\nu\|_{C^{1, \alpha}(\bar{\Omega})} + \|\log \nu\|_{L^\infty(\bar{\Omega})} \leq C \right\}\right) = 1.$$

*Then a CLT for empirical barycenters holds in  $H_\diamond^2(\mathbb{T}^d)$ .*

*Proof.* The proof is analogous to the proof of Corollary 3.5.3 once one identifies all objects on  $\mathbb{T}^d$  with periodic objects on  $\mathbb{R}^d$  and chooses  $\Phi_\nu := \frac{1}{2}|\cdot|^2 - \bar{\Phi}_\nu$  from Theorem 3.8.4 with  $\mathcal{D} = \mathcal{D}_{1, \alpha}$  from Section 3.8. The arguments in Proposition 3.4.2 can be extended to the periodic case as well by Theorem 3.8.4 to obtain uniform bounds in  $H_\diamond^2(\mathbb{T}^d)$ .  $\square$

### 3.6 Linearization of Monge-Ampère equations

We consider  $\nu, \mu \in \left\{ \varrho \in \mathcal{P}_{\text{ac}}(\bar{B}) : \|\varrho\|_{C^{0, \alpha}(\bar{B})} + \|\log \varrho\|_{L^\infty(\bar{B})} < \infty \right\}$  on a closed ball  $\bar{B} := \overline{B_R(0)}$  of radius  $R > 0$  for  $\alpha \in (0, 1)$ . Our goal is to linearize the following Monge-Ampère equation with a second boundary value condition

$$\begin{aligned} \det(D^2 u) \nu(\nabla u) &= \mu, \\ \nabla u(\bar{B}) &= \bar{B}, \end{aligned} \tag{3.6.1}$$

for some fixed  $\nu \in C^{1,\alpha}(\bar{B})$ . Note that thanks to Brenier's theorem there exists a unique convex solution satisfying (3.6.1) (a priori in the sense of  $\nabla u_{\#}\mu = \nu$ ), and it is  $C^{2,\alpha}(\bar{B})$  thanks to regularity theory for Monge-Ampère equations. We will need the following lemmas.

**Lemma 3.6.1.** *Let  $u \in C^1(\bar{B})$  be strictly convex. Then the following are equivalent*

- $\nabla u(\bar{B}) = \bar{B}$ ,
- $\nabla u(\partial B) \subset \partial B$ .

*Proof.* For the first direction assume by contradiction that there is  $p \in \partial B$  such that  $\nabla u(p) \in \mathring{B}$ . Note that at  $p$  there is an outer normal to  $\bar{B}$ , namely  $p$  itself. Take  $a > 0$  such that  $\nabla u(p) + ap \in B$ . Since  $\nabla u$  is surjective, there is  $q \in \bar{B}$  satisfying  $\nabla u(q) = \nabla u(p) + ap$ . Then

$$(q - p) \cdot (\nabla u(q) - \nabla u(p)) = a(q - p) \cdot p < 0,$$

which contradicts the monotonicity of  $\nabla u$ .

For the other direction, note that  $\nabla u(\partial B) \subset \partial B$  implies  $\nabla u(\partial B) = \partial B$  since the only subset of  $\partial B$  homeomorphic to  $\partial B$  is  $\partial B$  itself. Now, by a similar argumentation as above one can obtain that  $\nabla u(\partial B) \subset \partial \nabla u(\bar{B})$ . Furthermore, strict convexity of  $u$  yields that its conjugate  $u^* \in C^1(\mathbb{R}^d)$ , and recall that  $(\nabla u^*)^{-1}(\{x\}) = \{\nabla u(x)\}$  for any  $x \in \mathring{B}$ . Thus  $\nabla u$  maps  $\mathring{B}$  to the interior of  $\nabla u(\bar{B})$ . Therefore,  $\partial \nabla u(\bar{B}) = \nabla u(\partial B) = \partial B$ . Now, there is only one compact set in  $\mathbb{R}^d$  with non-empty interior and boundary  $\partial B$ :  $\bar{B}$ , so that we have  $\nabla u(\bar{B}) = \bar{B}$ .  $\square$

*Remark 3.6.2.* Note that the proof of Lemma 3.6.1 extends to the setting described in Remark 3.4.1. Keeping the same notation the statement changes to equivalence of

- $\nabla u(\bar{\Omega}) = \text{supp } \nu$ ,
- $\nabla u(\partial \Omega) \subset \partial \text{supp } \nu$ .

The contradicting argument reads in this case (since  $\nabla H(p)$  is the outer normal at  $p$ )

$$(q - p) \cdot (\nabla u(q) - \nabla u(p)) = a(q - p) \cdot \nabla H(p) < 0,$$

where the inequality is strict due to the strong convexity.

**Lemma 3.6.3.** *For  $u \in C^2(\bar{B})$  strongly convex such that  $|\nabla u(x)|^2 - R^2 = 0$  for  $x \in \partial B$ , there is  $\beta \in C(\partial B)$ ,  $\beta > 0$  such that  $(D^2u)^{-1}(x) \cdot x = \beta(x)\nabla u(x)$  for  $x \in \partial B$ . Furthermore, there exists  $\kappa > 0$  such that  $|\nabla u(x) \cdot x| \geq \kappa$  for all  $x \in \partial B$ .*

*Proof.* Note that the Legendre transform  $u^*$  is at least  $C^2(\bar{B})$ . Indeed, by standard regularity theory for convex functions  $u^* \in C^1(\bar{B})$  and since  $D^2u$  is invertible, the inverse function theorem applied to  $\nabla u$  yields differentiability for  $\nabla u^* = (\nabla u)^{-1}$ . Now note that  $\nabla u^*$  also satisfies (see Lemma 3.6.1)

$$\begin{aligned} |\nabla u^*(y)|^2 - R^2 &\leq 0 \quad \text{for all } y \in B \\ |\nabla u^*(y)|^2 - R^2 &= 0 \quad \text{for all } y \in \partial B. \end{aligned}$$

This implies by differentiating at a boundary point  $y$  that there is  $\tilde{\beta}(y) \geq 0$  such that

$$D^2u^*(y)\nabla u^*(y) = \tilde{\beta}(y)y.$$

By invertibility of  $D^2u^*(y)$ , we see that  $\tilde{\beta}(y) > 0$ . Substituting  $\nabla u(x) = y$  gives by using properties of Legendre transform

$$\begin{aligned} D^2u^*(\nabla u(x))\nabla u^*(\nabla u(x)) &= \tilde{\beta}(\nabla u(x))\nabla u(x), \\ \iff (D^2u)^{-1}(x)x &= \tilde{\beta}(\nabla u(x))\nabla u(x), \end{aligned}$$

for all  $x \in \partial B$ . Set  $\beta(x) := \tilde{\beta}(\nabla u(x))$  and note that  $\beta \in C(\partial B)$  since

$$\beta(x) = \frac{1}{R^2}(D^2u)^{-1}(x)x \cdot \nabla u(x).$$

The second statement follows since

$$|\nabla u(x) \cdot x| = \frac{1}{\beta(x)}(D^2u)^{-1}(x)x \cdot x \geq R^2K > 0,$$

where  $K$  is a constant only depending on  $\|D^2u\|_{L^\infty(B)}$  and  $\|(D^2u)^{-1}\|_{L^\infty(B)}$ .  $\square$

*Remark 3.6.4.* One may readily check that Lemma 3.6.3 extends to the setting described in Remark 3.4.1. Indeed, the proof uses that the defining convex functions of the ball are of the form  $|\cdot|^2 - R^2$  and the outer normal at a boundary point  $x$  is  $x$ .

From now on, we fix the constant by considering potentials in the set

$$C_{\diamond}^{k,\alpha}(\bar{B}) := \left\{ u \in C^{k,\alpha}(\bar{B}) : \int_B u = 0 \right\}$$

with  $k \in \mathbb{N}$ . Let us also define

$$\mathcal{M} = \{ u \in C_{\diamond}^{2,\alpha}(\bar{B}) : |\nabla u|^2 - R^2 = 0 \text{ on } \partial B \}.$$

We now prove that in a neighborhood of a strongly convex function  $u_0 \in \mathcal{M}$  this set is the graph of a  $C^1$ -function.

**Lemma 3.6.5.** *At  $u_0 \in \mathcal{M}$  strongly convex,  $\mathcal{M}$  is locally given by the image of a bijective  $C^1$ -function on a closed subspace of  $C_{\diamond}^{2,\alpha}(\bar{B})$ . More precisely, there exist open subsets  $V \subset F_0 := \{ h \in C_{\diamond}^{2,\alpha}(\bar{B}) : \nabla u_0 \cdot \nabla h = 0 \text{ on } \partial B \}$ ,  $U \subset C_{\diamond}^{2,\alpha}(\bar{B})$ , with  $u_0 \in U$ , and a bijective  $C^1$ -function:*

$$\chi_0: V \rightarrow U \cap \mathcal{M}.$$

Furthermore, for  $f_0 := \Pi_{F_0}(u_0)$ , where  $\Pi_{F_0}$  is the projection on  $F_0$  defined by (3.6.2), it holds  $\chi_0'(f_0) = \text{id}$ .

*Proof.* First, we show that  $C_{\diamond}^{2,\alpha}(\bar{B}) = F_0 \oplus G_0$ , where  $F_0, G_0$  are linear subspaces defined as

$$\begin{aligned} F_0 &:= \{ f \in C_{\diamond}^{2,\alpha}(\bar{B}) : \nabla u_0 \cdot \nabla f = 0 \text{ on } \partial B \}, \\ G_0 &:= \{ g \in C_{\diamond}^{2,\alpha}(\bar{B}) : \exists c \in \mathbb{R}, -\text{div}(A_0 \nabla g) = c \}, \end{aligned}$$

where  $A_0 = \text{cof}(D^2u_0)$  is the cofactor matrix of  $D^2u_0$ , and  $-\text{div}(A_0\nabla g) = c$  is to be understood in the distributional sense, i.e. for all  $\psi \in C_c^\infty(B)$  such that  $\int_B \psi = 0$

$$\int_B A_0\nabla g \cdot \nabla \psi = 0.$$

Take  $u \in C_\diamond^{2,\alpha}(\bar{B})$ . Define  $f$  to be a solution of

$$\begin{aligned} -\text{div}(A_0\nabla f) &= -\text{div}(A_0\nabla u) + \int_B \text{div}(A_0\nabla u) && \text{in } B, \\ \nabla u_0 \cdot \nabla f &= 0 && \text{on } \partial B, \end{aligned} \quad (3.6.2)$$

and  $g$  a solution of

$$\begin{aligned} -\text{div}(A_0\nabla g) &= -\int_B \text{div}(A_0\nabla u) && \text{in } B, \\ \nabla u_0 \cdot \nabla g &= \nabla u_0 \cdot \nabla u && \text{on } \partial B. \end{aligned} \quad (3.6.3)$$

Thanks to Lemma 3.6.3 the boundary conditions are uniformly oblique and compatible with the right hand side. Hence, both (3.6.2) and (3.6.3) admit a unique weak solution  $f, g \in H_\diamond^1(B)$  which is  $C_\diamond^{2,\alpha}(\bar{B})$  thanks to linear elliptic PDE theory (e.g. by a combination of [77, Theorem 5.54] and [61, Theorem 6.31]). Thus, we have found a decomposition  $u = f + g$  for  $f \in F_0$  and  $g \in G_0$ . It is also unique because  $F_0 \cap G_0 = \{0\}$ . To see that notice that every  $h \in F_0 \cap G_0$  satisfies

$$\begin{aligned} -\text{div}(A_0\nabla h) &= c && \text{in } B, \quad c \in \mathbb{R} \\ \nabla u_0 \cdot \nabla h &= 0 && \text{on } \partial B, \end{aligned}$$

whose unique solution is  $h = 0$ . In total, we obtain well-definedness of the projection operators  $\Pi_{F_0}: C^{2,\alpha}(\bar{B}) \rightarrow F_0$  and  $\Pi_{G_0}: C^{2,\alpha}(\bar{B}) \rightarrow G_0$ . Continuity of  $\Pi_{F_0}$  and  $\Pi_{G_0}$  in  $C^{2,\alpha}(\bar{B})$  follows by the open mapping theorem, see e.g. [19, Theorem 2.10].

Now we would like to apply the implicit function theorem to

$$\begin{aligned} \Gamma: F_0 \oplus G_0 &\rightarrow C^{1,\alpha}(\partial B), \\ (f, g) &\mapsto |\nabla(f + g)|^2 - R^2. \end{aligned}$$

Its partial derivative at  $u_0$  with respect to  $g_0 := \Pi_{G_0}(u_0)$  is given by

$$\frac{\partial}{\partial g} \Gamma(u_0)h = 2\nabla u_0 \cdot \nabla h \text{ on } \partial B, \quad h \in G_0.$$

Bijectivity of the derivative means existence and uniqueness of  $h \in C_\diamond^{2,\alpha}(\bar{B})$  such that

$$\begin{aligned} -\text{div}(A_0\nabla h) &= c \text{ on } B, \quad c \in \mathbb{R}, \\ \nabla u_0 \cdot \nabla h &= w \text{ on } \partial B, \end{aligned}$$

where  $w \in C^{1,\alpha}(\partial B)$ . By the same argumentation as above, this is the case if and only if  $c = -\frac{1}{|B|} \int_{\partial B} w \det(D^2u_0)\beta_0$  where  $\beta_0$  is as in Lemma 3.6.3. Continuity follows again by the open mapping theorem. Thanks to the implicit function theorem there are  $U_F \subset F_0$ ,  $U_G \subset G_0$  open ( $\Pi_F(u_0) \in U_F$ , resp.  $\Pi_G(u_0) \in U_G$ ) such that  $\tilde{\chi}_0: U_F \rightarrow U_G$  is  $C^1$  and

$$\Gamma(f, g) = 0 \text{ for } (f, g) \in U_F \oplus U_G \iff g = \tilde{\chi}_0(f).$$

### 3.6. LINEARIZATION OF MONGE-AMPÈRE EQUATIONS

This implies that  $\chi_0: U_F \rightarrow \mathcal{M} \cap U_F \oplus U_G$ ,  $f \mapsto f + \tilde{\chi}_0(f)$  is well-defined,  $C^1$  and bijective.

Finally, note that for  $f_0 := \Pi_{F_0}(u_0)$ ,  $h \in F_0$

$$0 = \frac{d}{df} \Gamma(f_0, \tilde{\chi}_0(f_0))h = 2 \underbrace{\nabla u_0 \cdot \nabla h}_{=0} + \frac{\partial}{\partial g} \Gamma(f_0, \tilde{\chi}_0(f_0)) \tilde{\chi}'_0(f_0)h.$$

By invertibility of  $\frac{\partial}{\partial g} \Gamma(f_0, \chi_0(f_0))$ , we conclude  $\tilde{\chi}'_0(f_0) = 0$ , hence  $\chi'_0(f_0) = \text{id}$ .  $\square$

Now for  $u_0 \in \mathcal{M}$  take  $U \subset C_{\diamond}^{2,\alpha}(\bar{B})$  from Lemma 3.6.5 (and possibly restrict it further such that any  $u \in U \cap \mathcal{M}$  is strongly convex) and consider the map

$$M_\nu: U \cap \mathcal{M} \rightarrow \left\{ u \in C^{0,\alpha}(\bar{B}) : \int_B u = 1 \right\} \\ u \mapsto \det(D^2u)\nu(\nabla u)$$

where  $\nu$  is a fixed probability density in the set  $\mathcal{Q}_{1,\alpha}$  defined in (3.4.1). Note that this map is well-defined by Lemma 3.6.1 and the fact that the push forward preserves the mass. We want to “take the derivative at  $u \in U \cap \mathcal{M}$ ” by pulling back  $M_\nu$  to the linear space  $F_0$  with the map  $\chi_0$  from Lemma 3.6.5.

**Proposition 3.6.6.** *In the setting of Lemma 3.6.5, let  $u \in U \cap \mathcal{M}$  be strongly convex. Then  $N_\nu := M_\nu \circ \chi_0$  is continuously differentiable at  $f := \Pi_{F_0}u$  and the derivative is given by*

$$N'_\nu(f): F_0 \rightarrow C_{\diamond}^{0,\alpha}(\bar{B}) \\ h \mapsto \text{tr}(A_\nu D^2(\chi'_0(f)h)) + \det(D^2u)\nabla\nu(\nabla u) \cdot \nabla(\chi'_0(f)h),$$

where  $F_0 = \left\{ h \in C_{\diamond}^{2,\alpha}(\bar{B}) : \nabla u_0 \cdot \nabla h = 0 \text{ on } \partial B \right\}$

and  $A_\nu := \nu(\nabla u)\text{cof}(D^2u)$ .

In addition, in the weak sense we have

$$N'_\nu(f)h = \text{div}(A_\nu \nabla(\chi'_0(f)h)).$$

*Proof.* Let  $h \in F_0$ , then the directional derivative is given by

$$\frac{d}{dt} N_\nu(f + th)|_{t=0} = \frac{d}{dt} \det(D^2\chi_0(f + th))\nu(\nabla\chi_0(f + th))|_{t=0} \\ = \text{tr}(A_\nu D^2(\chi'_0(f)h)) + \det(D^2u)\nabla\nu(\nabla u) \cdot \nabla(\chi'_0(f)h).$$

By continuity of  $\chi'_0$ , we can conclude that  $N_\nu$  is continuously differentiable. Now note that if  $u \in C^{3,\alpha}(\bar{B})$

$$\begin{aligned} \text{div}(A_\nu \nabla(\chi'_0(f)h)) &= \text{div}(\nu(\nabla u)\text{cof}(D^2u)\nabla(\chi'_0(f)h)) \\ &= D^2u\nabla\nu(\nabla u) \cdot \text{cof}(D^2u)\nabla(\chi'_0(f)h) \\ &\quad + \nu(\nabla u) \text{div}(\text{cof}(D^2u)\nabla(\chi'_0(f)h)) \\ &= \det(D^2u)\nabla\nu(\nabla u) \cdot \nabla(\chi'_0(f)h) \\ &\quad + \nu(\nabla u) \text{tr}(\text{cof}(D^2u)D^2(\chi'_0(f)h)), \end{aligned}$$

where, in the last line, we have used that  $\text{cof}(D^2u)$  has divergence-free columns (see Lemma p.462 in [51]). This yields

$$N'_\nu(f)h = \text{div}(A_\nu \nabla(\chi'_0(f)h)).$$

The same result follows for  $u \in C^{2,\alpha}(\bar{B})$  (in the weak sense) by density.  $\square$

For fixed  $\nu \in \mathcal{Q}_{1,\alpha}$ , consider now

$$\mathcal{S} = \left\{ \varrho \in \mathcal{P}_{\text{ac}}(\bar{B}) : \|\varrho\|_{C^{0,\alpha}(\bar{B})} + \|\log \varrho\|_{L^\infty(\bar{B})} < \infty \right\}$$

and the map

$$\begin{aligned} \Phi_\nu : \mathcal{S} &\rightarrow \mathcal{M}, \\ \mu &\rightarrow u, \text{ where } u \text{ strongly convex and } \nabla u \# \mu = \nu. \end{aligned} \quad (3.6.4)$$

Note that this is well defined thanks to Brenier's theorem (Theorem 2.1.18 and Remark 2.1.21) and regularity theory for Monge-Ampère equations (Theorem 2.1.23). Furthermore, by the considerations before we can now prove that it is continuously differentiable.

**Theorem 3.6.7.**  *$\Phi_\nu$  as defined in (3.6.4) is continuously differentiable. More precisely, for every  $\mu \in \mathcal{S}$ , the value of  $(\Phi_\nu)'(\mu)f$  at  $f \in C_\diamond^{0,\alpha}(\bar{B})$  is the unique solution  $h \in C_\diamond^{2,\alpha}(\bar{B})$  of the linearized equation*

$$\begin{aligned} \operatorname{div}(A_\nu \nabla h) &= f \text{ in } B, \\ \nabla u_0 \cdot \nabla h &= 0 \text{ on } \partial B, \end{aligned}$$

where  $u_0 = \Phi_\nu(\mu)$  and  $A_\nu = \nu(\nabla u_0) \operatorname{cof}(D^2 u_0)$ .

*Proof.* For  $u_0 = \Phi_\nu(\mu) \in \mathcal{M}$  the derivative of  $N_\nu$  at  $f_0 = \Pi_{F_0}(u_0)$  is given by Proposition 3.6.6. Invertibility of  $N'_\nu(f_0)$  is equivalent to finding, for every  $f \in C_\diamond^{0,\alpha}(\bar{B})$ , a unique

$$h \in F_0 = \left\{ u \in C_\diamond^{2,\alpha}(\bar{B}) : \nabla u_0 \cdot \nabla u = 0 \text{ on } \partial B \right\},$$

such that

$$\operatorname{div}(A_\nu \nabla h) = f \text{ in } B, \quad (3.6.5)$$

in the weak sense where we have used that  $\chi'_0(f_0) = \operatorname{id}$  by Lemma 3.6.5. As before, by strong convexity of  $u_0$  equation (3.6.5) is uniformly elliptic and the boundary conditions are compatible, so that by elliptic regularity theory there is a unique solution  $h \in C_\diamond^{2,\alpha}(\bar{B})$ , satisfying the boundary condition  $\nabla u_0 \cdot \nabla h = 0$  on  $\partial B$ . With the inverse function theorem we conclude that there is an open (in  $\mathcal{S}$ ) neighborhood  $U$  containing  $\mu$  such that  $N_\nu^{-1}|_U : U \rightarrow N_\nu^{-1}(U)$  is a  $C^1$ -diffeomorphism. By possibly further restricting  $U$  (such that  $N_\nu^{-1}(U) \subset V$  from Lemma 3.6.5), we see that  $\Phi_\nu|_U = \chi_0 \circ N_\nu^{-1}|_U$  is also  $C^1$  in a neighborhood of  $\mu$ . We employ again  $\chi'_0(f_0) = \operatorname{id}$  to conclude.  $\square$

### 3.7 Linearization in the semi-discrete case

Let  $\bar{B} = \overline{B_R(0)}$  for  $R > 0$ . In this section we are interested in linearizing the discrete equivalent of the Monge-Ampère equation by using the fine analysis developed in [68]. More precisely, in this section we assume  $\rho^* \in \mathcal{P}_{\text{ac}}(\bar{B})$  and  $\nu = \sum_{i=1}^{N_\nu} q_i^\nu \delta_{x_i^\nu} \in \mathcal{P}(\bar{B})$  to be discrete. Then the primal dual optimality conditions (Remark 2.1.11) motivate the study of the Laguerre tessellation for  $v \in \mathbb{R}^N$

$$\operatorname{Lag}_{x_i}(v) := \{x \in \bar{B} : \forall 1 \leq j \leq N, x \cdot x_i - v_i \geq x \cdot x_j - v_j\}, \quad i \in \{1, \dots, N\}.$$

Indeed, if  $u^*, v^*$  are optimal Kantorovich potentials (for cost function  $c(x, y) = -x \cdot y$ ), then for each  $i \in \{1, \dots, N\}$  on the interior of  $\operatorname{Lag}_{x_i}(v^*)$  the optimal transport map is given by  $\nabla u^* = x_i$   $\mathcal{L}^d$ -a.e. (see Theorem 2.1.18).

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Now, by Theorem 2.1.13 and Remark 2.1.20, there is actually a unique Kantorovich potential  $v^* \in \mathbb{R}_\diamond^N := \left\{ v \in \mathbb{R}^N : \sum_{i=1}^N v_i = 0 \right\}$  and by  $(\nabla u^*)_{\#} \rho^* = \nu$  we have

$$\rho^*(\text{Lag}_{x_i^\nu}(v^*)) = q_i^\nu \text{ for all } 1 \leq i \leq N. \quad (3.7.1)$$

This can be seen as a discrete version of the Monge-Ampère equation.

In order to linearize rigorously (3.7.1) we need to impose some assumptions on  $\nu$ . For this define for  $N \in \mathbb{N}^*$  and  $\varepsilon > 0$

$$\mathcal{D}_{\text{discr}}^{\varepsilon, N} := \left\{ \nu \in \mathcal{P}(\bar{B}) : \nu = \sum_{i=1}^{N_\nu} q_i^\nu \delta_{x_i^\nu}, q_i^\nu \geq \varepsilon, |x_i^\nu - x_j^\nu| \geq \varepsilon, N_\nu \leq N \right\}. \quad (3.7.2)$$

For,  $\nu \in \mathcal{D}_{\text{discr}}^{\varepsilon, N}$  the goal is to investigate regularity of

$$\begin{aligned} \Psi_\nu : \mathcal{P}_{\text{ac}}(\bar{B}) \cap C^{0, \alpha}(\bar{B}) &\rightarrow \mathbb{R}_\diamond^N \\ \rho^* &\mapsto v^* \text{ s.t. (3.7.1) holds.} \end{aligned}$$

Note that it is well-defined and indeed maps to a Brenier potential by Corollary 1.2 [68].

**Proposition 3.7.1.** *Assume that  $\nu \in \mathcal{D}_{\text{discr}}^{\varepsilon, N}$  for  $\varepsilon > 0$ ,  $N \in \mathbb{N}^*$  and  $\rho^* \in \mathcal{P}_{\text{ac}}(\bar{B}) \cap C^{0, \alpha}(\bar{B})$  for  $\alpha \in (0, 1)$  with  $\|(\rho^*)^{-1}\|_{L^\infty(\bar{B})} < \infty$ . Then  $\Psi_\nu$  is continuously differentiable at  $\rho^*$  and we have the following quantitative estimate*

$$|(\Psi_\nu)'(\rho^*)h| \leq \frac{1}{C\varepsilon^2} |q^\nu| \|\rho^*\|_{L^\infty(\bar{B})} \|(\rho^*)^{-1}\|_{L^\infty(\bar{B})} \|h\|_{L^2(\bar{B})},$$

where  $C$  is a fixed constant depending on  $\varepsilon$ ,  $\|\rho^*\|_{L^\infty(\bar{B})}$ ,  $\|(\rho^*)^{-1}\|_{L^\infty(\bar{B})}$  and the domain  $\bar{B}$ .

*Proof.* Define  $F_\nu : \mathcal{P}_{\text{ac}}(\bar{B}) \cap C^{0, \alpha}(\bar{B}) \times \mathbb{R}_\diamond^N \rightarrow \mathbb{R}_\diamond^N$  by

$$F_\nu(\rho, v) = \left( \rho(\text{Lag}_{x_i^\nu}(v)) - q_i^\nu \right)_{i=1}^N.$$

Since  $\text{spt } \rho^* = \bar{B}$ , by Remark 2.1.20 there is a unique potential  $v^* \in \mathbb{R}_\diamond^N$  satisfying (3.7.1). In particular, we have  $F_\nu(\rho^*, v^*) = 0$ . We want to apply the implicit function theorem in Banach spaces (see e.g. Theorem 4.B [114]) in order to get regularity of  $\Psi_\nu$ . For this we use the fine analysis of the Kantorovich functional  $K$  defined in Theorem 1.1 [68] (they call it  $\Phi$ ). Note that the quadratic cost function restricted to  $\bar{B} \times \mathbb{R}^N$  satisfies all the regularity assumptions required in the paper. Using Corollary 1.2 [68] we have in particular  $\nabla K(\cdot) = F_\nu(\rho^*, \cdot)$ .

By Theorem 4.1 [68] we deduce that  $F_\nu$  is continuously differentiable in  $v^*$ . Furthermore, we can apply Theorem 5.1 [68] since  $(\bar{B}, \rho^*)$  satisfies the Poincaré-Wirtinger inequality (PW) thanks to  $\|(\rho^*)^{-1}\|_{L^\infty(\bar{B})} < \infty$ . This implies that  $K$  is  $C^2$  and strongly concave and hence  $D_v F_\nu(\rho^*, v^*)$  exists and is bijective. The derivative in  $\rho$  can be directly computed and is given by

$$D_\rho F_\nu(\rho, v)h = \left( \int_{\text{Lag}_{x_i^\nu}(v)} h(x) \, dx \right)_{i=1}^N,$$

for  $h \in C_\diamond^{0,\alpha}(\bar{B})$ . Altogether this implies that there is an open subset  $U^*$  of  $\rho^*$  such that  $\Psi_\nu$  is continuously differentiable on  $U^*$  and

$$(\Psi_\nu)'(\rho^*) = -D_\nu F_\nu(\rho^*, \Psi_\nu(\rho^*))^{-1} D_\rho F_\nu(\rho^*, \Psi_\nu(\rho^*)).$$

Thanks to the quantitative concavity result in Theorem 5.1 [68] we have for  $h \in C_\diamond^{0,\alpha}(\bar{B})$

$$\begin{aligned} |(\Psi_\nu)'(\rho^*)h| &\leq \|D_\nu F_\nu(\rho^*, \Psi_\nu(\rho^*))^{-1}\|_{L(\mathbb{R}_\diamond^N, \mathbb{R}_\diamond^N)} |D_\rho F_\nu(\rho, \Psi_\nu(\rho^*))h| \\ &\leq \frac{1}{C\varepsilon^2} \|\rho^*\|_{L^\infty(\bar{B})} |D_\rho F_\nu(\rho, v)h|, \end{aligned}$$

where  $C$  depends on  $\varepsilon$ ,  $\|\rho^*\|_{L^\infty(\bar{B})}$ ,  $\|(\rho^*)^{-1}\|_{L^\infty(\bar{B})}$  and the domain  $\bar{B}$ .

Now note that by using Cauchy-Schwarz inequality

$$\begin{aligned} |D_\rho F_\nu(\rho, \Psi_\nu(\rho^*))h|^2 &= \sum_{i=1}^N \left( \int_{\text{Lag}_{x_i^\nu}(\Psi_\nu(\rho^*))} h(x) dx \right)^2 \\ &\leq \sum_{i=1}^N \mathcal{L}^d(\text{Lag}_{x_i^\nu}(\Psi_\nu(\rho^*)))^2 \|h\|_{L^2(\bar{B})}^2 \\ &\leq \|(\rho^*)^{-1}\|_{L^\infty(\bar{B})}^2 \|h\|_{L^2(\bar{B})}^2 \sum_{i=1}^N \rho^*(\text{Lag}_{x_i^\nu}(\Psi_\nu(\rho^*)))^2 \\ &= \|(\rho^*)^{-1}\|_{L^\infty(\bar{B})}^2 |q^\nu|^2 \|h\|_{L^2(\bar{B})}^2. \end{aligned}$$

□

For the central limit theorem we are interested in the map from  $\rho^*$  to the Legendre transform of the Brenier potential  $\Psi_\nu(\rho^*)$  of zero mean, hence the following lemma is needed.

**Lemma 3.7.2.** *The map*

$$\begin{aligned} T_\nu : \mathbb{R}_\diamond^N &\rightarrow L_\diamond^2(\bar{B}) \\ v &\mapsto \left( x \mapsto u_v(x) = \max_{1 \leq i \leq N} \{x \cdot x_i^\nu - v_i\} - \int_B \max_{1 \leq i \leq N} \{z \cdot x_i - v_i\} dz \right) \end{aligned}$$

is continuously differentiable. The following estimate on the derivative holds

$$\|(T_\nu)'(\bar{v})(h)\|_{L^2(B)} \leq C|h|,$$

for  $h \in \mathbb{R}_\diamond^d$  and  $C = \sqrt{\mathcal{L}^d(\bar{B})}$ .

*Proof.* Let  $v \in \mathbb{R}_\diamond^N$ . We start by differentiating the unnormalized version

$$S_\nu(v) := u_v(x) = \max_{1 \leq i \leq N} \{x \cdot x_i^\nu - v_i\},$$

at  $x \in \text{int}(\text{Lag}_{x_i^\nu}(v))$  for  $1 \leq i \leq N$  fixed. By definition of the Laguerre cells, we have

$$u_v(x) = x \cdot x_i^\nu - v_i > x \cdot x_j^\nu - v_j$$

for all  $j \neq i$ . Let  $h \in \mathbb{R}_\diamond^N$ . Then there is  $t_0 > 0$  such that for  $t \in (-t_0, t_0)$  we have

$$u_{v+th}(x) = x \cdot x'_i - v_i - th_i > x \cdot x'_j - v_j - th_j,$$

for all  $j \neq i$ . This implies that for such  $t$

$$\frac{u_{v+th}(x) - u_v(x)}{t} = -h_i.$$

Since  $\mathcal{L}^d \left( \bar{B} \setminus \bigcup_{j=1}^N \text{int}(\text{Lag}_{x'_j}(v)) \right) = 0$  (see for instance Section 1.2 [68]) we have for  $\mathcal{L}^d$ -a.e.  $x$

$$\lim_{t \rightarrow 0} \frac{u_{v+th}(x) - u_v(x) - t \sum_{i=1}^N \mathbb{1}_{\text{int}(\text{Lag}_{x'_i}(v))}(x) h_i}{t} = 0.$$

To get differentiability in  $L^2$  note that for any  $1 \leq j \leq N$

$$\begin{aligned} x \cdot x_j - v_j - th_j &\leq u_v(x) + t|h|_\infty \quad \text{and} \\ x \cdot x_j - v_j &\leq u_{v+th}(x) + t|h|_\infty. \end{aligned}$$

So that taking the maximum in  $j$  we obtain

$$|u_{v+th} - u_v| \leq t|h|_\infty.$$

In particular, we have

$$t^{-1} \left| u_{v+th} - u_v + t \sum_{i=1}^N \mathbb{1}_{\text{int}(\text{Lag}_{x'_i}(v))} h_i \right| \leq 2|h|_\infty,$$

and we conclude by Lebesgue's dominated convergence theorem

$$\lim_{t \rightarrow 0} \int_{\bar{B}} t^{-2} \left( u_{v+th} - u_v + t \sum_{i=1}^N \mathbb{1}_{\text{int}(\text{Lag}_{x'_i}(v))} h_i \right)^2 dx = 0.$$

The derivative in  $L^2$  is hence given by

$$(S_\nu)'(v)(h) = - \sum_{i=1}^N \mathbb{1}_{\text{int}(\text{Lag}_{x'_i}(v))} h_i.$$

Now consider the function  $N : L^2(B) \rightarrow L^2_\diamond(B)$

$$u \mapsto u - \int_B u(x) dx.$$

Its derivative evaluated at  $h \in L^2(B)$  is given by

$$N'(u)h = h - \int_B h(x) dx.$$

This implies in particular by minimality of the variance functional that

$$\|N'(u)h\|_{L^2(B)} \leq \|h\|_{L^2(B)}.$$

To conclude the estimate we compute

$$\int_{\bar{B}} ((S_\nu)'(v)(h))^2 dx = \int_{\bar{B}} \sum_{i=1}^N \mathbb{1}_{\text{int}(\text{Lag}_{x'_i}(v))} h_i^2 dx \leq C|h|^2,$$

where  $C = \mathcal{L}^d(\bar{B})$  and use the chain rule for  $T_\nu = N \circ S_\nu$ . □

To put it all together, consider

$$\begin{aligned} \Phi_\nu &: \mathcal{P}_{\text{ac}}(\bar{B}) \cap C^{0,\alpha}(\bar{B}) \rightarrow L^2_\diamond(B) \\ \rho &\mapsto u, \text{ where } u \text{ is convex, } \nabla u \# \rho = \nu. \end{aligned}$$

We obtain the following regularity of  $\Phi_\nu$ .

**Corollary 3.7.3.** *Assume that  $\rho^* \in \mathcal{P}_{\text{ac}}(\bar{B}) \cap C^{0,\alpha}(\bar{B})$  for  $\alpha \in (0, 1)$ ,  $\|(\rho^*)^{-1}\|_{L^\infty(B)} < \infty$  and  $\nu \in \mathcal{D}_{\text{discr}}^{\varepsilon, N}$  for  $\varepsilon > 0$ ,  $N \in \mathbb{N}^*$ . Then  $\Phi_\nu$  is continuously (Fréchet) differentiable at  $\rho^*$  and the derivative satisfies for  $h \in L^2_\diamond(B)$*

$$\|(\Phi_\nu)'(\rho^*)h\|_{L^2(B)} \leq C\|h\|_{L^2(B)},$$

where  $C$  only depends on  $B$ ,  $\varepsilon$ ,  $\|\rho^*\|_{L^\infty(B)}$  and  $\|(\rho^*)^{-1}\|_{L^\infty(B)}$ .

*Proof.* This follows since  $\Phi_\nu = T_\nu \circ \Psi_\nu$  in combination with Proposition 3.7.1 and Lemma 3.7.2.  $\square$

### 3.8 Linearization of the Monge-Ampère equation on the torus

In this section we consider the  $d$ -dimensional flat torus  $\mathbb{T}^d := \mathbb{R}^d/\mathbb{Z}^d$  equipped with the usual distance  $\mathbf{d}$  in quotient spaces, for  $x, y \in \mathbb{T}^d$

$$\mathbf{d}(x, y) := \inf_{p \in \mathbb{Z}^d} |\bar{x} - \bar{y} + p|,$$

where  $\bar{x}, \bar{y} \in \mathbb{R}^d$  are specific representatives of the equivalence classes  $x, y$ .

Note that  $(\mathbb{T}^d, \mathbf{d})$  is a compact metric space, and as such the theory from Chapter 2.1 applies. Furthermore, we can identify periodic functions and measures on  $\mathbb{R}^d$  with functions and measures on  $\mathbb{T}^d$ . In that setting, the regularity theory for Monge Ampère equations carries over as well as proven in [38].

We need the following integration by parts lemma

**Lemma 3.8.1.** *Let  $h \in C^2(\mathbb{T}^d)$ ,  $g \in C^1(\mathbb{T}^d)$  and  $A \in C^1(\mathbb{T}^d, \mathbb{R}^{d \times d})$*

$$\int_{\mathbb{T}^d} \text{div}(A \nabla h) g = \int_{\mathbb{T}^d} A \nabla h \cdot \nabla g$$

*Proof.* This follows by identifying the given functions by periodic functions on  $\mathbb{R}^d$  and applying the standard integration by parts with periodic boundary conditions.  $\square$

Consider  $\nu, \rho \in \left\{ \mu \in \mathcal{P}_{\text{ac}}(\mathbb{T}^d) : \|\mu\|_{C^{k,\alpha}(\mathbb{T}^d)} + \|\log \mu\|_{L^\infty(\mathbb{T}^d)} < \infty \right\} =: \mathcal{D}_{k,\alpha}$  for fixed  $\alpha \in (0, 1)$ . The goal of this section is to linearize the Monge-Ampère type equation on the torus. More precisely, for  $\nu \in \mathcal{D}_{1,\alpha}$  we consider the map

$$\begin{aligned} \bar{\Phi}_\nu : \mathcal{D}_{0,\alpha} &\rightarrow C^{2,\alpha}_\diamond(\mathbb{T}^d), \\ \rho &\mapsto \varphi, \text{ where } \bar{x} \mapsto \frac{|\bar{x}|^2}{2} - \varphi(x) \text{ convex and } \det(\text{Id} - D^2\varphi)\nu(x - \nabla\varphi) = \rho, \end{aligned} \tag{3.8.1}$$

where  $\bar{x} \in \mathbb{R}^d$  and  $x \in \mathbb{T}^d$  is its representative. Furthermore we use the short notation  $\det(\text{Id} - D^2\varphi)\nu(x - \nabla\varphi) = \rho$  for  $\det(\text{Id} - D^2\varphi(x))\nu(x - \nabla\varphi(x)) = \rho(x)$  for all  $x \in \mathbb{T}^d$  and

$$C^{k,\alpha}_\diamond(\mathbb{T}^d) := \left\{ f \in C^{k,\alpha}(\mathbb{T}^d) : \int_{\mathbb{T}^d} f = 0 \right\}.$$

*Remark 3.8.2.* Note carefully that here we have to pass to the Kantorovich potential  $u$  in order to be able to deal with a periodic function as requiring convexity on the torus would only yield constant functions. It is a priori only  $L^1(\mathbb{T}^d)$  but unique up to a constant by an argument as in Remark 2.1.20. A corresponding convex function (on  $\mathbb{R}^d$ ) is given by  $\bar{x} \mapsto \frac{|\bar{x}|^2}{2} - \varphi(x)$ , as one can see for instance in the proof of Theorem 1.25 [104].

We show that  $\bar{\Phi}_\nu$  is well-defined and continuously (Fréchet) differentiable (in the strong  $C^{0,\alpha}(\mathbb{T}^d)$  topology).

For well-definedness, identify all the quantities with their periodic counterpart on  $\mathbb{R}^d$  and use the version of Brenier's theorem for periodic measures on  $\mathbb{R}^d$ , Theorem 1 [38]. Hence, there is a unique (up to a constant) convex function  $u$  (on the whole  $\mathbb{R}^d$ ) satisfying  $\nabla u \# \rho = \nu$ , and it is  $C^{2,\alpha}$  thanks to Caffarelli's regularity theory for Monge-Ampère equations (Theorem 1 [38] summarizes this for the case on the torus). Fix the constant by requiring  $\bar{x} \mapsto \frac{|\bar{x}|^2}{2} - u(\bar{x})$  to be of zero mean. Now thanks to the relation  $\varphi(x) = \frac{|\bar{x}|^2}{2} - u(\bar{x})$ , where  $x \in \mathbb{T}^d$ ,  $\bar{x} \in \mathbb{R}^d$ , the regularity carries over to  $\varphi$ .

In order to do prove continuous differentiability fix  $\nu \in \mathcal{D}_{1,\alpha}$  for the remaining section and consider

$$M_\nu : C_\diamond^{2,\alpha}(\mathbb{T}^d) \rightarrow \left\{ f \in C^{0,\alpha}(\mathbb{T}^d) : \int_{\mathbb{T}^d} f = 1 \right\},$$

$$\varphi \mapsto \det(\text{Id} - D^2\varphi)\nu(x - \nabla\varphi) = \rho.$$

**Proposition 3.8.3.** *Let  $\nu \in \mathcal{D}_{1,\alpha}$  and  $\varphi_0 \in C_\diamond^{2,\alpha}(\mathbb{T}^d)$  be such that  $u_0 \in C^{2,\alpha}(\mathbb{R}^d)$  defined by  $u_0(\bar{x}) = \frac{|\bar{x}|^2}{2} - \varphi_0(x)$  is strongly convex. Then, there is neighborhood  $U_0$  (w.r.t. the strong  $C_\diamond^{2,\alpha}(\mathbb{T}^d)$ -topology) of  $\varphi_0$  such that for all  $\varphi \in U_0$  the function  $M_\nu$  is continuously (Fréchet) differentiable and the derivative is given by*

$$M'_\nu(\varphi) : C_\diamond^{2,\alpha}(\mathbb{T}^d) \rightarrow C_\diamond^{0,\alpha}(\mathbb{T}^d)$$

$$h \mapsto -\text{tr}(A_\nu(\varphi)D^2h) - \det(\text{Id} - D^2\varphi)\nabla\nu(x - \nabla\varphi) \cdot \nabla h,$$

where  $A_\nu(\varphi) = \nu(x - \nabla\varphi)\text{cof}(\text{Id} - D^2\varphi)^T$ . Furthermore, the derivative can be rewritten in divergence form, i.e. in the weak sense

$$M'_\nu(\varphi)h = -\text{div}(A_\nu(\varphi)\nabla h).$$

*Proof.* Choose  $U_0$  such that  $\varphi_0 \in U_0$  and for  $\varphi \in U_0$  the corresponding function  $u$  defined by  $u(\bar{x}) = \frac{|\bar{x}|^2}{2} - \varphi(x)$  are uniformly strongly convex on  $[0, 1]^d$ . We prove that  $M_\nu$  is Gâteaux-differentiable on  $U_0$  and that its Gateaux derivative  $D_G M_\nu \in C(U_0, L(C_\diamond^{2,\alpha}(\mathbb{T}^d), C_\diamond^{0,\alpha}(\mathbb{T}^d)))$ , where  $L(C_\diamond^{2,\alpha}(\mathbb{T}^d), C_\diamond^{0,\alpha}(\mathbb{T}^d))$  is the space of linear bounded operators from  $C_\diamond^{2,\alpha}(\mathbb{T}^d)$  to  $C_\diamond^{0,\alpha}(\mathbb{T}^d)$ . This concludes continuous differentiability.

Let  $\varphi \in U_0$ ,  $h \in C_\diamond^{2,\alpha}(\mathbb{T}^d)$ . Then by Lemma A.1 [54]

$$D_G M_\nu(\varphi)h = \frac{d}{dt} M_\nu(\varphi + th)|_{t=0}$$

$$= \frac{d}{dt} \det(\text{Id} - D^2(\varphi + th))\nu(x - \nabla(\varphi + th))|_{t=0}$$

$$= -\text{tr}(A_\nu(\varphi)D^2h) - \det(\text{Id} - D^2\varphi)\nabla\nu(x - \nabla\varphi) \cdot \nabla h,$$

for  $A_\nu(\varphi) = \nu(\nabla\varphi)\text{cof}(D^2\varphi)^T$ .

$D_G M_\nu(\varphi)$  is clearly linear and also bounded by strong convexity of  $u$ . It is as well continuous in  $\varphi$  (in the strong  $C^{2,\alpha}(\mathbb{T}^d)$  topology).

For reformulation in divergence form suppose  $\varphi \in C^{3,\alpha}(\mathbb{T}^d)$ . Then

$$\begin{aligned} \operatorname{div}(A_\nu(\varphi)\nabla h) &= \operatorname{div}(\nu(x - \nabla\varphi)\operatorname{cof}(Id - D^2\varphi)^T\nabla h) \\ &= (Id - D^2\varphi)^T\nabla\nu(x - \nabla\varphi) \cdot \operatorname{cof}(Id - D^2\varphi)^T\nabla h \\ &\quad + \nu(x - \nabla\varphi) \operatorname{div}(\operatorname{cof}(Id - D^2\varphi)^T\nabla h) \\ &= \det(Id - D^2\varphi)\nabla\nu(x - \nabla\varphi) \cdot \nabla h \\ &\quad + \sum_{j=1}^d \sum_{i=1}^d \partial_{x_j} \operatorname{cof}(Id - D^2\varphi)_{ji}^T \partial_{x_i} h \\ &\quad + \nu(x - \nabla\varphi) \operatorname{tr}(\operatorname{cof}(Id - D^2\varphi)^T D^2 h). \end{aligned}$$

Now note that  $Id - \operatorname{cof}(D^2\varphi)$  has divergence free columns by the lemma in Section 8.1.4b [51], so that

$$\sum_{j=1}^d \sum_{i=1}^d \partial_{x_j} \operatorname{cof}(Id - D^2\varphi)_{ji}^T \partial_{x_i} h = \sum_{i=1}^d \partial_{x_i} h \sum_{j=1}^d \partial_{x_j} \operatorname{cof}(Id - D^2\varphi)_{ji}^T = 0.$$

Hence, the equality holds in the weak sense by Lemma 3.8.1, i.e. for all  $g \in C^\infty(\mathbb{T}^d)$

$$\int_{\mathbb{T}^d} M'_\nu(\varphi)hg = \int_{\mathbb{T}^d} A_\nu\nabla h \cdot \nabla g. \quad (3.8.2)$$

Now take a subsequence in  $C^{3,\alpha}(\mathbb{T}^d)$  converging to  $\varphi \in C^{2,\alpha}(\mathbb{T}^d)$  in the  $C^{2,\alpha}(\mathbb{T}^d)$ -topology and use the continuity of the integrals in (3.8.2) to conclude.  $\square$

With this at hand, we can prove that  $\bar{\Phi}_\nu$  is continuously Fréchet differentiable.

**Theorem 3.8.4.** *Let  $\nu \in \mathcal{D}_{1,\alpha}$ . Then, the map  $\bar{\Phi}_\nu$  as defined in (3.8.1) is continuously Fréchet differentiable. More precisely, for every  $\rho \in \mathcal{D}_{0,\alpha}$ , the value of  $(\bar{\Phi}_\nu)'(\rho)f$  at  $f \in C_\diamond^{0,\alpha}(\mathbb{T}^d)$  is the unique solution  $h \in C_\diamond^{2,\alpha}(\mathbb{T}^d)$  of the linearized equation*

$$-\operatorname{div}(A_\nu\nabla h) = f \text{ on } \mathbb{T}^d,$$

where  $\varphi_0 = \bar{\Phi}_\nu(\rho)$  and  $A_\nu = \nu(x - \nabla\varphi_0)\operatorname{cof}(Id - D^2\varphi_0)^T$ .

*Proof.* Let  $\varphi_0 = \bar{\Phi}_\nu(\rho) \in C^{2,\alpha}(\mathbb{T}^d)$ . Considering Remark 3.8.2 and regularity for Monge-Ampère equations, we have that  $u_0 \in C^{2,\alpha}(\mathbb{R}^d)$  defined by  $u_0(\bar{x}) = \frac{|\bar{x}|^2}{2} - \varphi_0(x)$  is strongly convex. So the Fréchet derivative of  $M_\nu$  at  $\varphi_0$  is given by Proposition 3.8.3. Invertibility of  $M'_\nu(\varphi_0)$  is equivalent to finding, for every  $f \in C_\diamond^{0,\alpha}(\mathbb{T}^d)$ , a unique  $h \in C_\diamond^{2,\alpha}(\mathbb{T}^d)$  such that

$$-\operatorname{div}(A_\nu\nabla h) = f \text{ on } \mathbb{T}^d, \quad (3.8.3)$$

in the weak sense. By strong convexity of  $\varphi_0$  equation (3.8.3) is uniformly elliptic. This implies that there is a unique solution  $h \in H_\diamond^1(\mathbb{T}^d)$  which is also in  $C_\diamond^{2,\alpha}(\mathbb{T}^d)$  thanks to elliptic PDE regularity theory (use e.g. Lemma 6.5 [61] and Theorem 5.2 [61]). With the inverse function theorem we conclude that there is an open (in  $\mathcal{D}_{0,\alpha}$ ) neighborhood  $U$  containing  $\rho$  such that  $\bar{\Phi}_\nu$  is Fréchet differentiable on  $U$ .  $\square$

### 3.A Auxiliary probability results

**Lemma 3.A.1.** *Consider space  $C_b(\mathcal{X})$  of bounded continuous functions on a separable metric space  $\mathcal{X}$  endowed with the topology of pointwise convergence. Let  $f_1, f_2, \dots$  be i.i.d. (Borel) random functions from  $C_b(\mathcal{X})$  s.t.  $f_1(x^*) = 0$  a.s. and  $\mathbb{E} \sup_{x \in \mathcal{X}} |f_1(x)| < \infty$ . Let  $(X_n)_{n \in \mathbb{N}}$  be a sequence of r.v. convergent to  $x^*$  a.s. Then*

$$\frac{1}{n} \sum_{i=1}^n f_i(X_n) \rightarrow 0 \quad \text{a.s.}$$

*Proof.* Consider the modulus of continuity for  $f$  at point  $x^*$ :

$$\omega_f(\delta, x^*) := \begin{cases} \sup_{x \in B_\delta(x^*)} |f(x) - f(x^*)|, & \delta > 0, \\ 0, & \delta = 0. \end{cases}$$

Note that  $(f, \delta) \mapsto \omega_f(\delta, x^*)$  is measurable: indeed, take a countable dense set  $S \subset \mathcal{X}$ , then

$$\omega_f(\delta, x^*) = \sup_{x \in S} |f(x) - f(x^*)| \mathbb{1}[d(x, x^*) < \delta].$$

Since  $f_i(x^*) = 0$  a.s., we have for any fixed  $\delta > 0$

$$\begin{aligned} \left| \frac{1}{n} \sum_{i=1}^n f_i(X_n) \right| &\leq \frac{1}{n} \sum_{i=1}^n \omega_{f_i}(d(X_n, x^*), x^*) \\ &\leq \frac{1}{n} \sum_{i=1}^n (\omega_{f_i}(\delta, x^*) \mathbb{1}[d(X_n, x^*) \leq \delta] \\ &\quad + \sup_{x \in \mathcal{X}} |f_i(X_n)| \mathbb{1}[d(X_n, x^*) > \delta]). \end{aligned}$$

Further,  $\mathbb{E} \sup_{x \in \mathcal{X}} |f_1(x)| < \infty$ , therefore by the strong LLN

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n \sup_{x \in \mathcal{X}} |f_i(X_n)| &\xrightarrow{\text{a.s.}} \mathbb{E} \sup_{x \in \mathcal{X}} |f_1(x)|, \\ \frac{1}{n} \sum_{i=1}^n \omega_{f_i}(\delta, x^*) &\xrightarrow{\text{a.s.}} \mathbb{E} \omega_{f_1}(\delta, x^*) \leq \mathbb{E} \sup_{x \in \mathcal{X}} |f_1(x)|. \end{aligned}$$

Since  $\mathbb{1}[d(X_n, x^*) > \delta] \rightarrow 0$  a.s. it holds a.s. that

$$\limsup \frac{1}{n} \sum_{i=1}^n \omega_{f_i}(d(X_n, x^*), x^*) \leq \mathbb{E} \omega_{f_1}(\delta, x^*) \rightarrow 0 \quad \text{as } \delta \rightarrow 0$$

due to Lebesgue's dominated convergence theorem. The claim follows.  $\square$

The following result is a version of Slutsky's theorem for Hilbert space. We say that  $X_n \in H$  converge in probability to  $X$  ( $X_n \xrightarrow{P} X$ ), if  $\|X_n - X\| \xrightarrow{P} 0$ , i.e. for any  $\varepsilon > 0$  it holds that  $P(\|X_n - X\| > \varepsilon) \rightarrow 0$ .

**Lemma 3.A.2.** *Let  $(A_n)_{n \in \mathbb{N}}$  be a sequence of random bounded operators on a separable Hilbert space  $H$  convergent to a fixed operator  $A$  in SOT a.s. and bounded in probability (i.e. for any  $\varepsilon > 0$  there exists  $M_\varepsilon$  s.t.  $P(\|A_n\| > M_\varepsilon) \leq \varepsilon$  for all  $n$ ). Let  $(X_n)_{n \in \mathbb{N}}$  be a sequence of r.v. in  $H$ ,  $X_n \xrightarrow{d} X$ . Then  $A_n X_n \xrightarrow{d} AX$ .*

*Proof.* Let  $(e_n)_{n \in \mathbb{N}}$  be an o.n.b. in  $H$  and  $\Pi_k$  be the orthogonal projector onto the first  $k$  axes  $e_1, \dots, e_k$ . Then

$$A_n X_n = A X_n + (A_n - A) \Pi_k X_n + (A_n - A) (I - \Pi_k) X_n. \quad (3.A.1)$$

Since  $A_n \xrightarrow{\text{SOT}} A$  a.s., for any fixed  $k$  we have  $\|(A_n - A) \Pi_k\|_{op} \rightarrow 0$  a.s., thus

$$(A_n - A) \Pi_k X_n \xrightarrow{P} 0.$$

Moreover,

$$(I - \Pi_k) X_n \xrightarrow[n \rightarrow \infty]{d} (I - \Pi_k) X \xrightarrow[k \rightarrow \infty]{P} 0.$$

Since  $A_n$  are bounded in probability, the above equations imply that

$$(A_n - A) X_n \xrightarrow{P} 0.$$

This together with (3.A.1) and  $X_n \xrightarrow{d} X$  yields convergence  $A_n X_n \xrightarrow{d} A X$ .  $\square$

## Chapter 4

# Wasserstein medians

The following chapter is based on an ongoing work with G. Carlier and E. Chenchene, we refer to it with [29]. The images in this chapter have been provided by E. Chenchene.

Given the popularity of the Wasserstein barycenter (**B**) in several fields, as pointed out in the introduction and Section 2.3, it may already be enough as a statistical estimator. However, it has one drawback: it is not the most robust estimator in the sense that it is susceptible to outliers. Indeed, loosely speaking, it suffices that one of the given data probability measures moves “arbitrarily far” from the other samples, the Wasserstein barycenter will take into account this outlier and may become “arbitrarily far” from the uncorrupted Wasserstein barycenter. A way to capture this mathematically is the *break-down point*, which will make this notion precise and will be discussed in the sequel.

A way to circumvent this problem is to study the corresponding median problem. Again inspired by the Euclidean setting, minimizing the sum of all weighted Euclidean distances gives a notion of weighted median, which in the literature is commonly referred as point of Torricelli, Fermat-Weber point or geometric median, see e.g. [37] [85] [98]. As already pointed out in the introduction of this thesis, Fréchet generalized these definitions to a general metric space  $(X, d)$  in the seminal work *Les éléments aléatoires de nature quelconque dans un espace distancié* [56]. Let us also mention that the case of two measures has been studied in [82].

This motivates to define the Wasserstein median as any optimal solution to the following convex problem

$$\inf_{\rho \in \mathcal{P}_1(X)} \sum_{i=1}^N p_i W_1(\rho, \nu_i),$$

where  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(X)$  are probability measures and  $p_1, \dots, p_N \geq 0$  are non-negative weights that sum to one.

To illustrate the difference in robustness between Wasserstein barycenters and Wasserstein medians consider for instance the problem of averaging the five black-and-white pictures in Figure 4.1. It is clear from Figure 4.1, that the Wasserstein median shows some sort of robustness to the outlier (the spiral).

A more interesting example from the point of view of applications is shown in Figure 4.2, where both the Wasserstein barycenter and Wasserstein median of histograms are shown, the Wasserstein barycenter exhibiting more oscillations.



Figure 4.1 – Comparison between a Wasserstein barycenter (middle) and a Wasserstein median (right) for a sample of five measures (left) with uniform weights.

Our objective is to further investigate the notion of Wasserstein median highlighting the most important properties.

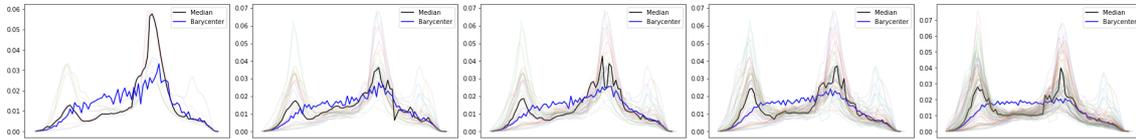


Figure 4.2 – Comparison between Wasserstein barycenters (blue) and Wasserstein medians (black) of the daily attendance distributions (x-axis: time from 2:00 am to 12:00 pm) of London's underground stations, with  $t = 9, 29, 39, 59, 81$ .

To this end we introduce the problem and justify its well-posedness in Section 4.1. Section 4.2 deals with the stability of the Wasserstein median subject to perturbations of the sample measures and we prove that its *break-down point* problem is  $\sim 1/2$ , i.e. to drastically corrupt the estimation of the Wasserstein median, at least half of the sample measures has to be modified. In Section 4.3 we study thoroughly the case where the probability measures are supported on the real line. We show in particular that if all the measures are absolutely continuous with bounded density, then there exists an absolutely continuous Wasserstein median whose density is in  $L^\infty$  with a linear dependency on the  $L^\infty$ -norms of the sample measures, which, as we show in a counterexample, is not true in higher dimensions. In Section 4.4, we present a dual and a multi-marginal formulation of the problem with some applications. In Section 4.5 we present a flow formulation of the Wasserstein median problem that leads to a PDE of Monge-Kantorovich type which characterizes the problem. For completeness, Section 4.A about the numerical simulations used for the images of this chapter is included. This work has been done by E. Chenchene.

## 4.1 Formulation and existence

Let  $(X, d)$  be a *proper* metric space, i.e. a metric space such that all the closed balls are compact. This implies that  $(X, d)$  is *Polish*, i.e. separable and complete. As we mentioned in the introduction, on  $(\mathcal{P}_1(X), W_1)$  we get a natural notion of median.

**Definition 4.1.1** (Wasserstein median). *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(X)$  and  $p_1, \dots, p_N$  positive weights such that  $p_1 + \dots + p_N = 1$ , we call (weighted) Wasserstein median any optimal*

solution to the following convex problem

$$\inf_{\rho \in \mathcal{P}_1(X)} \sum_{i=1}^N p_i W_1(\rho, \nu_i). \quad (\text{M})$$

We denote by  $\mathcal{F} : \mathcal{P}_1(X) \rightarrow \mathbb{R}$  the objective function and by  $\text{Med}_{\mathbf{p}}(\nu_1, \dots, \nu_N)$  the set of all Wasserstein medians of  $\nu_1, \dots, \nu_N$  with weights  $\mathbf{p} := (p_1, \dots, p_N)$ .

The existence of a solution of (M) follows from the standard Direct Method of Calculus of Variations which we detail for the sake of completeness.

**Theorem 4.1.2** (Existence of a solution). *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(X)$ ,  $\mathbf{p} = (p_1, \dots, p_N)$  positive weights such that  $p_1 + \dots + p_N = 1$  then there exists a minimizer of (M) and the set  $\text{Med}_{\mathbf{p}}(\nu_1, \dots, \nu_N)$  is a convex closed subset of  $\mathcal{P}_1(X)$ .*

*Proof.* Let  $(\rho^n)_{n \in \mathbb{N}}$  be a minimizing sequence of (M). There exists  $C > 0$  such that for all  $n \in \mathbb{N}$  we have  $\mathcal{F}(\rho^n) \leq C$ , thus for all  $n \in \mathbb{N}$ :

$$\sum_{i=1}^N p_i \inf_{\gamma_i \in \Pi(\rho^n, \nu_i)} \int d(x, y) d\gamma_i(x, y) \leq C. \quad (4.1.1)$$

By the triangular inequality we have for  $\bar{x} \in X$  and for all  $\gamma_i^n \in \Pi(\rho^n, \nu_i)$

$$\int d(x, \bar{x}) d\rho^n(x) \leq \sum_{i=1}^N p_i \int d(x, y) d\gamma_i^n(x, y) + \sum_{i=1}^N p_i \int d(y, \bar{x}) d\nu_i(y) \quad \forall n \in \mathbb{N}.$$

Hence, by (4.1.1) and the arbitrariness of  $\gamma_i^n$  the sequence  $(\rho^n)_{n \in \mathbb{N}}$  has uniformly bounded first moments. By Markov's inequality it follows that  $(\rho^n)_{n \in \mathbb{N}}$  is tight since  $X$  is proper. Hence  $(\rho^n)_{n \in \mathbb{N}}$  admits a narrowly converging subsequence, call  $\rho$  its limit. Since  $\mathcal{F}_1$  is lower semicontinuous with respect to the narrow convergence (see Lemma 7.1.4 in [7]),  $\rho$  is a Wasserstein median.

Convexity of  $\text{Med}_{\mathbf{p}}(\nu_1, \dots, \nu_N)$  follows by (standard) convexity of  $W_1$ .  $\square$

*Remark 4.1.3.* In the proof of Theorem 4.1.2 we proved that the set  $\text{Med}_{\lambda}(\nu_1, \dots, \nu_N)$  is narrowly compact. Actually, it is compact with respect to the topology induced by the  $W_1$  distance, as proven in Theorem 5.5 [71] in a much wider framework. A straightforward proof of this fact is given in Corollary 4.4.5 using the multi-marginal formulation in the case  $X = \mathbb{R}^d$ .

## 4.2 Stability and robustness

In this section, we introduce fundamental properties of Wasserstein medians which mainly rely on the metric side of the problem and can be generalized to *Fréchet medians*, we will highlight when this is possible.

### 4.2.1 Stability with respect to data

The stability with respect to random perturbation of the sample measures is a crucial property for any location estimator. We show in the sequel that if  $\nu_1, \dots, \nu_N$  are approximated by sequences  $(\nu_i^n)_{n \in \mathbb{N}} \in \mathcal{P}_1(X)^{\mathbb{N}}$  for  $i = 1, \dots, N$ , then the approximated medians narrowly converge, passing to a subsequence if necessary, to a Wasserstein median of the original measures. While this result is expected and can be established with quite standard techniques, it is important both for numerical purposes, and for theoretical reasons as it will enable us to circumvent the connectivity hypothesis on the support of the original measures in Theorem 4.3.9.

**Lemma 4.2.1.** *Let  $(p_1^n, \dots, p_N^n)_{n \in \mathbb{N}}$  with  $\sum_{i=1}^N p_i^n = 1$  be a sequence in  $[0, 1]^N$  converging to  $(p_1, \dots, p_N)$  and  $(\nu_1^n)_{n \in \mathbb{N}}, \dots, (\nu_N^n)_{n \in \mathbb{N}}$  be sequences converging to  $(\nu_1, \dots, \nu_N)$  in  $(\mathcal{P}_1(X), W_1)$ . Then the sequence of functionals of the Wasserstein median problem, i.e.,  $\mathcal{F}_n : \mathcal{P}_1(X) \rightarrow \mathbb{R}$  defined for  $n \in \mathbb{N}$*

$$\mathcal{F}_n(\rho) := \sum_{i=1}^N p_i^n W_1(\rho, \nu_i^n)$$

$\Gamma$ -converges with respect to the narrow convergence to the functional  $\mathcal{F}$  of the Wasserstein median problem (M).

*Proof.* The lim sup-inequality is guaranteed by taking the constant recovery sequence. For the lim inf-inequality let  $\mu \in \mathcal{P}_1(X)$  and  $(\mu^n)_{n \in \mathbb{N}}$  be a narrowly converging sequence to  $\mu$ . Then by joint lower semicontinuity of the Wasserstein functional (see e.g. Lemma 7.1.4 in [7])

$$\liminf_{n \rightarrow \infty} \mathcal{F}_n(\mu^n) \geq \sum_{i=1}^N p_i W_1(\mu, \nu_i).$$

□

With this at hand we can deduce the following stability result.

**Theorem 4.2.2** (Stability of Wasserstein medians). *Let  $\mathbf{p}^n = (p_1^n, \dots, p_N^n)_{n \in \mathbb{N}}$ ,  $\sum_{i=1}^N p_i^n = 1$ , be a sequence in  $[0, 1]^N$  converging to  $\mathbf{p} = (p_1, \dots, p_N)$  and  $(\nu_1^n)_{n \in \mathbb{N}}, \dots, (\nu_N^n)_{n \in \mathbb{N}}$  be sequences converging to  $(\nu_1, \dots, \nu_N)$  in  $(\mathcal{P}_1(X), W_1)$ . For all  $n \in \mathbb{N}$  let  $\rho^n \in \text{Med}_{\mathbf{p}^n}(\nu_1^n, \dots, \nu_N^n)$ . Then  $(\rho^n)_{n \in \mathbb{N}}$  admits a narrowly-converging subsequence and every limit point is a weighted Wasserstein median of  $(\nu_1, \dots, \nu_N)$  and weight  $\mathbf{p}$ .*

*Proof.* Similar to the proof of existence of a Wasserstein median, we can prove that  $(\rho^n)_{n \in \mathbb{N}}$  is tight. Indeed, for  $C > 0$  sufficiently large and  $\epsilon > 0$  there is an  $N \in \mathbb{N}$  such that for  $n \geq N$

$$\sum_{i=1}^N p_i^n W_1(\rho^n, \nu_i^n) \leq C, \quad |p_i^n - p_i| < \epsilon \quad \text{and} \quad W_1(\nu_i^n, \nu_i) < \epsilon.$$

Hence for a fixed  $x_0 \in X$  we obtain for  $n \geq N$

$$\int d(x, x_0) d\rho^n(x) \leq \sum_{i=1}^N p_i^n \left[ W_1(\rho^n, \nu_i^n) + W_1(\nu_i^n, \nu_i) + \int d(x_0, y) d\nu_i(y) \right] \leq \tilde{C},$$

for  $\tilde{C} > 0$  independent of  $n$ . This implies tightness of  $(\rho^n)_{n \in \mathbb{N}}$ . Optimality of an accumulation point now follows by the  $\Gamma$ -convergence from Lemma 4.2.1.  $\square$

*Remark 4.2.3.* Actually, one can improve the convergence of a suitable subsequence of minimizers  $(\rho^n)_{n \in \mathbb{N}}$  to convergence in  $(\mathcal{P}_1(X), W_1)$  by employing Theorem 5.5 [71] directly.

Another self-contained proof of this in the setting  $X = \mathbb{R}^d$  is given by combing the  $\Gamma$ -convergence from Lemma 4.2.1  $W_1$  and the precompactness of the sequence in  $(\mathcal{P}_1(X), W_1)$  by Corollary 4.4.5.

### 4.2.2 Robustness of Wasserstein medians

In statistics, an index which somewhat tries to capture the notion of robustness is the so called *break-down point*. Roughly speaking, it yields the largest fraction of the input data which could be corrupted (i.e., changed arbitrarily) without moving the estimation too far from the original estimation for the non-corrupted data. Let us give an example. Take  $N \geq 2$  points in  $\mathbb{R}$  and consider the usual (uniform) algebraic mean. It suffices to move only one of these points to  $+\infty$  for the mean to go to  $+\infty$ , too. In other words, corrupting arbitrarily only one input value the estimated mean could move arbitrarily far from the original mean value. The break-down point of the arithmetic mean is therefore  $1/N$ : it suffices to corrupt only one value to make the output information-less, unless we don't provide some error bounds on the corrupted data. It is well known (see Theorem 2.1 and 2.2 [78]) that the break-down point of geometric medians is approximately  $1/2$ , so that even corrupting half (minus one) of the data we can stay rather confident on the output. In this section we prove a similar result for Wasserstein medians. To do so, we should first recall some basic facts about break-down points, starting with a definition of break-down point that we adapted to the weighted case.

**Definition 4.2.4** (Break-down point). *Let  $(Y, d_Y)$  be a metric space,  $N \geq 2$  and  $\mathbf{p} = (p_1, \dots, p_N) \in [0, 1]^N$  with  $\sum_{i=1}^N p_i = 1$ . For a statistics function  $t_{\mathbf{p}} : Y^N \rightarrow Y$  we define its break-down point associated to the weights  $\mathbf{p}$  at  $\mathbf{x} = (x_1, \dots, x_N) \in Y^N$  by the following number*

$$b(t_{\mathbf{p}}(\mathbf{x})) := \min \left\{ \sum_{i \in I} p_i : I \subseteq \{1, \dots, N\}, \sup_{\mathbf{y}^I} d(t(\mathbf{y}^I), t(\mathbf{x})) = +\infty \right\},$$

where the sup is taken over all possible corrupted collections  $\mathbf{y}^I = (y_1, \dots, y_N)$  that are obtained from  $\mathbf{x}$  by replacing the points indexed by  $I$  by arbitrary values in  $Y$ .

*Remark 4.2.5* (“Arbitrarily far”). Let  $X$  be a bounded space (i.e.,  $\text{diam}X < \infty$ ). One could easily notice from the definition of the Wasserstein distance

$$W_1(\mu, \nu) \leq \text{diam}(X) := \sup\{d(x, y) \mid (x, y) \in X^2\},$$

which means that if the space is bounded, the breakdown point of any location estimator w.r.t. the metric  $W_1$  is always 1. This means that this index is only a useful indicator of robustness if we suppose the space to have infinite diameter. This assumption, which is clearly technical, has to be made in order to take advantages of the properties of the break-down index, which is sensible to robustness as far as perturbations are somewhat arbitrarily stressed.

We now state the main theorem for Wasserstein medians, where the reference metric space is  $\mathcal{P}_1(X)$  equipped with the  $W_1$  distance, and the statistics function is just the choice of one median in  $\text{Med}(\nu_1, \dots, \nu_N)$ . The proof is a generalization of the one of Theorem 2.2 in [78].

**Theorem 4.2.6** (Break-down point of Wasserstein medians). *Suppose  $\text{diam}(X) = \infty$ . Let  $N \geq 2$ ,  $\boldsymbol{\nu} := (\nu_1, \dots, \nu_N) \in \mathcal{P}_1(X)^N$  and  $\mathbf{p} := (p_1, \dots, p_N) \in [0, 1]^N$  with  $\sum_{i=1}^N p_i = 1$ . Denote by  $\mathcal{M}_{\mathbf{p}} : \mathcal{P}_1(X)^N \rightarrow \mathcal{P}_1(X)$  a function which gives a Wasserstein median for each  $\nu_1, \dots, \nu_N$  with associated weights  $\mathbf{p}$ . Then the break-down point of  $\mathcal{M}_{\mathbf{p}}$  satisfies*

$$b(\mathcal{M}_{\mathbf{p}}(\boldsymbol{\nu})) \geq \frac{1}{2}.$$

More precisely, if we take a corrupted collection  $\boldsymbol{\mu} := (\mu_1, \dots, \mu_N)$  by replacing components indexed by  $I \subset \{1, \dots, N\}$  with  $\sum_{i \in I} p_i < \frac{1}{2}$  we have

$$W_1(\mathcal{M}_{\mathbf{p}}(\boldsymbol{\nu}), \mathcal{M}_{\mathbf{p}}(\boldsymbol{\mu})) \leq \frac{2C\delta}{1-2\delta} + 2C \quad (4.2.1)$$

where  $C := \max_i W_1(\mathcal{M}_{\mathbf{p}}(\boldsymbol{\nu}), \nu_i)$  and

$$\delta := \sup \left\{ \sum_{j \in J} p_j : J \subset \{1, \dots, N\}, \sum_{j \in J} p_j < \frac{1}{2} \right\}.$$

*Proof.* Let us denote  $\rho = \mathcal{M}_{\mathbf{p}}(\nu_1, \dots, \nu_N)$ . Take  $I \subset \{1, \dots, N\}$  such that  $\sum_{i \in I} p_i < \frac{1}{2}$ . Denote by  $\boldsymbol{\mu} := (\mu_1, \dots, \mu_N)$  a corrupted collection obtained by replacing the points indexed by  $I$  of  $\boldsymbol{\nu} := (\nu_1, \dots, \nu_N)$ . We prove by contradiction that

$$W_1(\rho, \underbrace{\mathcal{M}_{\mathbf{p}}(\boldsymbol{\mu})}_{:=\mu}) \leq K,$$

for a constant  $K$  independent of  $I$ . In order to do so, define  $C := \max_i W_1(\rho, \nu_i)$  and let  $\mathcal{B} = B_{2C}(\rho)$  be the ball with center  $\rho$  and radius  $2C$  with respect to the  $W_1$  distance. Further, let

$$\xi := \text{Dist}(\mu, \mathcal{B}) := \inf_{\varrho \in \mathcal{B}} W_1(\mu, \varrho).$$

Then by the triangular inequality  $W_1(\mu, \rho) \leq \xi + 2C$ , so that for all  $j = 1, \dots, N$

$$W_1(\mu_j, \mu) \geq W_1(\mu_j, \rho) - W_1(\rho, \mu) \geq W_1(\mu_j, \rho) - (\xi + 2C). \quad (4.2.2)$$

Now suppose that  $\mu$  is far from  $\rho$ , more precisely by defining

$$\delta := \sup \left\{ \sum_{j \in J} p_j : J \subset \{1, \dots, N\}, \sum_{j \in J} p_j < \frac{1}{2} \right\},$$

suppose that

$$\xi > \frac{2C\delta}{1-2\delta}.$$

Then by using that  $(\mathcal{P}_1(X), W_1)$  is a geodesic space, see Lemma 4.2.8, we have for all  $j = 1, \dots, N$

$$W_1(\nu_j, \mu) \geq C + \xi \geq W_1(\nu_j, \rho) + \xi \quad (4.2.3)$$

Putting together the estimates in (4.2.2) and (4.2.3) yields

$$\begin{aligned}
 \sum_{j=1}^N p_j W_1(\mu_j, \mu) &\geq \sum_{j \in I} p_j (W_1(\mu_j, \rho) - (\xi + 2C)) + \sum_{j \notin I} p_j (W_1(\mu_j, \rho) + \xi) \\
 &= \sum_{j=1}^N p_j W_1(\mu_j, \rho) + \xi \left( \sum_{j \notin I} p_j - \sum_{j \in I} p_j \right) - 2C \sum_{j \in I} p_j \\
 &\geq \sum_{j=1}^N p_j W_1(\mu_j, \rho) + \xi(1 - 2\delta) - 2C\delta \\
 &> \sum_{j=1}^N p_j W_1(\mu_j, \rho),
 \end{aligned}$$

which contradicts  $\mu$  being a Wasserstein median for the corrupted collection  $\boldsymbol{\mu}$ . Note that this also implies that

$$\xi \leq \frac{2C\delta}{1 - \delta},$$

from which we deduce the estimate in (4.2.1).  $\square$

*Remark 4.2.7.* By inspecting the proof, we observe that actually the lower bound for the break-down point of  $\mathcal{M}_{\mathbf{p}}$  is given by

$$1 - \delta = \inf \left\{ \sum_{j \in J} p_j : J \subset \{1, \dots, N\}, \sum_{j \in J} p_j \geq \frac{1}{2} \right\}.$$

In case of uniform weights, i.e. with  $\mathbf{p} := (1/N, \dots, 1/N)$ , we have  $\delta = \lfloor \frac{N-1}{2} \rfloor / N$ . In this case we retrieve the classical estimate

$$b(\mathcal{M}_{\mathbf{p}}(\boldsymbol{\nu})) \geq \left\lfloor \frac{N+1}{2} \right\rfloor / N,$$

as proved in Theorem 2.2. in [78] for geometric medians on  $\mathbb{R}^d$ . Moreover, we have the following uniform estimate for  $k = \lfloor (N-1)/2 \rfloor$

$$\sup_{\boldsymbol{\mu}_k} W_1(\mathcal{M}_{\mathbf{p}}(\boldsymbol{\mu}_k), \mathcal{M}_{\mathbf{p}}(\boldsymbol{\nu})) \leq 2C \left\lfloor \frac{N+1}{2} \right\rfloor,$$

where  $C = \max_i W_1(\mathcal{M}_{\mathbf{p}}(\boldsymbol{\nu}), \nu_i)$  and the sup is taken over all possible corrupted collections  $\boldsymbol{\mu}_k = (\mu_1, \dots, \mu_N)$  that are obtained from  $\boldsymbol{\nu}$  by replacing  $k$  components of  $\boldsymbol{\nu}$  by arbitrary measures in  $\mathcal{P}_1(X)$ .

**Lemma 4.2.8.** *Let  $(X, d)$  be a Polish space. Then  $(\mathcal{P}_1(X), W_1)$  is a geodesic space.*

*Proof.* Let  $\mu_0, \mu_1 \in \mathcal{P}_1(X)$ . We claim that  $\mu_t = (1-t)\mu_0 + t\mu_1$  is a constant-speed geodesic in  $(\mathcal{P}_1(X), W_1)$ . Indeed, by employing Kantorovich-Rubinstein duality (Theorem 1.14 [112]), we have for  $0 \leq s \leq t \leq 1$

$$\begin{aligned}
 W_1(\mu_t, \mu_s) &= \sup \left\{ \int_X \varphi d(\mu_t - \mu_s) : \varphi \in L^1(|\mu_t - \mu_s|), \|\varphi\|_{\text{Lip}} \leq 1 \right\} \\
 &= (t-s) \sup \left\{ \int_X \varphi d(\mu_1 - \mu_0) : \varphi \in L^1(|\mu_1 - \mu_0|), \|\varphi\|_{\text{Lip}} \leq 1 \right\} \\
 &= (t-s)W_1(\mu_1, \mu_0),
 \end{aligned}$$

where  $\|\varphi\|_{\text{Lip}} := \sup_{x,y \in X} \frac{|\varphi(x) - \varphi(y)|}{d(x,y)}$ .

□

*Remark 4.2.9.* Theorem 4.2.6 can be adapted to Fréchet medians defined on *any* geodesic metric space. In fact, the proposed proof essentially relies on the triangular inequality, existence of a geodesic between two arbitrary elements and on the very first definition of a median.

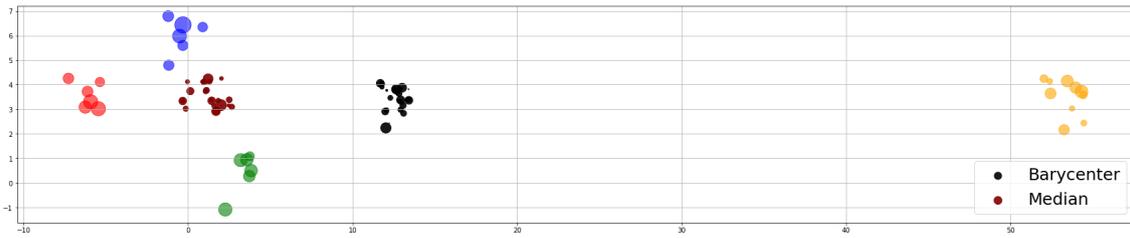


Figure 4.3 – Comparison of a Wasserstein median and a Wasserstein barycenter of four discrete measures (in blue, red, green, and yellow). The yellow sample measure could be thought as an outlier.

### 4.3 One dimensional Wasserstein medians

In this section, we study the case of Wasserstein medians on  $X = \mathbb{R}$  with distance  $d$  induced by the absolute value. Recall that in one dimension the Wasserstein space of order 1 can be identified as a Banach space since the Wasserstein distance of order 1 between two measures is equal to the  $L^1$ -distance between their cumulative or quantile distribution functions, see also Section 2.1 [104]. Hence, the Wasserstein median problem becomes more explicit. This allows to find few different explicit constructions of Wasserstein medians. In this section for all  $\nu \in \mathcal{P}_1(\mathbb{R})$  we denote by  $F_\nu$  its associated cumulative distribution function (cdf), which is defined by  $F_\nu(x) = \nu((-\infty, x])$  for all  $x \in \mathbb{R}$ . We also denote by  $q_\nu : [0, 1] \rightarrow \mathbb{R}$  its *pseudo-inverse* or quantile distribution function (qdf), which is defined by

$$q_\nu(t) := \inf\{x \in \mathbb{R} \mid F_\nu(x) \geq t\},$$

for  $t \in [0, 1]$ . More precisely, we have the following important characterization of the Wasserstein distance of order one on one dimensional domains, see for instance [104, Theorem 2.9]. Let  $\mu, \nu \in \mathcal{P}_1(\mathbb{R})$ , then we have:

$$\begin{aligned} W_1(\mu, \nu) &= \int_0^1 |q_\nu(t) - q_\mu(t)| dt = \|q_\nu - q_\mu\|_{L^1([0,1])} \\ &= \int_{\mathbb{R}} |F_\mu(t) - F_\nu(t)| dt = \|F_\nu - F_\mu\|_{L^1(\mathbb{R})}. \end{aligned}$$

We obtain immediately the following reformulations of the Wasserstein median problem

$$\inf(\mathbf{M}) = \inf_{\rho \in \mathcal{P}_1(\mathbb{R})} \int_{\mathbb{R}} \sum_{i=1}^N p_i |F_{\rho}(t) - F_{\nu_i}(t)| dt \quad (4.3.1)$$

$$= \inf_{\rho \in \mathcal{P}_1(\mathbb{R})} \int_0^1 \sum_{i=1}^N p_i |q_{\rho}(t) - q_{\nu_i}(t)| dt \quad (4.3.2)$$

which will be referred as *vertical* (4.3.1) and *horizontal* (4.3.2) *formulations*. The terminology will become clear in the sequel. Note that in this way the problem is equivalent to perform a proper selection of a 1D Euclidean weighted median of the cumulative or quantile distribution functions. Due to the continuity properties of cdfs and qdfs we can trace back to pointwise medians (as proved in Proposition 4.3.2) which is why the following lemma is useful in the sequel.

**Proposition 4.3.1** (Medians in  $\mathbb{R}$ ). *Let  $x_1 < \dots < x_N \in \mathbb{R}$  and  $\mathbf{p} = (p_1, \dots, p_N)$  positive weights which sum up to 1. Then  $x_k$  is a median if and only if  $k$  satisfies the following condition:*

$$\sum_{i \geq k} p_i \geq \frac{1}{2} \quad \text{and} \quad \sum_{i \leq k} p_i \geq \frac{1}{2}. \quad (4.3.3)$$

*If there exists a unique  $k$  such that (4.3.3) is satisfied then  $x_k$  is the unique weighted median. Finally, there exists at most two  $k$ s which satisfy (4.3.3), and they are consecutive: say  $x_k, x_{k+1}$ . In this case,  $\text{Med}_{\mathbf{p}}(x_1, \dots, x_N) = [x_k, x_{k+1}]$ .*

*Proof.* We look for  $x_k, k \in \{1, \dots, N\}$ , which minimizes the following convex function  $f(y) := \sum_{i=1}^N p_i |y - x_i|$ . By convexity this is equivalent to finding  $x_k$  such that

$$0 \in \partial f(x_k) = \sum_{i=1}^N p_i \partial |\cdot - x_i|(x_k) = \sum_{i < k} p_i + [-p_k, +p_k] - \sum_{i > k} p_i.$$

where we used a standard notation for the sum of sets. This can be rewritten as

$$\sum_{i < k} p_i - \sum_{i \geq k} p_k \leq 0 \leq \sum_{i \leq k} p_i - \sum_{i > k} p_i,$$

which in turn is equivalent to (4.3.3). The remaining statements are an immediate consequence of (4.3.3).  $\square$

This triggers a natural mild condition for uniqueness, i.e.

**Property.** Let  $p_1, \dots, p_N > 0$  be positive weights such that  $\sum_{i=1}^N p_i = 1$  and that

$$\text{there is no permutation } \sigma \text{ of } \{1, \dots, N\} \text{ and no index } k \text{ such that: } \sum_{i=1}^k p_{\sigma(i)} = \frac{1}{2}, \quad (4.3.4)$$

Condition (4.3.4) ensures uniqueness for 1D geometric medians by Proposition 4.3.1, and, therefore, also for Wasserstein medians on one dimensional domains by Proposition 4.3.2.

**Proposition 4.3.2.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(\mathbb{R})$  with cumulative distribution function  $F_1, \dots, F_N$  and quantile distribution function  $q_1, \dots, q_N$ ,  $\mathbf{p} := (p_1, \dots, p_N) \in [0, 1]^N$  with  $\sum_{i=1}^N p_i = 1$ . Let  $\rho \in \text{Med}_{\mathbf{p}}(\nu_1, \dots, \nu_N)$ , then*

$$F_\rho(x) \in \text{Med}_{\mathbf{p}}(F_1(x), \dots, F_N(x)) \quad \forall x \in \mathbb{R}, \text{ and } q_\rho(t) \in \text{Med}_{\mathbf{p}}(q_1(t), \dots, q_N(t)) \quad \forall t \in (0, 1). \quad (4.3.5)$$

*Conversely, given  $\rho \in \mathcal{P}_1(\mathbb{R})$ , if  $F_\rho$  is its cumulative distribution function and satisfies (4.3.5), or respectively its quantile distribution function  $q_\rho$  satisfies (4.3.5) then  $\rho$  is a Wasserstein median. Furthermore, if (4.3.4) holds, then there is a unique Wasserstein median.*

*Proof.* We show the first claim for cdfs. The same argument works for qdfs. Suppose that there is an  $x \in \mathbb{R}$  such that

$$F_\rho(x) \notin \text{Med}_\lambda(F_1(x), \dots, F_N(x)).$$

Then by right-continuity of all the cdfs there must be a  $\delta > 0$  such that for all  $y \in [x, x + \delta]$

$$F_\rho(y) \notin \text{Med}_\lambda(F_1(y), \dots, F_N(y)),$$

which contradicts  $F_\rho$  being the cdf of a Wasserstein median. The converse is immediate. Now uniqueness under (4.3.4) follows from the fact that in this case  $\text{Med}_{\mathbf{p}}(\xi_1, \dots, \xi_N)$  is always a singleton for every  $\xi_1, \dots, \xi_N \in \mathbb{R}$  by Proposition 4.3.1.  $\square$

Note that condition (4.3.4) holds for instance when we consider an odd number of sample measures with uniform weights. However, unlike the 1D Euclidean case this is not a necessary condition for uniqueness, even if it is still somehow tight. In fact, if (4.3.4) does not hold it is easy to build a sample for which uniqueness does not hold. Proposition 4.3.2, in particular (4.3.5), suggests also a natural way to construct a family of Wasserstein medians. The following definition will be helpful.

**Definition 4.3.3** (Upper and lower medians). *Let  $\Omega$  be a subset of  $\mathbb{R}$  and  $f_1, \dots, f_N : \Omega \rightarrow \mathbb{R}$  be  $N$  functions, we define*

$$g_+(x) := \max \text{Med}_\lambda(f_1(x), \dots, f_N(x)), \quad g_-(x) := \min \text{Med}_\lambda(f_1(x), \dots, f_N(x)) \quad \forall x \in \Omega.$$

$g_+$  will be called upper median and  $g_-$  lower median of  $f_1, \dots, f_N$ .

As before it is useful to look at properties of pointwise medians. Proposition 4.3.1 implies the following characterization for lower and upper medians which we use frequently in the proofs.

**Corollary 4.3.4.** *Let  $x_1, \dots, x_N \in \mathbb{R}$  and  $\mathbf{p} = (p_1, \dots, p_N)$  be (strictly) positive weights which sum up to 1. Then,*

- $x_+$  is the upper median, i.e.  $x_+ = \max \text{Med}_{\mathbf{p}}(x_1, \dots, x_N)$  iff  $x_+$  is a median and for all  $I \subset \{1, \dots, N\}$  with  $\sum_{i \in I} p_i \geq \frac{1}{2}$

$$x_+ \geq \min_{i \in I} x_i$$

- $x_-$  is the lower median, i.e.  $x_- = \min \text{Med}_{\mathbf{p}}(x_1, \dots, x_N)$  iff  $x_-$  is a median and for all  $I \subset \{1, \dots, N\}$  with  $\sum_{i \in I} p_i \geq \frac{1}{2}$

$$x_- \leq \max_{i \in I} x_i$$

*Proof.* By reordering and relabeling the points we can always assume that  $x_1 < \dots < x_M$  and  $M \leq N$ . Indeed, reordering the given points to  $\bar{x}_1 < \dots < \bar{x}_M$  (by possibly dropping points with equal value) with weights  $\bar{p}_i = \sum_{k \in A_i} p_k$  where  $A_i = \{k \in \{1, \dots, N\} : x_k = \bar{x}_i\}$  yields the result.

So, assume that  $x_1 < \dots < x_M$  and corresponding (strictly) positive weights  $(p_i)_{i=1}^M$  with  $M \leq N$ .

We only prove the first assertion, the second one is analogous. Let  $x_+$  be the upper median. Then, by Proposition 4.3.1 there is  $k \in \{1, \dots, M\}$  such that  $x_+ = x_k$  with  $\sum_{i \geq k} p_i \geq \frac{1}{2}$  and  $\sum_{i \leq k} p_i \geq \frac{1}{2}$ . Now, assume that there is  $I \subset \{1, \dots, N\}$  with  $\sum_{i \in I} p_i \geq \frac{1}{2}$  and

$$x_+ < \min_{i \in I} x_i.$$

Observe that necessarily  $I \subset \{k+1, \dots, M\}$  and  $\sum_{i \geq k+1} p_i = \frac{1}{2}$  since  $\sum_{i \geq k+1} p_i \geq \sum_{i \in I} p_i \geq \frac{1}{2}$  and  $\sum_{i \geq k+1} p_i = 1 - \sum_{i \leq k} p_i \leq \frac{1}{2}$ . This implies that  $I = \{k+1, \dots, M\}$ . Since  $\sum_{i \leq k+1} p_i \geq \frac{1}{2}$  and  $\sum_{i \geq k+1} p_i \geq \frac{1}{2}$ , Proposition 4.3.1 gives that  $x_{k+1} > x_+$  is a median as well, contradicting the fact that  $x_+$  is the upper median.

Let now  $x_+$  be a median. If there is a unique median, then clearly  $x_+$  is the upper median. Otherwise, there is  $k \in \{1, \dots, M\}$  such that  $\text{Med}_{\mathbf{p}}(x_1, \dots, x_N) = [x_k, x_{k+1}]$  and  $\sum_{i \geq k+1} p_i \geq \frac{1}{2}$  by Proposition 4.3.1. But then by our assumption  $x_+ \geq x_{k+1}$  which concludes that  $x_+$  is the upper median.  $\square$

The following technical lemma summarizes the elements to justify our Median selection procedure and states properties we need for the higher regularity in the sequel.

**Lemma 4.3.5** (Median selection). *Let  $\Omega$  be a (possibly unbounded) interval of  $\mathbb{R}$  and  $f_1, \dots, f_N : \Omega \rightarrow \mathbb{R}$  be non-decreasing functions. Let  $g_+, g_-$  be the upper and the lower medians of  $f_1, \dots, f_N$ . Define*

$$g_\theta = \theta g_+ + (1 - \theta) g_- \quad \text{for } \theta \in [0, 1].$$

*Then it holds that*

1.  $g_\theta$  is non-decreasing for all  $\theta \in [0, 1]$ , hence, differentiable almost everywhere.
2. If  $f_1, \dots, f_N$  are all strictly increasing then  $g_\theta$  is strictly increasing for all  $\theta \in [0, 1]$ .
3. If  $f_1, \dots, f_N$  are all right (resp. left) continuous, then  $g_\theta$  is right (resp. left) continuous.
4. Assume that  $\theta \in \{0, 1\}$ . Denote by  $\mathcal{I}_0(x) = \{i \in \{1, \dots, N\} \mid g_\theta(x) = f_i(x)\}$ . Then we have that

$$\min_{i \in \mathcal{I}_0(x)} f'_i(x) \leq g'_\theta(x) \leq \max_{i \in \mathcal{I}_0(x)} f'_i(x) \quad \text{for a.e. } x \in \Omega.$$

*Proof.* It suffices to prove the points 1., 2. and 3. for  $\theta \in \{0, 1\}$ . For all  $t \in \Omega$  denote  $\mathcal{I}_+(t) := \{i \in \{1, \dots, N\} : f_i(t) \geq g_+(t)\}$ . Since all the  $f_i$ 's are non-decreasing, we obtain for  $h > 0$  such that  $t+h \in \Omega$ , and all  $i \in \mathcal{I}_+(t)$

$$f_i(t+h) \geq g_+(t).$$

Now, note that by Corollary 4.3.4 with  $\sum_{i \in \mathcal{I}_+(t)} p_i \geq \frac{1}{2}$  we have

$$g_+(s) \geq \min_{i \in I} f_i(s).$$

This implies  $g_+(t+h) \geq g_+(t)$  as desired. For the lower median a similar strategy with the set  $\mathcal{I}_-(t+h) := \{i \in \{1, \dots, N\} : f_i(t+h) \leq g_-(t+h)\}$  and part 2 of Corollary 4.3.4 yields the result. For 2. the argument is analogous and therefore omitted.

For 3. consider  $g_+$  and  $t \in \Omega$ ,  $(t_n)_{n \in \mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$  with  $t_n \geq t$  and  $t_n \rightarrow t$  as  $n \rightarrow \infty$ . Then  $(g_+(t_n))_{n \in \mathbb{N}}$  is bounded and hence there is a converging subsequence. Denote the sequence by  $(n_k)_{k \in \mathbb{N}}$  and its limit by  $\tilde{g}_+(t)$ . By passing to the limit  $k \rightarrow \infty$  the fact that all the  $g_+(t_{n_k})$  are medians we have for all  $x \in \mathbb{R}$

$$\sum_{i=1}^N p_i |\tilde{g}_+(t) - f_i(t)| \leq \sum_{i=1}^N p_i |x - f_i(t)|.$$

Hence  $\tilde{g}_+(t)$  is a median as well. To conclude that it is the upper median take  $I \subset \{1, \dots, N\}$  such that  $\sum_{i \in I} p_i \geq \frac{1}{2}$ , then

$$g_+(t_{n_k}) \geq \min_{i \in I} f_i(t_{n_k}),$$

and passing to the limit  $k \rightarrow \infty$  concludes that  $\tilde{g}_+(t)$  is the upper median, hence  $\tilde{g}_+(t) = g_+(t)$ . Now that we know that every subsequence has a converging subsequence towards  $g_+(t)$  we can conclude that the whole sequence converges. The proof for the lower median and for the left continuity is analogous.

Let us now focus on 4. Let  $\Omega' \subset \Omega$  be a set of full Lebesgue measure where  $g_\theta$ ,  $f_i$  with  $i \in \{1, \dots, N\}$  are all differentiable and consider  $x \in \Omega'$ . By the continuity of all the functions  $g_\theta$  and  $f_1, \dots, f_N$  in  $x$  and Proposition 4.3.1 (recall  $\theta \in \{0, 1\}$ ), for all sufficiently small  $h \in \mathbb{R}$ ,  $g_\theta(x+h) = f_j(x+h)$  for some  $j \in \mathcal{I}_0(x)$ , which we denote by  $j_h$ . Furthermore, by the differentiability of  $g_\theta$  and all  $f_i$  in  $x$  we have for  $\epsilon > 0$

$$\begin{aligned} g'_\theta(x) &\leq |g'_\theta(x) - f'_{j_h}(x)| + f'_{j_h}(x) \\ &\leq \underbrace{\left| \frac{g_\theta(x+h) - g_\theta(x)}{h} - \frac{f_{j_h}(x+h) - f_{j_h}(x)}{h} \right|}_{=0} + \epsilon + f'_{j_h}(x), \end{aligned}$$

where we have possibly chosen  $h$  even smaller to ensure  $\epsilon$ -closedness of the difference quotients to the derivative. This yields

$$g'_\theta(x) \leq \max_{j \in \mathcal{I}_0(x)} \{f'_j(x)\} + \epsilon,$$

and we conclude the upper estimate on the derivative by  $\epsilon \rightarrow 0$ . The lower bound is analogous.  $\square$

Given  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(\mathbb{R})$  with cdf  $F_{\nu_1}, \dots, F_{\nu_N}$  and qdf  $q_{\nu_1}, \dots, q_{\nu_N}$  we can now select two (a priori different) Wasserstein medians by taking

$$q_\theta := \theta q_+ + (1 - \theta) q_-, \quad F_\theta := \theta F_+ + (1 - \theta) F_-, \quad (4.3.6)$$

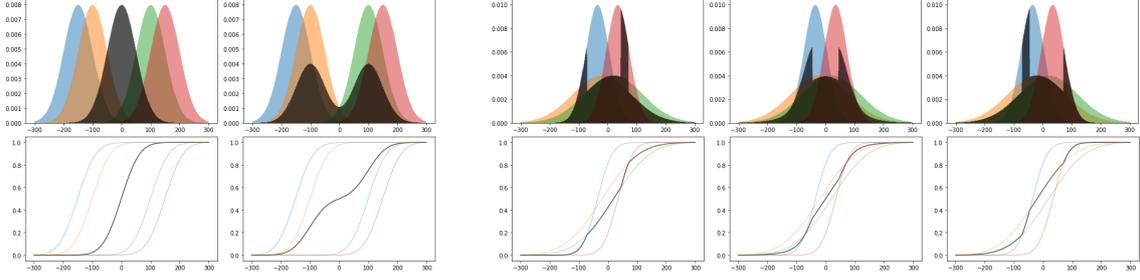


Figure 4.4 – Two numerical examples: (Left) The horizontal selection compared to the vertical selection with parameter  $\theta = 1/2$ . (Right) Three vertical selections with parameters  $\theta = 0, 1/2, 1$  for a different sample of four measures. (Down) their cumulative distribution functions.

with  $\theta \in [0, 1]$ . They will be referred to as *horizontal* and *vertical selections*. We call *horizontal upper*, *horizontal lower*, *vertical upper*, *vertical lower Wasserstein medians* the medians given by  $q_+, q_-, F_+, F_-$  respectively. Note that thanks to Lemma 4.3.5  $F_\theta$  and  $q_\theta$  are indeed cdfs and qdfs respectively (the fact that the limits carry over is immediate). We furthermore obtain a regularity result as detailed in the following.

**Proposition 4.3.6.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(\mathbb{R})$  and fix  $\theta \in [0, 1]$  then  $F_\theta : \mathbb{R} \rightarrow [0, 1]$  and  $q_\theta : [0, 1] \rightarrow \bar{\mathbb{R}}$  given by (4.3.6) are two well defined cumulative and quantile distribution functions which define two Wasserstein medians  $\rho^\theta$  and  $\mu^\theta$  respectively. Moreover, we have the following*

1. *If  $\nu_1, \dots, \nu_N$  are all atomless (resp. discrete) then  $\rho^\theta$  and  $\mu^\theta$  are atomless (resp. discrete);*
2. *If  $\nu_1, \dots, \nu_N$  have connected support, then  $\rho^\theta$  and  $\mu^\theta$  have connected support.*

*Proof.* The proof is a direct consequence of Lemma 4.3.5 and the following well known characterizations. We know that  $\mu$  being atomless is equivalent to  $F_\mu$  being continuous as well as  $q_\mu$  being strictly increasing, see Theorem 4.3 (m) [48]. Similarly, by Theorem 4.3 (p) [48]  $\mu$  has connected support if and only if  $F_\mu$  is strictly increasing on  $\{\mu > 0\}$ , if and only if  $q_\mu$  is continuous.  $\square$

In addition, if the regularity of *all* the sample measures improves further, then the regularity of the vertical and horizontal selections of a Wasserstein median improves as well, as shown in the following theorems. Let us first discuss the vertical selections.

**Theorem 4.3.7.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(\mathbb{R})$  and let  $F_\theta : \mathbb{R} \rightarrow [0, 1]$  be given by (4.3.6) for  $\theta \in [0, 1]$ . If  $\nu_1, \dots, \nu_N$  are all absolutely continuous with densities  $f_1, \dots, f_N \in L^p(\mathbb{R})$  with  $p \in [1, \infty]$  then  $\rho^\theta$ , the measure given by  $F_\theta$ , is absolutely continuous with density  $f_{\rho^\theta} \in L^p(\mathbb{R})$ , and the following quantitative estimate on the density holds*

$$f_{\rho^\theta}(x) \leq \max_{1 \leq i \leq N} \{f_i(x)\}, \quad \text{for a.e. } x \in \mathbb{R}.$$

*In particular, its  $L^p$ -norm is finite and the following estimate holds*

$$\|f_{\rho^\theta}\|_{L^p(\mathbb{R})} \leq \sum_{i=1}^N \|f_i\|_{L^p(\mathbb{R})}. \quad (4.3.7)$$

*Proof.* Let us assume now that all the sample measures are absolutely continuous with densities  $f_1, \dots, f_N \in L^p(\mathbb{R})$ . Consider first  $\theta \in \{0, 1\}$ . Let  $I \subset \mathbb{R}$  be a non-trivial interval. We prove that  $F_\theta$  is absolutely continuous on  $I$  by using its equivalence to being continuous, of bounded variation and satisfying Lusin's property, which states that for any measurable set  $N$  with  $\mathcal{L}^1(N) = 0$  we have  $\mathcal{L}^1(F_\theta(N)) = 0$ , see for instance [12, 5.8.51].

Indeed, continuity and being of bounded variation (more precisely being non-decreasing) is carried over to  $F_\theta$  thanks to Lemma 4.3.5. For the Lusin's property, observe that by Proposition 4.3.1 for all  $x \in \mathbb{R}$   $F_\theta(x) \in \{F_{\nu_1}(x), \dots, F_{\nu_N}(x)\}$ , so that we have

$$F_\theta(N) \subset \bigcup_{i=1}^N F_{\nu_i}(N),$$

for any measurable set  $N$ . If now  $\mathcal{L}^1(N) = 0$ , then by absolute continuity of the  $F_{\nu_i}$ , we have  $\mathcal{L}^1(F_{\nu_i}(N)) = 0$ , hence also  $\mathcal{L}^1(F_\theta(N)) = 0$ . We proved that  $F_1$  and  $F_0$  yield two absolutely continuous Wasserstein medians. Since  $F_\theta = \theta F_1 + (1 - \theta)F_0 = \theta F_+ + (1 - \theta)F_-$  we also retrieve the same result for all  $\theta \in (0, 1)$ . Finally, the estimate on the derivative  $f_\theta$  follows by Lemma 4.3.5 point 4.  $\square$

Let us now turn our attention to the horizontal selections, the following refined stability property will be useful.

**Lemma 4.3.8.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(\mathbb{R})$  be probability measures. For all  $i \in \{1, \dots, N\}$  let  $(\nu_i^n) \in \mathcal{P}_1(\mathbb{R})^{\mathbb{N}}$  be sequences that converge to  $\nu_i$  in  $(\mathcal{P}_1(\mathbb{R}), W_1)$ . Denote by  $\mu^n \in \text{Med}_p(\nu_1^n, \dots, \nu_N^n)$  the horizontal lower (resp. upper) weighted medians for all  $n \in \mathbb{N}$ , then  $\mu^n$  converges narrowly to the horizontal lower (resp. upper) median of  $\nu_1, \dots, \nu_N$ .*

*Proof.* Let us denote by  $q^n$  the quantile function associated to  $\mu^n$ , where w.l.o.g.  $\mu^n$  are the horizontal lower medians. It is a general result (cfr. Theorem 4.2.2) that  $\mu^n$  admits a narrowly-converging subsequence  $(\nu^{n_k})_{k \in \mathbb{N}}$  whose limit is a Wasserstein median of the limit sample. Then, denoting by  $q^\infty$  the quantile distribution function of the limit, it follows that  $q^{n_k}(t) \rightarrow q^\infty(t)$  as  $k \rightarrow \infty$  for all  $t \in (0, 1)$  where  $q^\infty$  is continuous (see for instance proof of Proposition 5 on page 250 [55]). Since  $q^\infty$  is non-decreasing, the set of discontinuities of  $q^\infty$  is  $\mathcal{L}^1$ -negligible, therefore  $q^{n_k}$  converges almost-everywhere to  $q^\infty$ . Let now  $I \subset \{1, \dots, N\}$  with  $\sum_{i \in I} p_i \geq \frac{1}{2}$ . By Corollary 4.3.4 we have for all  $k \in \mathbb{N}$  and all  $t \in (0, 1)$

$$q^{n_k}(t) \leq \max_{i \in I} q^n(t).$$

By a.e. convergence we obtain hence for a.e.  $t \in (0, 1)$

$$q^\infty(t) \leq \max_{i \in I} q^\infty(t).$$

By again employing Corollary 4.3.4 and Proposition 4.3.2 together with left-continuity of  $q^\infty$  we get that  $q^\infty$  is indeed the horizontal lower median. Since every subsequence contains a convergence subsequence converging to the horizontal lower median, the same is true for the whole sequence.  $\square$

We are ready to prove the main theorem regarding the regularity of the horizontal selections.

**Theorem 4.3.9.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(\mathbb{R})$  and let  $q_\theta : \mathbb{R} \rightarrow [0, 1]$  given by (4.3.6) for  $\theta \in [0, 1]$ . If  $\nu_1, \dots, \nu_N$  are all absolutely continuous with densities  $f_1, \dots, f_N \in L^p(\mathbb{R})$  with  $p \in (1, \infty]$  then  $\mu^\theta$ , the measure given by  $q_\theta$ , is absolutely continuous with density  $f_{\mu^\theta} \in L^p(\mathbb{R})$ , and the following quantitative estimate on the  $L^p$ -norm of the density holds*

$$\|f_{\mu^\theta}\|_{L^p(\mathbb{R})} \leq \sum_{i=1}^N \|f_i\|_{L^p(\mathbb{R})}. \quad (4.3.8)$$

*Proof.* We apply a similar strategy to the one in the proof of Theorem 4.3.7 but with the additional assumption that all the sample measures have connected support and on their support  $F'_i = f_i > 0$  a.e. This implies (see for instance [12, 5.8.52]) that all the qdfs are absolutely continuous on  $[a, b]$  with  $[a, b] \subset (0, 1)$ . Using the same argument as in the proof of Theorem 4.3.7, we find that for  $\theta \in \{0, 1\}$  the horizontal median  $q_\theta$  is absolutely continuous on any closed interval  $[a, b] \subset (0, 1)$ . Therefore, since  $q_\theta = \theta q_+ + (1 - \theta)q_-$ , the same holds for any  $\theta \in [0, 1]$ . This implies (by again employing [12, 5.8.52]) absolute continuity of the respective cdfs on compact intervals, and hence absolute continuity of the median measure.

Now fix  $\theta \in \{0, 1\}$  and let us denote by  $\mu^\theta$  the corresponding Wasserstein median and  $F_{\mu^\theta}$  its cdf. In order to give an  $L^p$  estimate on the derivative almost everywhere of  $F_{\mu^\theta}$ , which we call  $f_{\mu^\theta}$  note that for almost every  $t \in (0, 1)$   $q'_i(t) = [f_i(q_i(t))]^{-1}$  for all  $i \in \{1, \dots, N\}$  and  $q'_\theta(t) = [f_{\mu^\theta}(q_\theta(t))]^{-1}$ . Therefore, using point 4. of Lemma 4.3.5, we get

$$f_{\mu^\theta}(q_\theta(t)) = \frac{1}{q'_\theta(t)} \leq \frac{1}{\min_{\mathcal{I}_0(t)} \{q'_i(t)\}} \leq \max_{i \in \mathcal{I}_0(t)} \{f_i(q_i(t))\} \quad \text{for a.e. } t \in (0, 1), \quad (4.3.9)$$

where  $\mathcal{I}_0(t) = \{i \in \{1, \dots, N\} \mid q_i(t) = q_\theta(t)\}$ . Let us denote by  $\mathcal{A}$  the set of full measure where (4.3.9) holds. Since  $q_\theta$  satisfies Lusin's property,  $q_\theta(\mathcal{A})$  has full measure. Then, using that  $q_\theta(F_{\mu^\theta}(x)) = x$ , for all  $x \in q_\theta(\mathcal{A})$  we obtain

$$f_{\mu^\theta}(x) \leq \max_{i \in \mathcal{I}_0(F_{\mu^\theta}(x))} \{f_i(q_i(F_{\mu^\theta}(x)))\} \leq \max_{1 \leq i \leq N} \{f_i(x)\},$$

where we used that  $q_i(F_{\mu^\theta}(x)) = q_\theta(F_{\mu^\theta}(x)) = x$  for all  $i \in \mathcal{I}_0(F_{\mu^\theta}(x))$ . Hence we get the desired  $L^p$  estimate for  $\theta \in \{0, 1\}$ .

To get rid of the additional assumption on the support of the sample measures we use an approximation argument. Let  $\mathbf{g}$  be the standard Gaussian measure on  $\mathbb{R}$  and introduce the following approximating sequences:

$$\nu_i^n := \left(1 - \frac{1}{n}\right) \nu_i + \frac{1}{n} \mathbf{g} \quad \forall i \in \{1, \dots, N\}, \quad \forall n \in \mathbb{N}^*.$$

We have that  $(\nu_i^n)_{n \in \mathbb{N}^*}$  is a sequence of absolutely continuous measures with connected support and positive density  $\mathcal{L}^1$ -a.e. which converges in  $W_1$  to  $\nu_i$  for every  $i$ . The upper (resp. lower) horizontal Wasserstein median  $\nu^n$  of  $(\nu_1^n, \nu_2^n, \dots, \nu_N^n)$  is absolutely continuous for all  $n \in \mathbb{N}^*$ , let us call its density  $f^n$ . By Lemma 4.3.8 the sequence  $(\nu^n)_{n \in \mathbb{N}^*}$  converges to the upper (resp. lower) median of  $(\nu_1, \dots, \nu_N)$ . We also have that for any  $n$  the estimate (4.3.8) holds. Therefore we have

$$\|f^n\|_p \leq \sum_{i=1}^N \left\| \left(1 - \frac{1}{n}\right) f_i + \frac{1}{n} g \right\|_p \leq \left(1 - \frac{1}{n}\right) \sum_{i=1}^N \|f_i\|_p + \frac{1}{n} \|g\|_p.$$

Hence  $(f^n)_{n \in \mathbb{N}^*}$  converges weakly-\* (i.e. in  $\sigma(L^p(\mathbb{R}), L^{\frac{p}{p-1}}(\mathbb{R}))$ ) and using that the  $L^p$  norm is lower semicontinuous with respect to the weak-\* convergence then we get (4.3.8). In the general case for  $\theta \in (0, 1)$  the  $L^p$ -bound on  $f_{\mu^\theta}$  follows from Lemma 4.3.10 with  $V(x) = x^p$ .  $\square$

The hypothesis of the following lemma is reminiscent of McCann's condition for displacement convexity, which boils down to convexity of the function inside the integral in 1D as specified below. This is not at all surprising, indeed the horizontal medians correspond to McCann's displacement interpolation between the horizontal lower and upper median.

**Lemma 4.3.10.** *Let  $V : [0, \infty) \rightarrow \mathbb{R}$  be a convex function. Then in the setting of Theorem 4.3.9*

$$\int_{\mathbb{R}} V(f_{\mu^\theta}(x)) dx \leq \theta \int_{\mathbb{R}} V(f_+(x)) dx + (1 - \theta) \int_{\mathbb{R}} V(f_-(x)) dx.$$

*Proof.* First, note that since  $V$  is convex implies  $\phi : (0, \infty) \ni t \mapsto tV(t^{-1})$  convex as well. Indeed,  $\phi$  coincides with the perspective function of  $V$ ,  $P : (0, \infty) \times [0, \infty) \rightarrow \mathbb{R}$ ,  $P(t, x) \mapsto tV(xt^{-1})$ , evaluated at  $(t, 1)$ . This is convex by for instance Proposition 8.25 [8]. We now have the following estimate

$$\begin{aligned} \int_{\mathbb{R}} V(f_{\mu^\theta}(x)) dx &= \int_0^1 V(q'_\theta(t)^{-1})q'_\theta(t) dt \\ &\leq \int_0^1 \theta V(q'_+(t)^{-1})q'_+(t) + (1 - \theta)V(q'_-(t)^{-1})q'_-(t) dt \\ &= \theta \int_{\mathbb{R}} V(f_+(x)) dx + (1 - \theta) \int_{\mathbb{R}} V(f_-(x)) dx, \end{aligned}$$

where in the inequality we have used convexity of  $\phi$ .  $\square$

*Remark 4.3.11.* Note that, in contrast to the Wasserstein barycenter case, we need regularity of the whole sample to guarantee existence of a regular Wasserstein median. Counterexamples can be easily designed even in 1D. Furthermore, the estimates (4.3.7) and (4.3.8) are only valid in dimension one, see Example 4.4.9 for a counterexample to  $L^p$  bounds in higher dimensions.

## 4.4 Multi-marginal and dual formulations

### 4.4.1 Multi-marginal formulation

An important feature of Wasserstein medians is that (M) admits a multi-marginal reformulation, which, as we shall detail in the following, enlightens a connection with the median problem on  $(X, d)$ .

**Definition 4.4.1.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(X)$  and  $p_1, \dots, p_N$  positive weights such that  $p_1 + \dots + p_N = 1$ , the multi-marginal problem is given by*

$$\inf_{\rho, \gamma \in \Pi(\rho, \nu_1, \dots, \nu_N)} \int \sum_{i=1}^N p_i d(x, x_i) d\gamma(x, x_1, \dots, x_N), \quad (\text{MMP})$$

where  $\Pi(\rho, \nu_1, \dots, \nu_N)$  is the set of all Radon probability measures on  $X^{N+1}$  with marginals  $\rho, \nu_1, \dots, \nu_N$ . A slightly different variant is

$$\inf_{\gamma \in \Pi(\nu_1, \dots, \nu_N)} \int \inf_{x \in X} \sum_{i=1}^N p_i d(x, x_i) d\gamma(x_1, \dots, x_N). \quad (\overline{\text{MMP}})$$

The problems (MMP) and ( $\overline{\text{MMP}}$ ) can be proven to be equivalent to (M), as detailed in the following adaptation of Proposition 3 [33] for Wasserstein medians.

**Theorem 4.4.2.** *The following hold*

1.  $\inf(\text{M}) = \inf(\text{MMP}) = \inf(\overline{\text{MMP}})$ .
2. If  $\rho$  is a solution to (M), then there is  $\gamma \in \Pi(\rho, \nu_1, \dots, \nu_N)$  solving (MMP), and conversely, for an optimal solution  $\gamma$  of (MMP) the first marginal  $\pi_{0\#}\gamma$  is a Wasserstein median.
3. For any measurable function  $M_\lambda : X^N \rightarrow X$  such that for all  $(x_1, \dots, x_N) \in X^N$

$$M_\lambda(x_1, \dots, x_N) \in \arg \min_{x \in X} \sum_{i=1}^N p_i d(x, x_i), \quad (4.4.1)$$

and any  $\gamma$  that minimizes ( $\overline{\text{MMP}}$ ), the measure  $\rho := (M_\lambda)_\# \gamma$  is a Wasserstein median.

4. If  $\gamma$  is an optimal solution of (MMP), then  $\pi_{0,j\#}\gamma$  is an optimal transport plan between the corresponding marginals.

The proof is analogous to the one of Proposition [33]. Note however that there is not a straightforward generalization of point 3. in Proposition 3 [33] (corresponding to a converse of 3. here) to Wasserstein medians due to the fact that the set of minimizers in (4.4.1) is not in general single-valued.

This is not only a technicality: consider for instance  $X = [-1, 1]$  equipped with the usual Euclidean distance and let  $\nu_1 = \delta_{-1/2}$  and  $\nu_2 = \delta_{1/2}$  with uniform weights. Then  $\text{Med}_\lambda(\nu_1, \nu_2)$  is the set of all probability measures supported on  $[-1/2, 1/2]$  whereas if we take  $\gamma$  admissible for ( $\overline{\text{MMP}}$ ) then necessarily  $\gamma = \delta_{(-1/2, 1/2)}$  and the Wasserstein medians obtained with the above procedure are all discrete  $\rho = (M_\lambda)_\# \delta_{(-1/2, 1/2)} = \delta_{M_\lambda(-1/2, 1/2)} = \delta_c$  for some  $c \in [-1/2, 1/2]$ . It turns out, that a sufficient condition for the converse of 3. to hold is the following

**Property.** Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(X)$  and positive weights  $\mathbf{p} = (p_1, \dots, p_N)$  such that  $\sum_{i=1}^N p_i = 1$ , we say that there is *essentially one* function that satisfies (4.4.1) relative to  $\nu_1, \dots, \nu_N$  and  $\mathbf{p}$  if for all  $\gamma \in \text{Opt}(\overline{\text{MMP}})$

$$\text{if } M_\mathbf{p} \text{ and } M'_\mathbf{p} \text{ are measurable and satisfy (4.4.1) then } M_\mathbf{p} = M'_\mathbf{p} \gamma - a.e. \quad (4.4.2)$$

The following proposition further characterizes the structure of optimal solutions of the multi-marginal problems and establishes the converse of 3. in Theorem 4.4.2 under the assumption of *essential uniqueness* as stated in (4.4.2).

**Proposition 4.4.3.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(X)$ , let  $\mathbf{p} = (p_1, \dots, p_N)$  be positive weights such that  $\sum_{i=1}^N p_i = 1$ , and  $\rho \in \mathcal{P}(X)$  be a Wasserstein median. Let  $\gamma \in \Pi(\rho, \nu_1, \dots, \nu_N)$  be an optimal solution to (MMP) associated to  $\rho$ . We have the following*

1. *For  $\gamma$ -almost every  $(x, x_1, \dots, x_N) \in X^{N+1}$  there is  $M_\lambda$  which satisfies (4.4.1) such that*

$$x = M_\lambda(x_1, \dots, x_N). \quad (4.4.3)$$

2. *If there exists essentially one function  $M_\lambda$  that satisfies (4.4.1) relative to  $\nu_1, \dots, \nu_N$  and  $\mathbf{p}$ , then for any Wasserstein median  $\rho \in \mathcal{P}(X)$  there exists an optimal solution  $\gamma$  to (MMP) such that  $\rho = (M_\lambda)_\# \gamma$ .*

*Proof.* Let us start from point 1. Denote by  $\eta$  the projection of  $\gamma$  onto the last  $N$  components. We have that

$$\inf(\mathbf{M}) = \int \sum_i p_i d(x, x_i) d\gamma \geq \int \inf_y \sum_i p_i d(y, x_i) d\eta \geq \inf(\mathbf{M}). \quad (4.4.4)$$

The latter inequality is due to the fact that  $\eta$  is feasible for (MMP). (4.4.4) yields that

$$\sum_i p_i d(x, x_i) = \inf_y \sum_i p_i d(y, x_i) \quad \gamma - a.e.$$

Hence there is  $M_\lambda$  which satisfies (4.4.1) such that (4.4.3) holds. Let us now discuss point 2. Let  $\rho$  be a Wasserstein median and  $\gamma$  an optimal solution to (MMP) associated to  $\rho$ . Let us denote by  $\eta$  the projection of  $\gamma$  onto the last  $N$  components. Note that in (4.4.4) we proved that  $\eta$  is optimal for (MMP). By 1. and the *essential uniqueness* of  $M_\lambda$  we have that the support of  $\gamma$  is included in the graph of  $M_\lambda$ . It follows that  $\gamma = (M_\lambda, Id)_\# \eta$ , and specifically that  $\rho = (\pi_0)_\# (M_\lambda, Id)_\# \eta = (M_\lambda)_\# \eta$ .  $\square$

Theorem 4.4.2 and Proposition 4.4.3 entail the following interesting applications.

**Corollary 4.4.4.** *Let  $X = \mathbb{R}^d$ . If all the sample measures are supported on a convex subset  $\mathcal{K} \subset \mathbb{R}^d$ , then every Wasserstein median  $\rho \in \text{Med}_\lambda(\nu_1, \dots, \nu_N)$  is supported on  $\mathcal{K}$  too. Moreover, for  $p \geq 1$  we have the following bound on the  $p$ -moments:*

$$\int_{\mathbb{R}^d} |x|^p d\rho \leq \sum_{i=1}^N \int_{\mathbb{R}^d} |x|^p d\nu_i \quad \forall \rho \in \text{Med}_\lambda(\nu_1, \dots, \nu_N). \quad (4.4.5)$$

*Proof.* The first claim follows directly from (4.4.3) and the convexity of  $\mathcal{K}$ . Now, pick  $\rho \in \text{Med}_\lambda(\nu_1, \dots, \nu_N)$  and let  $\gamma$  the optimal solution to (MMP) given by point 2. in Theorem 4.4.2. By (4.4.3) for  $\gamma$ -almost every  $(x, x_1, \dots, x_N)$  the first component  $x$  can be written as a convex combination of the latter  $N$  components  $x_1, \dots, x_N$ . In particular, we have by convexity of  $|\cdot|^p$

$$|x|^p \leq \sum_{i=1}^N |x_i|^p \quad \text{for } \gamma - a.e. (x, x_1, \dots, x_N) \in (\mathbb{R}^d)^N.$$

Integrating over  $\gamma$  we get (4.4.5).  $\square$

The following corollary improves the results in Theorems 4.1.2 and 4.2.2 by passing from the narrow topology to the topology induced by the Wasserstein distance.

**Corollary 4.4.5.** *Let  $\mathbf{p}^n = (p_1^n, \dots, p_N^n)_{n \in \mathbb{N}}$  with  $\sum_{i=1}^N p_i^n = 1$  be a sequence in  $[0, 1]^N$  converging to  $\mathbf{p} = (p_1, \dots, p_N)$  and  $(\nu_1^n)_{n \in \mathbb{N}}, \dots, (\nu_N^n)_{n \in \mathbb{N}}$  be sequences converging to  $(\nu_1, \dots, \nu_N)$  in  $(\mathcal{P}_1(X), W_1)$ . Then any sequence  $\rho^n \in \text{Med}_\lambda(\nu_1^n, \dots, \nu_N^n)$  admits a subsequence that converges in  $(\mathcal{P}_1(X), W_1)$  to a weighted median of  $\nu_1, \dots, \nu_N$ . In particular,  $\text{Med}_\lambda(\nu_1, \dots, \nu_N)$  is a convex compact subset of  $(\mathcal{P}_1(\Omega), W_1)$ .*

*Proof.* Let  $\rho^n \in \text{Med}_\lambda(\nu_1^n, \dots, \nu_N^n)$ , as in the proof of Corollary 4.4.4 we consider  $\gamma^n \in \Pi(\rho^n, \nu_1^n, \dots, \nu_N^n)$  an optimal solution to (MMP) associated  $\rho^n$ . By point 1. of Proposition 4.4.3 we have that for  $\gamma^n$ -almost every  $(x, x_1, \dots, x_N)$  the first component  $x$  can be written as convex combination of  $x_1, \dots, x_N$ . Thus, we have for  $C > 0$  by quasi-convexity of  $y \mapsto |y| \mathbf{1}_{\{|y| \geq C\}}$  that

$$|x| \mathbf{1}_{\{|x| \geq C\}} \leq \sum_{i=1}^N |x_i| \mathbf{1}_{\{|x_i| \geq C\}}.$$

Integrating with respect to  $\gamma^n$  we get

$$\int_{\Omega} |x| \mathbf{1}_{\{|x| \geq C\}} d\rho^n \leq \sum_{i=1}^N \int_{\Omega} |x_i| \mathbf{1}_{\{|x_i| \geq C\}} d\nu_i^n \quad \forall n, C > 0.$$

The right-hand-side is uniformly bounded by the uniform integrability of  $(\nu_i^n)_{n \in \mathbb{N}}$  for all  $i \in \{1, \dots, N\}$ , thus, the sequence  $(\rho^n)_{n \in \mathbb{N}}$  is uniformly integrable, too. Together with being narrowly precompact by Theorem 4.2.2, it is also precompact with respect to the topology induced by  $W_1$  by Proposition 7.1.5 [7].

The same argument yields precompactness of  $\text{Med}_\lambda(\nu_1, \dots, \nu_N)$  and hence compactness by Theorem 4.1.2.  $\square$

**Corollary 4.4.6.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(X)$  and  $p_1, \dots, p_N$  be positive weights that sum to one. If there exists  $j \in \{1, \dots, N\}$  such that  $p_j > 1/2$ , then the Wasserstein median of  $(\nu_1, \dots, \nu_N)$  is unique and coincides with  $\nu_j$ .*

*Proof.* Let  $\rho$  be a weighted median of  $(\nu_1, \dots, \nu_N)$ . By a straightforward application of the triangle inequality applied to the metric  $d$  of  $X$  there exists a unique function  $M_\lambda$  such that (4.4.1) holds, and it is equal to

$$M_\lambda(x_1, \dots, x_N) = x_j \quad \forall (x_1, \dots, x_N) \in X^N,$$

which coincides with the projection onto the  $j^{\text{th}}$  factor.

Indeed, suppose w.l.o.g. that  $p_N > \frac{1}{2}$ . Assume that a weighted median of  $(x_1, \dots, x_N) \in X$  is given by  $\bar{x} \neq x_N$ , i.e.

$$\bar{x} \in \arg \min_{x \in X} \sum_{i=1}^N p_i d(x, x_i).$$

But then

$$\sum_{i=1}^N p_i d(x_N, x_i) = \sum_{i=1}^{N-1} p_i d(x_N, x_i) \leq \sum_{i=1}^{N-1} p_i [d(x_N, \bar{x}) + d(\bar{x}, x_i)] < \sum_{i=1}^N p_i d(\bar{x}, x_i),$$

contradicting minimality of  $\bar{x}$ .

Now by point 2. of Proposition 4.4.3, every Wasserstein median  $\rho$  is given by  $\rho = (\mathbb{M}_\lambda)_\# \gamma$ , where  $\gamma \in \Pi(\nu_1, \dots, \nu_N)$  is an optimal solution to (MMP). Since  $\gamma \in \Pi(\nu_1, \dots, \nu_N)$  we get  $\rho = (\pi_j)_\# \gamma = \nu_j$ .  $\square$

*Remark 4.4.7.* The case of two measures is a somewhat remarkable special case of this threshold effect. Indeed, as soon as  $p_1 > p_2$  the measure  $\nu_1$  is the unique median. On the other hand, in case of equality of the weights  $p_1 = p_2 = \frac{1}{2}$  any point on a  $W_1$ -geodesic between  $\nu_1$  and  $\nu_2$  is a median since by reparametrizing to a constant-speed geodesic it can be seen that it saturates the triangular inequality. And vice versa, if  $\rho$  is a Wasserstein median, then it lies on a geodesic curve. Indeed just concatenate two properly rescaled constant speed geodesics between  $\rho$  and  $\nu_1$  and between  $\rho$  and  $\nu_2$  and use  $W_1(\nu_1, \nu_2) = W_1(\nu_1, \rho) + W_1(\rho, \nu_2)$ .

*Remark 4.4.8.* In fact, the result of Corollary 4.4.6 can be directly proved by using the triangle inequality of  $W_1$ . Nevertheless, we decided to keep this proof because using the same argument enables us to lift certain properties of the weighted median on  $X$  to the Wasserstein median.

We also use this strategy in Example 4.4.9 to show that the  $L^\infty$ -norm of a Wasserstein median (if it is finite) cannot depend linearly on the  $L^\infty$ -norms of the given measures  $\nu_1, \dots, \nu_N$ . This is in contrast to what is true for Wasserstein barycenters (see Theorem 5.1 [1]).

**A counterexample to regularity.** Unlike the case of Wasserstein barycenters, in the case of Wasserstein medians it is not sufficient that one of the given measures is regular, say absolutely continuous or  $L^\infty$ , for a median to inherit this property. One can construct counterexamples in the one dimensional case. If all of the given measures have  $L^p$ -integrable densities, then this carries over to a median in one dimension in some cases, see Section 4.3. The situation seems to be more intricate in higher dimension. The following example shows that a linear  $L^\infty$ -bound cannot hold.

*Example 4.4.9.* Take four absolutely continuous measures with bounded density on  $\mathbb{R}^2$  as follows. For  $0 < \epsilon < 1$  define  $\nu_1$  by its density  $\frac{1}{\epsilon} \mathbf{1}_{[1,2] \times [-\frac{\epsilon}{2}, \frac{\epsilon}{2}]}$ , and the other three measures are obtained by successive rotation by  $90^\circ$ , see Figure 4.5. By using the multi-marginal formulation, we show that any uniform (i.e. with uniform weights) Wasserstein median has to be concentrated on a set of Lebesgue measure of order  $\epsilon^2$ , and hence, even if it is absolutely continuous with respect to the Lebesgue measure, its density cannot have a linear dependence of the  $L^\infty$ -bound of the given measures.

For this observe that by Theorem 4.4.2 any Wasserstein median  $\rho$  with a corresponding optimal multi-marginal plan  $\gamma$  satisfies that  $x$  is a geometric median of  $(x_1, \dots, x_4)$  for  $\gamma$ -a.e.  $(x, x_1, \dots, x_4)$ .

Now note that with this construction four points  $x_i \in \text{spt } \nu_i$  with  $i = 1, \dots, 4$  always form a convex quadrilateral, and hence their unique median is the intersection of the two segments generated by  $x_1, x_3$  and  $x_2, x_4$ . This follows from what is known for geometric medians in two dimensions, see for instance Theorem 1.1.2 (c) [37]. It is easy to see that all these intersections happen in the square  $[-\frac{\epsilon}{2}, \frac{\epsilon}{2}]^2$ , yielding that  $\text{spt } \rho \subset [-\frac{\epsilon}{2}, \frac{\epsilon}{2}]^2$ .

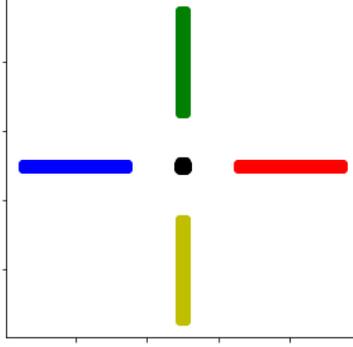


Figure 4.5 – Schematic depiction of the support of the four measures  $\nu_i$  from Example 4.4.9 in colors and admissible support of any Wasserstein median in black

#### 4.4.2 Dual formulation

To introduce the dual formulation of (M) we fix a point  $x_0 \in X$  and define the spaces

$$Y_0 := \left\{ f \in C(X) : \lim_{d(x, x_0) \rightarrow \infty} \frac{f(x)}{1 + d(x, x_0)} = 0 \right\},$$

$$Y_b := \left\{ f \in C(X) : \sup_{x \in X} \frac{f(x)}{1 + d(x, x_0)} < \infty \right\}.$$

Note that the space is independent of the choice  $x_0$  and that the dual is

$$(Y_0)^* =: \mathcal{M}_1(X) = \{ \mu \in \mathcal{M}(X) : (1 + d(x, x_0))\mu \in \mathcal{M}(X) \}.$$

With this at hand, we define the following problem (which is strictly speaking the pre-dual of (M))

$$\sup \left\{ \sum_{i=1}^N \int_X \varphi_i^{c_i} d\nu_i : \varphi_i \in Y_0, \sum_{i=1}^N \varphi_i = 0 \right\}, \quad (\text{M}_0^*)$$

where  $\varphi_i^{c_i}$  is the  $c_i$ -transform of  $\varphi_i$  for  $c_i = p_i d$ , that is defined as  $\varphi_i^{c_i}(y) := \inf_{x \in X} p_i d(x, y) - \varphi_i(x)$  for all  $y \in X$  and  $i = 1, \dots, N$ , and its relaxed version

$$\sup \left\{ \sum_{i=1}^N \int_X \varphi_i^{c_i} d\nu_i : \varphi_i \in Y_b, \sum_{i=1}^N \varphi_i = 0 \right\}. \quad (\text{M}^*)$$

By definition of the  $c_i$ -transform we clearly have the following weak duality relation

$$\inf (\text{M}) \geq \sup (\text{M}^*) \geq \sup (\text{M}_0^*).$$

With a standard argument, we can establish a strong duality and an existence result.

**Proposition 4.4.10.** *We have that  $\inf (\text{M}) = \sup (\text{M}^*) = \sup (\text{M}_0^*)$ . Moreover, there exists a minimizer of  $(\text{M}^*)$ .*

The proof is essentially the same as the proof of Proposition 2.2 and 2.3 in [1] for the Wasserstein barycenter case. Moreover, in the proof we can also notice that we can always consider  $N - 1$  potentials to be  $c_i$ -concave, with  $c_i = p_i d$ , i.e.,  $\varphi_i = \varphi_i^{c_i}$ , which, thanks to the following lemma, actually means Lipschitz in our context.

**Lemma 4.4.11.** *Let  $\lambda > 0$  and let  $c = \lambda d$ , if  $\varphi : X \rightarrow \mathbb{R}$  is  $c$ -concave then  $\varphi$  is  $\lambda$ -Lipschitz. We write  $\varphi \in \text{Lip}_\lambda(X)$ . Moreover,  $\varphi^c = -\varphi$ .*

For a proof, see for instance Proposition 3.1 [104].

If we want all the optimal potentials to be Lipschitz, then we have to relax the constraint, as shown in the following.

**Proposition 4.4.12.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(X)$  and  $p_1, \dots, p_N$  be positive weights such that  $\sum_{i=1}^N p_i = 1$ . Define the following*

$$\sup \left\{ \sum_{i=1}^N \int_X \psi_i d\nu_i \mid \psi_i \in \text{Lip}_{p_i}(X), i = 1, \dots, N, \sum_{i=1}^N \psi_i \leq 0 \right\}. \quad (\text{ML}^*)$$

We have the following equivalence

$$\inf(\mathbf{M}) = \sup(\mathbf{M}_0^*) = \sup(\mathbf{M}^*) = \sup(\text{ML}^*).$$

Moreover, the right hand side has a global maximizer and it can be derived from the solution of  $(\mathbf{M}^*)$  taking the  $c_i$ -concavification of each  $\psi_i$ .

*Proof.* We prove that  $\sup(\mathbf{M}^*) \geq \sup(\text{ML}^*)$  and then  $\sup(\text{ML}^*) \geq \sup(\mathbf{M}^*)$ . Let  $(\psi_1, \dots, \psi_N)$  be admissible for  $(\text{ML}^*)$  and define

$$\varphi = (\varphi_1, \dots, \varphi_N) := \left( -\psi_1, \dots, -\psi_{N-1}, \sum_{n=1}^{N-1} \psi_n \right).$$

Clearly,  $\varphi$  is admissible for  $(\mathbf{M}^*)$  and we have

$$\sum_{i=1}^N \int \psi_i d\nu_i = \sum_{i=1}^{N-1} \int (-\varphi_i) d\nu_i + \int \psi_N d\nu_N.$$

Since for every  $i = 1, \dots, N-1$  it holds  $\varphi_i \in \text{Lip}_{p_i}(X)$ , thanks to Lemma 4.4.11 we have  $-\varphi_i = \varphi_i^{c_i}$ . For  $i = N$ , we have

$$\varphi_N = \sum_{n=1}^{N-1} \psi_n \leq -\psi_N,$$

thus,  $\varphi_N^{c_N} \geq \psi_N$ . Putting all together we get

$$\sum_{i=1}^N \int \psi_i d\nu_i \leq \sum_{i=1}^N \int \varphi_i^{c_i} d\nu_i.$$

This proves the first inequality. For the converse, let  $\varphi = (\varphi_1, \dots, \varphi_N)$  be admissible for  $(\mathbf{M}^*)$ . Consider

$$\psi = (\psi_1, \dots, \psi_N) = (\varphi_1^{c_1}, \dots, \varphi_N^{c_N}).$$

It follows that  $\psi$  is admissible for  $(\text{ML}^*)$  because  $\psi_i$  are all  $p_i$ -Lipschitz functions and we have:

$$\sum_{i=1}^N \int \psi_i(x) d\nu_i = \sum_{i=1}^N \int \varphi_i^{c_i}(x) d\nu_i = \sum_{i=1}^N \inf_{y \in X} \{p_i d(x, y) - \varphi_i(y)\} \leq - \sum_{i=1}^N \int \varphi_i(x) d\nu_i = 0.$$

The two objective functions, since  $\psi_i = \varphi_i^{c_i}$  for all  $i = 1, \dots, N$  coincide.  $\square$

The set of optimal points of  $(\text{ML}^*)$  is a convex subset of  $C(X)$  whose elements are called *Kantorovich potentials*. The reason is contained in the following.

**Theorem 4.4.13** (Optimality conditions). *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(X)$  and  $p_1, \dots, p_N$  be positive weights such that  $\sum_{i=1}^N p_i = 1$ . Let  $\rho \in \mathcal{P}_1(X)$ ,  $\gamma_i \in \Pi(\rho, \nu_i)$ ,  $\psi_i \in \text{Lip}_{p_i}(X)$  for all  $i \in \{1, \dots, N\}$ .*

*Then,  $\rho$  is a Wasserstein median,  $\gamma_i \in \Pi(\rho, \nu_i)$  are OT plans for all  $i \in \{1, \dots, N\}$ , and  $(\psi_1, \dots, \psi_N)$  solve  $(\text{ML}^*)$  if and only if they satisfy the following system of Primal-Dual conditions*

1. *For all  $i \in \{1, \dots, N\}$ , it holds  $\psi_i(y) - \psi_i(x) = p_i d(x, y)$  for  $\gamma_i$ -almost every  $(x, y) \in X^2$ .*

2. *It holds that:*

$$\sum_{i=1}^N \psi_i \leq 0, \quad \sum_{i=1}^N \psi_i = 0 \quad \rho - \text{a.e.}$$

Moreover,  $\psi_i/p_i \in \text{Lip}_1(X)$  are optimal Kantorovich potentials for the OT problem with cost function  $c = d$  between  $\nu_i$  and  $\rho$  for all  $i \in \{1, \dots, N\}$ .

*Proof.* Let  $\rho$  be a Wasserstein median,  $(\psi_1, \dots, \psi_N)$  an optimal solution to the dual problem  $(\text{ML}^*)$  and  $\gamma_i \in \Pi(\rho, \nu_i)$  optimal transportation plans. By duality (Proposition 4.4.12) we have

$$\sum_{i=1}^N \int_{X^2} p_i d(x, y) d\gamma_i(x, y) = \sum_{i=1}^N \int_X \psi_i d\nu_i, \quad \text{thus, } \sum_{i=1}^N \int_{X^2} \left( p_i d(x, y) - \psi_i(y) \right) d\gamma_i(x, y) = 0.$$

Since  $\psi_i$  is  $p_i$ -Lipschitz for all  $i \in \{1, \dots, N\}$ , and  $\sum_i \psi_i \leq 0$  we have

$$0 \leq - \int \sum_{i=1}^N \psi_i(x) d\rho(x) \leq \sum_{i=1}^N \int_{X^2} \left( p_i d(x, y) - \psi_i(y) \right) d\gamma_i(x, y) = 0.$$

Hence  $\sum_{i=1}^N \psi_i = 0$   $\rho$ -a.e. It follows that

$$\sum_{i=1}^N \int_{X^2} \left( p_i d(x, y) - \psi_i(y) + \psi_i(x) \right) d\gamma_i(x, y) = 0,$$

and since  $\psi_i \in \text{Lip}_{p_i}(X)$  we have  $p_i d(x, y) + \psi_i(x) - \psi_i(y) \geq 0$ , which implies 1. For the 'if'-part suppose that  $\psi_i$  are  $p_i$ -Lipschitz functions which satisfy 1. and 2. Then the latter equation is true, and by the weak duality we obtain optimality. The fact that  $\psi_i/p_i$  are Kantorovich potentials between  $\nu_i$  and  $\rho$  follows immediately from 1.  $\square$

## 4.5 Beckmann minimal flow formulation

In this section, we consider the median problem on a compact convex domain  $\bar{\Omega} \subset \mathbb{R}^d$ .

### 4.5.1 The Beckmann problem

**Definition 4.5.1.** Let  $\nu_1, \dots, \nu_N \in \mathcal{P}_1(\bar{\Omega})$  and  $p_1, \dots, p_N$  be positive weights such that  $\sum_{i=1}^N p_i = 1$ . The Beckmann minimal flow problem consists of minimizing the weighted sum of the total variation norm of  $\sigma_1, \dots, \sigma_N$  satisfying an appropriate divergence constraint, namely

$$\inf_{(\sigma_1, \dots, \sigma_N, \rho) \in \mathcal{M}_{\text{div}}(\bar{\Omega}, \mathbb{R}^d)^N \times \mathcal{P}(\bar{\Omega})} \left\{ \sum_{i=1}^N p_i \|\sigma_i\|_{\text{TV}} : \nabla \cdot \sigma_i + \nu_i = \rho, i \in \{1, \dots, N\} \right\}, \quad (\text{MB})$$

where  $\|\cdot\|_{\text{TV}}$  is the total variation norm. Here the divergence operator is to be intended in the weak sense with zero Neumann boundary conditions. More precisely, for all  $i \in \{1, \dots, N\}$  we write  $\nabla \cdot \sigma_i + \nu_i = \rho$  in short if for all  $\phi \in C^1(\bar{\Omega})$

$$- \int_{\bar{\Omega}} \nabla \phi \cdot d\sigma_i + \int_{\bar{\Omega}} \phi d\nu_i = \int_{\bar{\Omega}} \phi d\rho.$$

Each admissible  $\sigma_i$  is called transport flow from  $\rho$  to  $\nu_i$ .

The Beckmann problem is equivalent to the Wasserstein median problem, as detailed in the following theorem.

**Theorem 4.5.2.** Let  $\nu_1, \dots, \nu_N \in \mathcal{P}(\bar{\Omega})$ ,  $\mathbf{p} = (p_1, \dots, p_N)$  be positive weights such that  $\sum_{i=1}^N p_i = 1$ . Then (MB) admits a solution and  $\inf(\text{MB}) = \inf(\text{M})$ . Furthermore,  $\rho$  is a Wasserstein median if and only if there are transport flows  $(\sigma_i)_{i=1}^N$  such that  $(\sigma_1, \dots, \sigma_N, \rho)$  is an optimal solution to (MB).

*Proof.* For all  $i \in \{1, \dots, N\}$ , we know from e.g. Theorem 4.6 [104] that

$$W_1(\rho, \nu_i) = \inf_{\sigma_i \in \mathcal{M}_{\text{div}}(\bar{\Omega}, \mathbb{R}^d)} \{ \|\sigma_i\|_{\text{TV}} : \nabla \cdot \sigma_i + \nu_i = \rho \}. \quad (4.5.1)$$

Hence, the Wasserstein median problem rewrites

$$\begin{aligned} \inf(\text{M}) &= \inf_{\rho \in \mathcal{P}_1(\bar{\Omega})} \sum_{i=1}^N p_i W_1(\rho, \nu_i), \\ &= \inf_{\rho \in \mathcal{P}_1(\bar{\Omega})} \sum_{i=1}^N p_i \inf_{\sigma_i \in \mathcal{M}_{\text{div}}(\bar{\Omega}, \mathbb{R}^d)} \{ \|\sigma_i\|_{\text{TV}} : \nabla \cdot \sigma_i + \nu_i = \rho \} \\ &= \inf_{(\sigma_1, \dots, \sigma_N, \rho) \in \mathcal{M}_{\text{div}}(\bar{\Omega}, \mathbb{R}^d)^N \times \mathcal{P}(\bar{\Omega})} \left\{ \sum_{i=1}^N p_i \|\sigma_i\|_{\text{TV}} : \nabla \cdot \sigma_i + \nu_i = \rho, i \in \{1, \dots, N\} \right\} \\ &= \inf(\text{MB}). \end{aligned}$$

For existence, fix a Wasserstein median  $\rho$  and note that Theorem 4.6 [104] also provides existence of a transport flow  $\sigma_i$  for the Beckmann flow problem between  $\rho$  and  $\nu_i$ . By optimality the vector  $(\sigma_1, \dots, \sigma_N, \rho)$  is a solution for (MB). This also proves that if  $(\sigma_1^*, \dots, \sigma_N^*, \rho^*)$  is an optimal solution to (MB), then  $\rho^* \in \text{Med}_{\mathbf{p}}(\nu_1, \dots, \nu_N)$ .  $\square$

Note that if we fix a Wasserstein median  $\rho \in \mathcal{P}(\Omega)$ , then (MB) totally decouples in  $N$  optimal transport problems according to (4.5.1). Therefore, all the classical theory on

the flow formulation of Optimal Transport applies here. An overview of this theory can be found in Sections 4.2 [104]. For instance, given an OT plan  $\gamma_i$  from  $\rho$  to  $\nu_i$  we can find an optimal transport flow  $\sigma_{\gamma_i}$  defined as follows (see proof of Theorem 4.6 [104])

$$\langle \sigma_{\gamma_i}, \theta \rangle := \int_{\overline{\Omega} \times \overline{\Omega}} \int_0^1 \theta((1-t)x + ty)(y-x) dt d\gamma_i(x, y), \quad (4.5.2)$$

for every  $\theta \in C(\overline{\Omega}, \mathbb{R}^d)$ , and we can call transportation density the quantity  $\eta_{\gamma_i}$

$$\langle \eta_{\gamma_i}, \phi \rangle := \int_{\overline{\Omega} \times \overline{\Omega}} \int_0^1 \phi((1-t)x + ty)|y-x| dt d\gamma_i(x, y). \quad (4.5.3)$$

for every  $\phi \in C(\Omega)$ . The two quantities are related in the following sense. Let  $\varphi_i$  be a Kantorovich potential from  $\rho$  to  $\nu_i$ , then

$$\sigma_{\gamma_i} = -\nabla \varphi_i \eta_{\gamma_i}. \quad (4.5.4)$$

Note that this expression is well-defined because by the theory of transport rays from Section 3.1.3 [104] or more precisely Lemma 3.6 [104] and strong duality  $\varphi_i$  is differentiable at  $(1-t)x + ty$  for  $t \in (0, 1)$  and  $(x, y) \in \text{spt } \gamma_i$  with  $x \neq y$ .

The construction of optimal solutions to (MB) from optimal transportation plans in the sense of (4.5.2) can be generalized to the Wasserstein median setup by considering the vector valued measure  $\sigma_\gamma = ((\sigma_\gamma)_1, \dots, (\sigma_\gamma)_N) \in \mathcal{M}(\overline{\Omega}, \mathbb{R}^d)^N$  for given  $\rho \in \mathcal{P}(\Omega)$  and  $\gamma \in \Pi(\rho, \nu_1, \dots, \nu_N)$  defined by

$$\langle \sigma_\gamma, \theta \rangle := \int_{\overline{\Omega}^{N+1}} \left( \sum_{j=1}^N \int_0^1 \theta_j((1-t)x + tx_j)(x_j - x) dt \right) d\gamma(x, x_1, \dots, x_N), \quad (4.5.5)$$

for each  $\theta \in C(\overline{\Omega}, \mathbb{R}^d)^N$ . The corresponding transport density is defined analogous to (4.5.3) as  $\eta_\gamma \in \mathcal{M}(\overline{\Omega}, \mathbb{R})^N$  given by

$$\langle \eta_\gamma, \phi \rangle := \int_{\overline{\Omega}^{N+1}} \left( \sum_{j=1}^N \int_0^1 \phi_j((1-t)x + tx_j)|x_j - x| dt \right) d\gamma(x, x_1, \dots, x_N), \quad (4.5.6)$$

for  $\phi \in C(\overline{\Omega})^N$ . Let us now generalize the relation (4.5.4) to the Wasserstein median setting.

**Proposition 4.5.3.** *Let  $\rho \in \mathcal{P}(\overline{\Omega})$ , and  $\gamma \in \Pi(\rho, \nu_1, \dots, \nu_N)$  such that  $(\rho, \gamma)$  is optimal for (MMP), then the transport flow  $\sigma_\gamma \in \mathcal{M}(\overline{\Omega}, \mathbb{R}^d)^N$  defined by (4.5.5) is an admissible optimal solution for (MB) and satisfies for any optimal Kantorovich potentials  $(\psi_1, \dots, \psi_N)$ , i.e. solutions of (ML\*)*

$$(\sigma_\gamma)_i = \frac{1}{p_i} \nabla \psi_i \cdot (\eta_\gamma)_i,$$

where  $\eta_\gamma \in \mathcal{M}(\overline{\Omega}, \mathbb{R})^N$  is the corresponding density from (4.5.6).

*Proof.* The proof goes along the lines of the proof of Theorem 4.6 [104] by noticing that the multi-marginal decouples to the bimarginal setting thanks to Theorem 4.4.2. To check

feasibility let us start computing  $\nabla \cdot (\sigma_\gamma)_i$  for  $i = 1, \dots, N$ . Denote  $\gamma_i = (\pi_{0,i})_\# \gamma$ . Then for  $\theta_i \in C^1(\Omega)$  we have

$$\begin{aligned} \langle \nabla \cdot (\sigma_\gamma)_i, \theta_i \rangle &= - \int_{\bar{\Omega}^2} \left( \int_0^1 \frac{d}{dt} \theta_i((1-t)x + tx_i)(x_i - x) dt \right) d\gamma_i(x, x_i) \\ &= - \int_{\bar{\Omega}^2} (\theta_i(x_i) - \theta_i(x)) d\gamma_i(x, x_i) = \int_{\bar{\Omega}} \theta_i d(\rho - \nu_i). \end{aligned}$$

This implies  $\nabla \cdot (\sigma_\gamma)_i + \nu_i = \rho$  in the weak sense for all  $i = 1, \dots, N$ . To prove optimality note that

$$\begin{aligned} \sum_{i=1}^N p_i \|(\sigma_\gamma)_i\|_{\text{TV}} &= \sum_{i=1}^N p_i \sup_{\substack{\theta_i \in C(\bar{\Omega}, \mathbb{R}^d), \\ \|\theta_i\|_{L^\infty(\Omega, \mathbb{R}^d)} \leq 1}} \langle (\sigma_\gamma)_i, \theta_i \rangle = \sum_{i=1}^N \sup_{\substack{\theta_i \in C(\bar{\Omega}, \mathbb{R}^d), \\ \|\theta_i\|_{L^\infty(\Omega, \mathbb{R}^d)} \leq 1}} \langle (\sigma_\gamma)_i, p_i \theta_i \rangle \\ &= \sup_{\substack{\theta_i \in C(\bar{\Omega}, \mathbb{R}^d), \\ \|\theta_i\|_{L^\infty(\Omega, \mathbb{R}^d)} \leq 1}} \langle ((\sigma_\gamma)_1, \dots, (\sigma_\gamma)_N), (p_1 \theta_1, \dots, p_N \theta_N) \rangle \\ &= \sup_{\substack{\theta_i \in C(\bar{\Omega}, \mathbb{R}^d), \\ \|\theta_i\|_{L^\infty(\Omega, \mathbb{R}^d)} \leq 1}} \int_{\bar{\Omega}^{N+1}} \left( \sum_{i=1}^N \int_0^1 p_i \theta_i((1-t)x + tx_i)(x_i - x) dt \right) d\gamma \\ &\leq \int_{\bar{\Omega}^{N+1}} \left( \sum_{j=1}^N p_j |x_j - x| \right) d\gamma(x, x_1, \dots, x_N) = \inf(\text{MMP}) = \inf(\text{MB}). \end{aligned}$$

Now let  $(\psi_1, \dots, \psi_n)$  be a solution of (ML\*). By Theorem 4.4.13 one observes that the  $c_i$ -transform  $\psi^{c_i}/p_i = -\psi_i/p_i$  (for  $c_i = p_i|\cdot - \cdot|$ ) is a Kantorovich potential from  $\rho$  to  $\nu_i$  w.r.t. the Euclidean distance for all  $i = 1, \dots, N$ . Hence using (4.5.4) we obtain (since  $(\eta_\gamma)_i = \eta_{\gamma_i}$  from (4.5.3))

$$(\sigma_\gamma)_i = \frac{1}{p_i} \nabla \psi_i \cdot (\eta_\gamma)_i.$$

□

Note that in the setting of Proposition 4.5.3, each component of  $\sigma_\gamma$  is the optimal transport flow from  $\rho$  to  $\nu_i$  according to (4.5.2) associated to the optimal transportation plan  $\gamma_i = (\pi_{0,i})_\# \gamma$ .

As in the classical transportation theory, the converse of Proposition 4.5.3 is true as well.

**Proposition 4.5.4.** *If  $\sigma = (\sigma_1, \dots, \sigma_N) \in \mathcal{M}_{\text{div}}(\bar{\Omega}, \mathbb{R}^d)^N$  and  $\rho \in \mathcal{P}(\bar{\Omega})$  are such that  $(\sigma_1, \dots, \sigma_N, \rho)$  is optimal for (MB), then there exists an optimal multi-marginal transportation plan  $\gamma \in \Pi(\rho, \nu_1, \dots, \nu_N)$  of (MMP) such that  $\sigma = \sigma_\gamma$ .*

*Proof.* As  $\sigma_i$  is an optimal transport flow from  $\rho$  to  $\nu_i$ , by Theorem 4.13 [104] there exists an optimal transportation plan  $\gamma_i \in \Pi(\rho, \nu_i)$  such that:  $\sigma_i = \sigma_{\gamma_i}$ . Using the Gluing Lemma (see e.g. Lemma 5.3.4 [7]) we obtain  $\gamma \in \Pi(\rho, \nu_1, \dots, \nu_N)$  such that:  $(\pi_{0,i})_\# \gamma = \gamma_i$  for all

$i = 1, \dots, N$ . Therefore for  $\boldsymbol{\theta} \in C(\overline{\Omega}, \mathbb{R}^d)^N$

$$\begin{aligned} \langle \boldsymbol{\sigma}, \boldsymbol{\theta} \rangle &= \sum_{i=1}^N \langle \boldsymbol{\sigma}_i, \boldsymbol{\theta}_i \rangle \\ &= \sum_{i=1}^N \int_{\overline{\Omega} \times \overline{\Omega}} \left( \int_0^1 \boldsymbol{\theta}_i((1-t)x + tx_i)(x_i - x) dt \right) d\gamma_i(x, x_i) \\ &= \int_{\overline{\Omega}^{N+1}} \left( \sum_{i=1}^N \int_0^1 \boldsymbol{\theta}_i((1-t)x - tx_i)(x_i - x) dt \right) d\boldsymbol{\gamma}(x, x_1, \dots, x_N) \end{aligned}$$

Hence  $\boldsymbol{\sigma} = \boldsymbol{\sigma}_\boldsymbol{\gamma}$ . Optimality of  $\boldsymbol{\gamma}$  follows from

$$\begin{aligned} \inf (\text{MMP}) &= \sum_{i=1}^N p_i W_1(\rho, \nu_i) \\ &= \sum_{i=1}^N p_i \int_{\overline{\Omega}^2} |x - x_i| d\gamma_i(x, x_i) \\ &= \int_{\overline{\Omega}^{N+1}} \sum_{i=1}^N p_i |x - x_i| d\boldsymbol{\gamma}(x, x_1, \dots, x_N). \end{aligned}$$

□

Relying on the theory on summability of the transport density, given in Theorem 4.14, Corollary 4.15, Theorem 4.16 and Theorem 4.20 in [104], we deduce the following one-sided higher regularity results.

**Theorem 4.5.5.** *Let  $\rho \in \mathcal{P}(\overline{\Omega})$  be a Wasserstein median. Then we have the following.*

- *If  $\nu_1, \dots, \nu_N \in \mathcal{P}(\overline{\Omega})$  are absolutely continuous, then the transportation flows  $\boldsymbol{\sigma}_i$  between  $\rho$  and  $\nu_i$  do not depend on the choice of the optimal transport plan  $\gamma_i$  between  $\rho$  and  $\nu_i$  and their corresponding transport densities  $\boldsymbol{\eta}_i$  are absolutely continuous.*
- *If furthermore  $\nu_1, \dots, \nu_N \in L^p(\Omega)$ , then if  $p < d' = d/(d-1)$ , the unique optimal transport density  $\eta_i$  associated to the transport from  $\rho$  to  $\nu_i$  belongs to  $L^p(\Omega)$  as well, and if  $p \geq d'$  it belongs to any space  $L^q(\Omega)$  for  $q < d'$ . By (4.5.4) this integrability carries over to the unique transportation flow  $\sigma_i$ .*

The significance of the previous Theorem is that if all our data  $\nu_i \in L^p(\Omega)$ , then we obtain some regularity for the transportation flow, namely  $\boldsymbol{\sigma}_i \in L^{1+\epsilon}(\Omega; \mathbb{R}^d)$  for some  $\epsilon > 0$  for all  $i \in \{1, \dots, N\}$ , without having to assume any regularity of the Wasserstein median.

In the next section we derive a PDE of Monge-Kantorovich type characterizing the Wasserstein median. Without any regularity assumptions it quite intricate to properly define a gradient. Thanks to Theorem 4.5.5 we can give a simpler version of this PDE system.

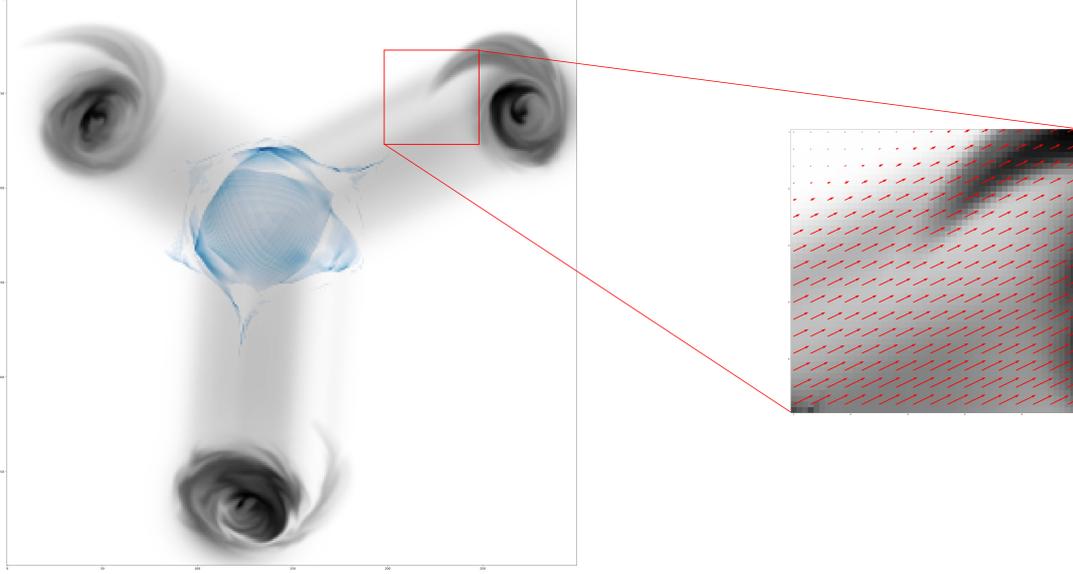


Figure 4.6 – Left: a Wasserstein median (blue) of three sample measures (black) and the three optimal transport densities (in gray) (i.e. the Total Variation measure according to REF) computed via Douglas-Rachford on a  $300 \times 300$  grid. Right: a zoom of a  $50 \times 50$  portion of the picture, where we highlighted (in red) the transport flow.

#### 4.5.2 PDE formulation of the Wasserstein median problem

Let  $\nu_1, \dots, \nu_N \in \mathcal{P}(\overline{\Omega})$ , we consider the following system of PDEs which is reminiscent of the Monge-Kantorovich equation related to the  $W_1$ -distance as stated in Section 5 [4].

**Definition 4.5.6** (The Monge-Kantorovich problem (MK)). *Given  $\nu_1, \dots, \nu_N \in \mathcal{P}(\overline{\Omega})$ , and  $p_1, \dots, p_N > 0$  such that  $\sum_{i=1}^N p_i = 1$ . The Monge-Kantorovich problem consists of finding  $\psi_i \in \text{Lip}_{p_i}(\Omega)$ ,  $\eta_i \in \mathcal{M}_+(\Omega)$  for  $i \in \{1, \dots, N\}$  and  $\rho \in \mathcal{P}_1(\Omega)$  such that*

1. *For each  $i \in \{1, \dots, N\}$  there exist a sequence of smooth functions  $(\psi_i^n)_{n \in \mathbb{N}}$  uniformly converging to  $\psi_i$  on  $\overline{\Omega}$  such that the functions  $\nabla \psi_i^n$  converge in  $L^2(\eta_i)^d$  to a function  $\nabla_{\eta_i} \psi_i$  satisfying*

$$|\nabla_{\eta_i} \psi_i| = p_i \quad \eta_i - \text{a.e. in } \Omega.$$

2. *The following PDE is satisfied in the weak sense with Neumann boundary conditions*

$$\frac{1}{p_i} \nabla \cdot (\eta_i \nabla_{\eta_i} \psi_i) + \nu_i = \rho \quad \text{in } \Omega \quad \forall i \in \{1, \dots, N\}.$$

3. *The following obstacle problem holds*

$$\sum_i \psi_i \leq 0, \quad \sum_i \psi_i = 0 \quad \rho\text{-a.e.}$$

*Remark 4.5.7* (Tangential gradient). The function  $\nabla_{\eta_i} \psi_i$  in point 1. of MK is called *tangential gradient* of  $\psi_i$ , introduced in [15, 14] and [52], see also Remark 5.1 [4]. The notion of tangential gradient is necessary to be able to give meaning to  $\nabla \cdot (\eta_i \nabla_{\eta_i} \psi_i)$ . Indeed,

under no additional assumptions even the product  $\eta_i \nabla \psi_i$  may a priori not be well-defined due to  $\eta_i$  not necessarily being absolutely continuous. In Theorem 4.5.8 we will see thanks to the equivalence to the Wasserstein median problem that  $\nabla_{\eta_i} \psi_i = \nabla \psi_i$   $\eta_i$ -a.e.

Note furthermore that the definition is well posed because given  $\psi_i \in \text{Lip}_{p_i}(\Omega)$ ,  $\eta_i \in \mathcal{M}_+(\overline{\Omega})$  for  $i \in \{1, \dots, N\}$  and  $\rho \in \mathcal{P}(\overline{\Omega})$  which solve MK, there is at most one tangential gradient  $\nabla_{\eta_i} \psi_i$ . Indeed, consider two sequences of smooth functions  $(\psi_i^n)_{n \in \mathbb{N}}$ ,  $(\widehat{\psi}_i^n)_{n \in \mathbb{N}}$  uniformly converging to  $\psi_i$  on  $\overline{\Omega}$  with  $\nabla \psi_i^n \rightarrow \nabla_{\eta_i} \psi_i$  and  $\nabla \widehat{\psi}_i^n \rightarrow \widehat{\nabla_{\eta_i} \psi_i}$  in  $L^2(\eta_i)^d$  as  $n \rightarrow \infty$ . We have by 2. from Definition 4.5.6

$$\int_{\overline{\Omega}} \nabla_{\eta_i} \psi_i \cdot \widehat{\nabla_{\eta_i} \psi_i} \, d\eta_i = \lim_{n \rightarrow \infty} \int_{\overline{\Omega}} \nabla_{\eta_i} \psi_i \cdot \nabla_{\eta_i} \widehat{\psi}_i^n \, d\eta_i = p_i \lim_{n \rightarrow \infty} \langle \nu_i - \rho, \widehat{\psi}_i^n \rangle = p_i \langle \nu_i - \rho, \psi_i \rangle.$$

So by taking the difference

$$\begin{aligned} \int_{\overline{\Omega}} |\nabla_{\eta_i} \psi_i - \widehat{\nabla_{\eta_i} \psi_i}|^2 \, d\eta_i &= \int_{\overline{\Omega}} |\nabla_{\eta_i} \psi_i|^2 \, d\eta_i + \int_{\overline{\Omega}} |\widehat{\nabla_{\eta_i} \psi_i}|^2 \, d\eta_i - 2 \int_{\overline{\Omega}} \nabla_{\eta_i} \psi_i \cdot \widehat{\nabla_{\eta_i} \psi_i} \, d\eta_i \\ &= \lim_{n \rightarrow \infty} \left( \int_{\overline{\Omega}} \nabla_{\eta_i} \psi_i \cdot \nabla_{\eta_i} \psi_i^n \, d\eta_i + \int_{\overline{\Omega}} \widehat{\nabla_{\eta_i} \psi_i} \cdot \nabla_{\eta_i} \widehat{\psi}_i^n \, d\eta_i \right) - 2p_i \langle \nu_i - \rho, \psi_i \rangle \\ &= \lim_{n \rightarrow \infty} p_i \langle \nu_i - \rho, \psi_i^n \rangle + \lim_{n \rightarrow \infty} p_i \langle \nu_i - \rho, \widehat{\psi}_i^n \rangle - 2p_i \langle \nu_i - \rho, \psi_i \rangle = 0. \end{aligned}$$

Hence  $\nabla_{\eta_i} \psi_i = \widehat{\nabla_{\eta_i} \psi_i}$   $\eta_i$ -a.e.

We now prove equivalence of MK and (MB), hence with the Wasserstein median problem.

**Theorem 4.5.8.** *Let  $\nu_1, \dots, \nu_N \in \mathcal{P}(\overline{\Omega})$ , and  $p_1, \dots, p_N > 0$  such that  $\sum_{i=1}^N p_i = 1$ .*

- *If  $\psi_i \in \text{Lip}_{p_i}(\Omega)$  are dual potentials, i.e. solve (ML\*) and  $\eta_i \in \mathcal{M}_+(\overline{\Omega})$  for  $i \in \{1, \dots, N\}$  are transport densities, i.e.  $\sigma_i := \frac{1}{p_i} \nabla \psi_i \eta_i$  solve (MB), then they solve the Monge-Kantorovich system with  $\rho := \nabla \cdot \sigma_i + \nu_i$  (this is independent of  $i$ ) and  $\nabla_{\eta_i} \psi_i = \nabla \psi_i$   $\eta_i$ -a.e.*
- *If  $\rho \in \mathcal{P}(\overline{\Omega})$ ,  $\psi_i \in \text{Lip}_{p_i}(\Omega)$  and  $\eta_i \in \mathcal{M}_+(\overline{\Omega})$  solve the Monge-Kantorovich system, then  $\rho$  solves (M),  $\psi_i$  solve (ML\*) and  $\sigma_i := \frac{1}{p_i} \nabla_{\eta_i} \psi_i \eta_i$  solve (MB). Moreover, in this case  $\nabla_{\eta_i} \psi_i = \nabla \psi_i$   $\eta_i$ -a.e.*

*Proof.* We start with the first implication. So let  $\psi_i \in \text{Lip}_{p_i}(\Omega)$  be dual potentials and  $\eta_i \in \mathcal{M}_+(\overline{\Omega})$  for  $i \in \{1, \dots, N\}$  transport densities,  $\sigma_i := \frac{1}{p_i} \nabla \psi_i \eta_i$  the corresponding transport flows. Point 2. of MK in Definition 4.5.6 simply follows since  $\sigma_i$  is a feasible solution for the Beckmann problem by construction (see Proposition 4.5.3). Validity of point 3., the obstacle problem, follows directly by the optimality conditions in Proposition 4.4.13.

For the first point take a convolution kernel  $(k_n)_{n \in \mathbb{N}^*}$  (i.e.  $k_n \in C_c^\infty(\mathbb{R}^d)$ ,  $\text{spt } k_n \subset \overline{B_{\frac{1}{n}}(0)}$ ,  $k_n \geq 0$  and  $\int_{\mathbb{R}^d} k_n \, dx = 1$ ) and define  $\psi_i^n := k_n * \psi_i$ , where the convolution is to be intended applied to the Lipschitz extension of  $\psi_i$  to the whole  $\mathbb{R}^d$ . Then since  $|\nabla \psi_i * k_n| \leq p_i$

$$\begin{aligned} p_i W_1(\rho, \nu_i) &= - \int_{\overline{\Omega}} \psi_i \, d(\rho - \nu_i) = - \lim_{n \rightarrow \infty} \int_{\overline{\Omega}} \psi_i * k_n \, d(\rho - \nu_i) \\ &= \lim_{n \rightarrow \infty} \frac{1}{p_i} \int_{\overline{\Omega}} \nabla \psi_i * k_n \cdot \nabla \psi_i \, d\eta_i \leq p_i \|\sigma_i\|_{\text{TV}} = p_i W_1(\rho, \nu_i). \end{aligned}$$

In particular  $\lim_{n \rightarrow \infty} \frac{1}{p_i} \int_{\Omega} \nabla \psi_i \star k_n \cdot \nabla \psi_i \, d\eta_i = \lim_{n \rightarrow \infty} p_i \int_{\Omega} \nabla \psi_i \star k_n \, d\sigma_i = p_i W_1(\rho, \nu_i)$ . Therefore with  $|\nabla \psi_i| = p_i$  and  $|\nabla \psi_i \star k_n| \leq p_i$  and optimality of all the quantities

$$\begin{aligned} \lim_{n \rightarrow \infty} \int_{\Omega} |\nabla \psi_i - \nabla \psi_i \star k_n|^2 \, d\eta_i &= \int_{\Omega} |\nabla \psi_i|^2 \, d\eta_i + \lim_{n \rightarrow \infty} \int_{\Omega} |\nabla \psi_i \star k_n|^2 \, d\eta_i \\ &\quad - 2 \lim_{n \rightarrow \infty} \int_{\Omega} \nabla \psi_i \star k_n \cdot \nabla \psi_i \, d\eta_i \\ &\leq 2p_i^2 \|\sigma_i\|_{\text{TV}} - 2p_i^2 W_1(\rho, \nu_i) = 0 \end{aligned}$$

This implies that  $\nabla \psi_i$  is a tangential gradient. Now note that there is a multi-marginal transport plan  $\gamma$  solution to (MMP) with  $\eta = \eta_\gamma$  by Proposition 4.5.4. Since  $\eta_i \ll \pi_{0, i \#} \gamma$  we obtain by the optimality conditions (Theorem 4.4.13)

$$|\nabla \psi_i| = p_i \quad \eta_i\text{-a.e. in } \Omega.$$

For the converse take a sequence of smooth functions  $(\psi_i^n)_{n \in \mathbb{N}}$  from the definition of the tangential gradient and test the PDE with  $\psi_i^n$  to obtain for  $i = 1, \dots, N$

$$-\frac{1}{p_i} \int_{\Omega} \nabla_{\eta_i} \psi_i \nabla \psi_i^n \, d\eta_i + \int_{\Omega} \psi_i^n \, d\nu_i = \int_{\Omega} \psi_i^n \, d\rho.$$

By taking the limit  $n \rightarrow \infty$  and summing over all  $i$  we get

$$-\sum_{i=1}^N \frac{1}{p_i} \int_{\Omega} |\nabla_{\eta_i} \psi_i|^2 \, d\eta_i + \int_{\Omega} \sum_{i=1}^N \psi_i \, d\nu_i = \int_{\Omega} \sum_{i=1}^N \psi_i \, d\rho.$$

This yields using  $|\nabla_{\eta_i} \psi_i| = p_i$   $\eta_i$ - a.e. and  $\sum_{i=1}^N \psi_i = 0$   $\rho$ -a.e.

$$-\sum_{i=1}^N p_i \eta_i(\bar{\Omega}) + \int_{\Omega} \sum_{i=1}^N \psi_i \, d\nu_i = 0.$$

Now

$$\sum_{i=1}^N p_i \|\sigma_i\|_{\text{TV}} \leq \sum_{i=1}^N p_i \eta_i(\bar{\Omega}) = \int_{\Omega} \sum_{i=1}^N \psi_i \, d\nu_i,$$

which concludes optimality of  $\rho$ ,  $\psi_i$  and  $\sigma_i$  by weak duality.

In order to obtain  $\nabla_{\eta_i} \psi_i = \nabla \psi_i$   $\eta_i$ - a.e. use optimality of the quantities and proceed as in the first direction with convolution.  $\square$

Of course, if we can assume that any solution  $\eta_i$  is absolutely continuous then the usual weak gradient  $\nabla \psi_i \in L^\infty(\Omega)$  would automatically be in  $L^2(\eta_i)$  and it would coincide with the tangential gradient  $\eta_i$ -a.e. if  $\psi_i$  is a solution to MK. By proving equivalence with the Beckmann problem in Theorem 4.5.8 we see that the assumption  $\nu_1, \dots, \nu_N \in L^p(\Omega)$  is sufficient for  $\eta_i \in L^1(\Omega)$  by Theorem 4.5.5. In that case we can replace the general Monge-Kantorovich system from Definition 4.5.6 by its regular version.

**Regular Monge-Kantorovich problem.** Given  $\nu_1, \dots, \nu_N \in \mathcal{P}_{\text{ac}}(\Omega)$  with densities in  $L^p(\Omega)$ ,  $p > 1$  and  $p_1, \dots, p_N > 0$  such that  $\sum_{i=1}^N p_i = 1$ .

Find:  $\psi_i \in W^{1,\infty}(\Omega)$ ,  $\eta_i \in L^1_+(\Omega)$  for  $i \in \{1, \dots, N\}$  and  $\rho \in \mathcal{P}(\Omega)$ , such that:

1. For each  $i \in \{1, \dots, N\}$  it holds that  $|\nabla \psi_i| \leq p_i$  in  $\Omega$ ,  $|\nabla \psi_i| = p_i$   $\eta_i$  - a.e.

2. The following PDE is satisfied in the weak sense with Neumann boundary conditions

$$\frac{1}{p_i} \nabla \cdot (\eta_i \nabla \psi_i) + \nu_i = \rho \quad \text{in } \Omega \quad \forall i \in \{1, \dots, N\}$$

3. The following obstacle condition holds.

$$\sum_i \psi_i \leq 0, \quad \sum_i \psi_i = 0 \quad \rho\text{-a.e.}$$

## 4.A Numerics

Indication: This part has been executed by my collaborator E. Chenchene. As I cannot cite another source (in form of a preprint or paper) yet, this draft is included here to show how the images in chapter have been created.

Despite having gathered an increasing interest due to its high potential for applications, the computation of Wasserstein means and median is still considered an important challenge and a definitive computational strategy is yet far from being established. In this section, we describe the algorithms we employed to compute all the above numerical examples and present a fairly new approach based on a Douglas-Rachford method on the Beckman flow formulation, which turned out to be particularly competitive with the state-of-art.

**One dimensional case.** Assume we have  $N \geq 2$  discrete measures supported on a ordered grid of  $n \geq 2$  points in  $\mathbb{R}$ . Recall from Section 4.3 that if  $X = \mathbb{R}$  the problem admits a closed form solution which can be computed directly with simple sorting procedures. Let us consider the vertical selection median according to (4.3.1). First, for each  $i \in \{1, \dots, N\}$  we define  $F_i$  to be the cumulative distribution function corresponding to  $\nu_i$ . For each point  $x$  of the grid we implement a sorting procedure to find the median interval of  $\{F_1(x), \dots, F_N(x)\}$ , which takes  $O(N \log(N))$  time. Let  $F_-(x)$  and  $F_+(x)$  be the lower and upper median respectively, and define  $F_\theta = \theta F_+ + (1 - \theta) F_-$  for  $\theta \in [0, 1]$ . By Theorem 4.3.2,  $F_\theta$  is the cumulative distribution function of a Wasserstein median  $\nu$  defined for each  $x_i$  in the grid as  $\nu(x_i) := (F_\theta(x_{i+1}) - F_\theta(x_i)) / |x_{i+1} - x_i|$ .

### 4.A.1 Wasserstein medians in two dimensions.

Consider now a grid  $X = \{(h, k) \in \mathbb{R}^2 \mid h, k = 1, \dots, p\}$ . Each element can represent for instance the coordinates of a pixel in a digital picture. We equip  $X$  with a cost function  $c$ , such as the Euclidean  $\ell^1$  or the  $\ell^2$  distance. Let  $n = p^2$  and fix an ordering of the elements of  $X$ , say  $X := \{x_1, \dots, x_n\}$ . Fix  $N \geq 2$  discrete measures  $\mu_1, \dots, \mu_N \in \mathcal{P}(X)$ . In this case, the multi-marginal formulation of the Wasserstein median problem according to (MMP) is a finite dimensional linear problem with  $Nn^2$  variables and  $Nn(n+2)+1$  linear constraints. Subsequently, (MMP) can become quickly intractable, especially considering that  $n = p^2$ . For this reason, LP tools to compute Wasserstein medians have for long been deprecated. More recently, S. Gualandi et al. provided new competitive LP schemes to tackle the Wasserstein median problem formulated on a network flow form *à la Beckmann* which run instead of  $O(n^3 \log(n))$  in  $(n^2 \log(n))$  time.

The celebrated Sinkhorn algorithm is nowadays the most popular approach to tackle Optimal Transport problems in higher dimensions. It could be thought as an instance of the *Iterative Bregman Projections* (IBP) scheme applied to an entropy-regularized variant of the discrete (MMP) formulation depending on a parameter  $\varepsilon > 0$  which has to be tuned as small as possible to get sufficiently close to a solution. While having many important computational advantages, such as an highly parallelizable structure and a fast IBP convergence behaviour, as a main drawback we would deal with non-exact outputs, in general blurred, and important numerical instabilities when we look for more and more precise solutions.

### Douglas-Rachford on the Beckmann formulation.

Given a square domain  $\Omega$ , and  $N \geq 2$  measures  $\nu_1, \dots, \nu_N \in \mathcal{P}(\Omega)$ , the Beckmann minimal flow formulation of the Wasserstein median according to (MB) is a convex minimization problem on a convex set. We discretize (MB) employing the grid  $\mathcal{G}_h$  with step-length  $h$ . We introduce the discrete spaces  $\mathcal{M}_h := \{\mu : \mathcal{G} \rightarrow \mathbb{R}\}$  and  $\mathcal{S}_h := \{\sigma : \mathcal{G} \rightarrow \mathbb{R}^2\}$  and consider the usual discretization of the gradient  $\nabla_h : \mathcal{U} \rightarrow \mathcal{S}$  defined via forward differences. The discrete divergence operator is the opposite adjoint of  $\nabla_h$ , that we denote with  $\nabla_h \cdot = -\nabla_h^*$ . We consider the following discretized Beckman problem. Let

$$\mathcal{D}_h := \left\{ (\sigma_1, \dots, \sigma_N, \nu) \mid \forall k : \sigma_k \in \mathcal{S}_h, \nu \in \mathcal{M}_h, \nabla_h \cdot \sigma_k + \nu_k = \nu, \right\}$$

Then, (MB) turns into the following discrete formulation

$$\inf_{(\sigma_1, \dots, \sigma_N, \nu) \in \mathcal{D}_h} \sum_{k=1}^N p_k \|\sigma_k\|_{1,2} + \mathbb{I}(\nu \in \Delta) \quad (4.A.1)$$

Where  $\Delta$  is the unit simplex, and  $\|\cdot\|_{1,2}$  is the  $\ell_{1,2}$  distance on  $\mathcal{S}$ , also known as *group-Lasso* penalty, namely, for all  $\sigma \in \mathcal{S}$ ,  $\|\sigma\|_{1,2} = \sum_{n=1}^n \|\sigma(x_i)\|$ , where, now  $\|\cdot\|$  is the usual  $\ell_2$  distance on  $\mathbb{R}^n$ .

To solve (4.A.1), we apply a Douglas-Rachford method with the functions defined by  $g_1(\sigma_1, \dots, \sigma_N, \nu) = \sum_{k=1}^N p_k \|\sigma_k\|_{1,2} + \mathbb{I}(\nu \in \Delta)$ ,  $g_2(\sigma_1, \dots, \sigma_N, \nu) = \mathbb{I}((\sigma_1, \dots, \sigma_N, \nu) \in \mathcal{D}_h)$ . The Douglas-Rachford method is an instance of the proximal point algorithm, which can be employed to solve a minimization problem consisting of the sum of two, or more, convex lower semi continuous functions which are accessible through evaluation of their proximity operators. In our case, the proximity operator of  $g_1$  consists in a projection onto the unit simplex for the discrete measure  $\nu$  and on the application of the proximal operator of the group-Lasso penalty (that we denote by  $\text{Shrink}_\tau$ ) on each component  $\sigma_i$ , which is computable via Moreau formula.

The proximity operator of  $g_2$  coincides with the projection onto  $\mathcal{D}_h$ , which is much more delicate, as we now describe. It is well known that given a linear map  $A : \mathbb{R}^n \rightarrow \mathbb{R}^m$  and a vector  $b \in \mathbb{R}^m$ , the projection onto the set of solution to the linear system  $Ax = b$  is given by  $P_r(x) = x - A^*\xi$  where  $\xi$  solves  $(AA^*)\xi = Ax - b$ . In our case, we have  $b = [-\nu_1, \dots, -\nu_N]^T$  and the linear operators  $A$  and  $AA^*$  can be written in block form as

$$A = \begin{bmatrix} \nabla_h \cdot & & & -I \\ & \ddots & & \vdots \\ & & \nabla_h \cdot & -I \end{bmatrix}, \quad AA^* = \begin{bmatrix} -\Delta_h + I & I & \cdots & I \\ I & \ddots & & \vdots \\ \vdots & & & I \\ I & I & \cdots & -\Delta_h + I \end{bmatrix}, \quad (4.A.2)$$

where  $\Delta_h$  represents the discrete Laplacian operator, namely  $\Delta_h = (\nabla_h \cdot) \nabla_h$ .

**Proposition 4.A.1.** *Let  $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_N) \in \mathcal{S}_h^N$  and  $\nu \in \mathcal{M}_h \cap \Delta$ , then the projection  $(\tilde{\boldsymbol{\sigma}}, \tilde{\nu})$  of  $(\boldsymbol{\sigma}, \nu)$  onto  $\mathcal{D}_h$  is given by*

$$\tilde{\sigma}_i = \sigma_i + \nabla_h \xi_i, \quad \tilde{\nu} = \nu + \sum_{i=1}^N \xi_i,$$

where  $\xi_i = \xi'_i - (I - \frac{1}{N} \Delta_h)^{-1} \left( \frac{1}{N} \sum_{j=1}^N \xi'_j \right)$  and  $\xi'_i$  solves for all  $i \in \{1, \dots, N\}$

$$-\Delta_h \xi'_i = \nabla_h \cdot \sigma_i + \nu_i - \nu.$$

*Proof.* We only need to show that  $A(\tilde{\boldsymbol{\sigma}}, \tilde{\nu}) = b$  and that  $\boldsymbol{\xi} = (\xi_1, \dots, \xi_N)$  solves  $AA^* \boldsymbol{\xi} = A(\boldsymbol{\sigma}, \nu) - b$  where  $A$  and  $AA^*$  are defined in (4.A.2). Let us start from the latter. Denoting  $\bar{\xi}' = 1/N \sum_{i=1}^N \xi'_i$ , we have for all  $i \in \{1, \dots, N\}$  that

$$\begin{aligned} -\Delta_h \xi_i + \sum_{j=1}^N \xi_j &= -\Delta_h \xi'_i + \Delta_h \left( I - \frac{1}{N} \Delta_h \right)^{-1} \bar{\xi}' + N \bar{\xi}' - N \left( I - \frac{1}{N} \Delta_h \right)^{-1} \bar{\xi}' \\ &= \nabla_h \cdot \sigma_i + \nu_i - \nu + N \bar{\xi}' - N \left( I - \frac{1}{N} \Delta_h \right) \left( I - \frac{1}{N} \Delta_h \right)^{-1} \bar{\xi}' \\ &= \nabla_h \cdot \sigma_i + \nu_i - \nu. \end{aligned}$$

Hence  $AA^* \boldsymbol{\xi} = A(\boldsymbol{\sigma}, \nu) - b$ . Regarding the feasibility constraint, we have

$$\begin{aligned} \nabla_h \cdot \tilde{\sigma}_i + \nu_i &= \nabla_h \cdot \sigma_i + \Delta_h \xi_i + \nu_i = \nabla_h \cdot \sigma_i + \Delta_h \xi'_i - \Delta_h \left( I - \frac{1}{N} \Delta_h \right)^{-1} \bar{\xi}' + \nu_i \\ &= \nu - \Delta_h \left( I - \frac{1}{N} \Delta_h \right)^{-1} \bar{\xi}' = \nu + N \bar{\xi}' - N \left( I - \frac{1}{N} \Delta_h \right)^{-1} \bar{\xi}' = \tilde{\nu}, \end{aligned}$$

which concludes the proof.  $\square$

Proposition 4.A.1 allows us to implement a Douglas-Rachford scheme on (4.A.1), which we summarize in Algorithm 1. In Algorithm 1, we are required to solve two sparse (elliptic) linear systems, which we tackled with generic sparse linear solvers, e.g. `spsolve` in `scipy`. However, one should put adequate care when trying to solve the first Laplacian system. Indeed, if the projection onto the simplex is not computed sufficiently well, the right hand side can be out of the range of the Laplacian. For this reason, in our numerical implementation, we smoothed out all possible numerical errors with a further projection of the right hand side onto the set of discrete measure with total mass equal to one.

The computational cost required to solve the aforementioned linear systems is overall balanced with a very fast iteration-wise convergence behaviour. Most importantly, note that there is no need to store dense  $n \times n$  matrices. This makes the proposed method suitable for highly large-scale instances, which using state of art methods are far from being tractable.

**Data:** A collection of discrete probability measures  $\nu_1, \dots, \nu_N \in \mathcal{S}_h$ , step-size  $\tau > 0$ .

**Result:**  $\nu = \lim \nu^k$ ,  $\sigma_q = \lim \sigma_q^k$  for  $q \in \{1, \dots, N\}$  solution to (4.A.1).

**Initialize:**  $\eta_1^0, \dots, \eta_N^0 \in \mathcal{S}_h$  and  $\mu^0 \in \mathcal{M}_h \cap \Delta$ ;

**while** *not convergent* **do**

$\sigma_q^{k+1} = \text{Shrink}_\tau(\eta_q^k)$  for all  $q \in \{1, \dots, N\}$  ;

$\nu^{k+1} = \text{Proj}_\Delta(\mu^k)$ ;

**for**  $q \in \{1, \dots, N\}$  **do**

**Solve:**  $-\Delta_h \xi_q^t = \nabla_h \cdot (2\sigma_q^{k+1} - \eta_q^k) + \nu_i - 2\nu^{k+1} + \mu^k$ ;

$\xi_q = \xi_q^t - (I - \frac{1}{N}\Delta_h)^{-1} \left( \frac{1}{N} \sum_{j=1}^N \xi_j^t \right)$

**end**

$\eta_q^{k+1} = (1 - \theta_k)\eta_q^k + \theta_k (\sigma_q^{k+1} + \nabla_h \xi_q)$  for all  $q \in \{1, \dots, N\}$ ;

$\mu^{k+1} = (1 - \theta_k)\mu^k + \theta_k \left( \nu^{k+1} + \sum_{q=1}^N \xi_q \right)$ .

**end**

**Algorithm 1:** Douglas-Rachford for the Wasserstein median problem

**Convergence.** Douglas-Rachford benefits from robust convergence guarantees, without any condition neither on the starting point, nor on the step-size  $\tau > 0$ . In particular, we have that if  $\sigma_q^k$ ,  $\nu^k$ ,  $\eta^k$  and  $\mu^k$  are generated by Algorithm 1, then for each  $q \in \{1, \dots, N\}$ , we have  $\sigma_q^k \rightarrow \sigma_q^*$  and  $\nu^k \rightarrow \nu^*$  and  $(\sigma_1^*, \dots, \sigma_N^*, \nu^*)$  solves (4.A.1). Furthermore, defining  $\tilde{\sigma}_q^{k+1} = 2\sigma_q^{k+1} - \eta_q^k + \nabla_h \xi_q$  and  $\tilde{\nu}^{k+1} = 2\nu^{k+1} - \mu^k + \sum_{q=1}^N \xi_q$ , we have that, up to numerical tolerances  $(\tilde{\sigma}_1^{k+1}, \dots, \tilde{\sigma}_N^{k+1}, \tilde{\nu}^{k+1}) \in \mathcal{D}_h$ , i.e. is always feasible for (4.A.1), and  $\tilde{\sigma}_q^k \rightarrow \sigma_q^*$ ,  $\tilde{\nu}^k \rightarrow \nu^*$  for every  $q \in \{1, \dots, N\}$ . Thus, it makes sense to measure the relative decrease of objective function on  $\tilde{\sigma}_1^k, \dots, \tilde{\sigma}_N^k$ , namely  $r^k = (f^{k+1} - f^k)/f^k$  with  $f^{k+1} = \sum_{q=1}^N p_q \|\tilde{\sigma}_q^{k+1}\|_{1,2}$  and setting  $r^k < \text{tol}$  as stopping criterion.

Interestingly, in our implementation we noticed that the larger  $\tau$ , the sparser the limit of  $(\nu^k)_{k \in \mathbb{N}}$  and that a good choice of the step-size is  $\tau = 10^{-3}$ , which even at different scales, always provided very fast convergence behaviours.

Matrix-free method, i.e. without the need to ever solve any linear system exists and can be applied to solve (4.A.1) as well. Indeed, we implemented the Primal Dual Hybrid Gradient method popularized by Chambolle and Pock, with different step-size selection strategies, such as *backtracking*, *adaptive* and *fixed* step-sizes, which, however, always provided very slow behaviours, and therefore, we disregarded it.

## Chapter 5

# Constrained Wasserstein interpolation

This chapter is based on joint work with G. Buttazzo and G. Carlier from the preprint [20].

The goal is to investigate a class of problems as a mathematical model for the optimal location of a parking region around a city. In this context, one is given two probability measures  $\mu_0$  and  $\mu_1$ , which may be interpreted as a distribution of residents and a distribution of services respectively. A resident living at  $x_0$  reaching a service located at  $x_1$  may either walk directly to  $x_1$  for the cost  $c_1(x_0, x_1)$  or drive to an intermediate parking location  $x$  and then walk from  $x$  to  $x_1$  paying the sum  $c_0(x_0, x) + c_1(x, x_1)$ . In this model, detailed in Section 5.1, the pivot or parking measure  $\rho$  may have total mass less than 1, and one may decompose  $\mu_0$  and  $\mu_1$  as  $\mu_i = \mu_i - \nu_i + \nu_i$  with  $0 \leq \nu_i \leq \mu_i$  denoting the *driving* part of  $\mu_i$  and the unknowns are  $\nu_0$ ,  $\rho$  and  $\nu_1$  (with same total mass). The goal is then to minimize the overall cost

$$W_{c_1}(\mu_0 - \nu_0, \mu_1 - \nu_1) + W_{c_0}(\nu_0, \rho) + W_{c_1}(\rho, \nu_1),$$

subject to possible additional constraints on  $\rho$ , such as

- location constraints, where the support of  $\rho$ ,  $\text{spt } \rho$ , is required to be contained in a given region  $K \subset \mathbb{R}^d$ ;
- density constraints, where the measure  $\rho$  is required to be absolutely continuous and with a density not exceeding a prescribed function  $\phi$ .

Let us remark that if  $(\nu_0, \nu_1, \rho)$  solves this parking problem, then  $\rho$  minimizes the reduced problem

$$W_{c_0}(\nu_0, \cdot) + W_{c_1}(\cdot, \nu_1),$$

subject to the same location or density constraints. We call this corresponding problem the (constrained) Wasserstein interpolation problem and study fine properties of solutions in detail in Sections 5.4 and 5.5. These qualitative properties will be directly applicable to optimal parking measures.

Certain classes of constrained Wasserstein interpolation problems have been studied in the past. Notably, [83] considers the problem of location constraint for cost functions given by Finsler distances, while in [84] the case of density constraint for Euclidean cost

functions is analyzed. The paper [64] considers a more general density constraint problem again for the Euclidean cost, where the measure  $\rho$  is required not to exceed a given measure  $\Theta \in \mathcal{M}_+(\mathbb{R}^d)$ . Without additional constraint on the measure  $\rho$ , the minimization of the functional  $W_{c_0}(\nu_0, \cdot) + W_{c_1}(\cdot, \nu_1)$ , or its generalizations to more than two prescribed measures, arise in different applied settings such as multi-population matching [33] or Wasserstein barycenters [1]. In particular, in the quadratic case where  $c_0(x, y) = c_1(x, y) = |x - y|^2$ , minimizers of  $W_{c_0}(\nu_0, \cdot) + W_{c_1}(\cdot, \nu_1)$  are the midpoints of McCann's displacement interpolation [86] between  $\nu_0$  and  $\nu_1$  i.e. geodesics for the quadratic Wasserstein metric. Our goal is to investigate the effect of location and density constraints on such Wasserstein interpolation problems. Let us also mention that the minimization of  $W_{c_0}(\nu_0, \rho)$  with respect to  $\rho$  in a class of measures which are singular with respect to  $\nu_0$  was addressed in [21].

The remaining chapter is organized as follows. In Section 5.1, we introduce the problem related to the optimization of a parking area. Section 5.2 considers the general Wasserstein interpolation problem (WI) and after solving an explicit example, we prove existence and discuss uniqueness of solutions. Dual formulations are introduced in Section 5.3. In Section 5.4, the particular case of distance-like costs is studied, while Section 5.5 deals with the case of strictly convex cost functions. In these sections we study various qualitative properties of the solutions, in particular their integrability. Finally, in Section 5.6, we present some numerical simulations thanks to an entropic approximation scheme and compare the solutions of interpolation and parking problems.

## 5.1 A parking location model

In this section, we introduce a mathematical model for the optimal location of a parking area in a city. We fix:

- a compactly supported probability measure on  $\mathbb{R}^d$ ,  $\mu_0$  which represents the distribution of residents in a given area;
- a compactly supported probability measure on  $\mathbb{R}^d$ ,  $\mu_1$  which represents the distribution of services.

The goal is to determine a measure  $\rho$  which represents the density of parking places, in order to minimize a suitable total transportation cost. All the residents travel to reach the services, but some of them may simply walk (which will cost  $c_1(x, y)$  to go from  $x$  to  $y$ ), while some other ones may use their car to reach a parking place (which will cost  $c_0(x, y)$  to go from  $x$  to the parking place  $y$ ) and then walk from the parking place to the services (which will cost  $c_1(y, z)$  to go from  $y$  to  $z$ ). We consider two cost functions  $c_0$  and  $c_1$  and the corresponding Wasserstein functionals  $W_{c_0}$  and  $W_{c_1}$ , defined as in (OT), respectively representing the cost of moving by car and the cost of walking. It may be natural to assume that walking is more costly than driving i.e.  $c_1 \geq c_0$ , for instance we may take  $p \geq 1$  and

$$c_0(x, y) = |x - y|^p, \quad c_1(x, y) = \lambda|x - y|^p \text{ with } \lambda \geq 1.$$

Assuming that  $\nu_0 \leq \mu_0$  denotes the distribution of driving residents and  $\nu_1 \leq \mu_1$  the corresponding services they reach for, the total cost we consider is

$$F(\nu_0, \nu_1, \rho) = W_{c_1}(\mu_0 - \nu_0, \mu_1 - \nu_1) + W_{c_0}(\nu_0, \rho) + W_{c_1}(\rho, \nu_1). \quad (5.1.1)$$

## 5.1. A PARKING LOCATION MODEL

The optimization problems we consider are then the minimization of  $F(\nu_0, \nu_1, \rho)$ , subject to the constraints

$$0 \leq \nu_0 \leq \mu_0, \quad 0 \leq \nu_1 \leq \mu_1, \quad \text{and } \nu_0(\mathbb{R}^d) = \nu_1(\mathbb{R}^d) = \rho(\mathbb{R}^d),$$

and additional constraints as:

- no other constraints on the parking measure  $\rho$ ;
- location constraints, that is  $\text{spt } \rho \subset K$ , with a compact set  $K \subset \mathbb{R}^d$  a priori given;
- density constraints, that is  $\rho \leq \phi$ , for a given non-negative and integrable function  $\phi$ .

This optimization problem in the case of a location constraint can also be reformulated as a linear program in the following way

$$\begin{aligned} & \inf_{\gamma, \tilde{\gamma} \geq 0,} \int_{\mathbb{R}^d \times \mathbb{R}^d} c_1(x_0, x_1) d\gamma(x_0, x_1) + \int_{\mathbb{R}^d \times \mathbb{R}^d \times K} (c_0(x_0, x) + c_1(x, x_1)) d\tilde{\gamma}(x_0, x, x_1). \\ & \gamma + \pi_{0,1}^{\#} \tilde{\gamma} \in \Pi(\mu_0, \mu_1) \end{aligned} \tag{5.1.2}$$

It is indeed easy to see that the optimal solution to minimizing the functional in (5.1.1) is given by  $\pi_{\text{piv}}^{\#} \tilde{\gamma}$ . Hence to incorporate a density constraint in the formulation (5.1.2) one needs to add the constraint  $\pi_{\text{piv}}^{\#} \tilde{\gamma} \leq \phi$ .

Figure 5.1 gives an example of the optimal parking problem where both  $\gamma$  and  $\tilde{\gamma}$  are non-trivial.

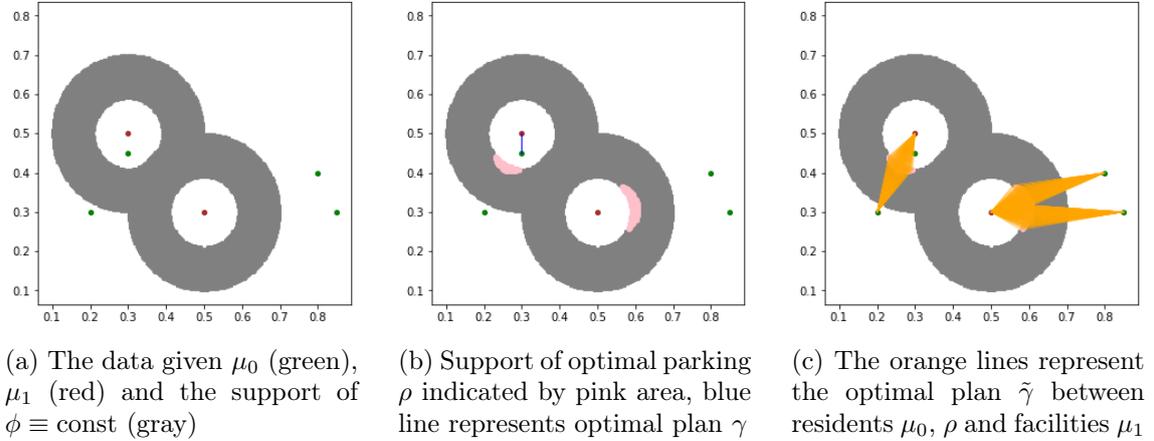


Figure 5.1 – Parking location problem with density constraint.

The problem with location constraint is actually equivalent to a standard optimal transport problem with cost function

$$C(x_0, x_1) := \min \left\{ c_1(x_0, x_1), \inf_{x \in K} \{c_0(x_0, x) + c_1(x, x_1)\} \right\}.$$

More precisely, consider

$$\inf_{\beta \in \Pi(\nu_0, \nu_1)} \int_{\mathbb{R}^d \times \mathbb{R}^d} C(x_0, x_1) d\beta(x_0, x_1). \tag{5.1.3}$$

Then both (5.1.2) and (5.1.3) admit solutions and they are equivalent in the following sense

- $\inf (5.1.2) = \inf (5.1.3)$ ,
- if  $\gamma, \tilde{\gamma}$  are optimal for (5.1.2), then  $\beta := \gamma + \pi_{0,1}^\# \tilde{\gamma}$  is optimal for (5.1.3),
- if  $\beta$  is optimal for (5.1.3), then defining

$$V_1 := \left\{ (x_0, x_1) \in \mathbb{R}^d \times \mathbb{R}^d : c_1(x_0, x_1) = C(x_0, x_1) \right\}$$

$\gamma := \beta|_{V_1}$  and  $P : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$  (measurable)

$$P(x_0, x_1) \in \arg \min_{x \in K} \{c_0(x_0, x) + c_1(x, x_1)\},$$

and

$$d\tilde{\gamma}(x_0, x_1, x) := \delta_{P(x_0, x_1)}(x) \otimes d\beta|_{\mathbb{R}^d \setminus V_1}(x_0, x_1),$$

then  $\gamma$  and  $\tilde{\gamma}$  are optimal for (5.1.2).

*Remark 5.1.1.* Note that the solutions  $(\nu_0, \nu_1, \rho)$  to minimizing (5.1.1), (respectively the solutions  $\gamma$  and  $\tilde{\gamma}$  to (5.1.2)) are not necessarily probability measures. The optimal common total mass of  $\tilde{\gamma}$ ,  $\nu_0$  and  $\nu_1$  represents the fraction of  $\mu_0$  which uses the parking. In order to analyse further properties of a parking measure  $\rho$ , we consider in the next sections the following Wasserstein interpolation problem

$$\inf \{W_{c_0}(\nu_0, \rho) + W_{c_1}(\rho, \nu_1) : \mu \in \mathcal{A}\},$$

where  $\mathcal{A} \subset \mathcal{P}(\mathbb{R}^d)$  encodes the location or density constraints imposed on  $\rho$ . The parking problem is a generalization of this interpolation problem, as the Wasserstein interpolation problem corresponds to imposing that the parking measure is of full mass.

## 5.2 Wasserstein interpolation with constraints

Let  $\nu_0, \nu_1 \in \mathcal{P}(\mathbb{R}^d)$  be two probabilities with compact support, and let  $c_0, c_1 : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}_+$  be two continuous cost functions. For a class  $\mathcal{A} \subset \mathcal{P}(\mathbb{R}^d)$  we are interested in solving the optimization problem

$$\inf \{W_{c_0}(\nu_0, \rho) + W_{c_1}(\rho, \nu_1) : \mu \in \mathcal{A}\}. \quad (\text{WI})$$

Here  $W_{c_i}(\mu_0, \mu_1)$  denotes the value of the optimal transport problem between two measures  $\mu_0, \mu_1 \in \mathcal{P}(\mathbb{R}^d)$ , obtained by means of the Wasserstein functionals defined in (OT). In order to simplify the presentation, by an abuse of notation, if  $\rho$  is a measure and  $\phi$  is a non-negative Lebesgue integrable function, by  $\rho \leq \phi$  we mean that  $\rho$  is absolutely continuous and its density, again denoted  $\rho$ , satisfies  $\rho \leq \phi$  Lebesgue a.e. Also, for a measure  $\varrho \in \mathcal{P}(\mathbb{R}^d)$  we often write by abuse of notation  $\varrho \in \mathcal{P}(\bar{\Omega})$  if  $\text{spt } \varrho \subset \bar{\Omega}$  for a closed subset  $\bar{\Omega} \subset \mathbb{R}^d$ .

Typical cases for the class  $\mathcal{A}$  of admissible choices are:

- (i) no constraint, that is  $\mathcal{A} = \mathcal{P}(\mathbb{R}^d)$ ;
- (ii) location constraints, that is  $\mathcal{A} = \mathcal{P}(K)$  for a non-empty compact subset  $K$  of  $\mathbb{R}^d$ ;
- (iii) density constraints, that is  $\mathcal{A} = \{\rho \in \mathcal{P}_{\text{ac}}(\mathbb{R}^d) : \rho \leq \phi\}$  for an  $L^1$ -function  $\phi : \mathbb{R}^d \rightarrow \mathbb{R}_+$  with compact support and  $\int_{\mathbb{R}^d} \phi dx > 1$ .

### 5.2.1 Explicit one-dimensional examples

Before going to the general case, let us illustrate our problem in a simple one-dimensional case.

*Example 5.2.1.* Consider the one-dimensional case and the measures

$$\nu_0(x) = \mathbb{1}_{[0,1]}(x), \quad \nu_1(x) = \mathbb{1}_{[5,6]}(x).$$

We first look at the case where the cost functions are given by distances:

$$c_0(x, y) = (1 - t)|x - y|, \quad c_1(x, y) = t|x - y| \quad \text{with } t \in ]0, 1[.$$

The following results can be easily seen by rephrasing the problem in terms of the distribution functions  $f, f_0, f_1$  of the probabilities  $\rho, \nu_0, \nu_1$  (see for instance Chapter 2 of [104]):

$$\inf \left\{ \int_0^6 (1 - t)|f_0 - f| + t|f - f_1| dx : f \text{ non-decreasing, } f(0) = 0, f(6) = 1 \right\}$$

with the constraints

- (i) no additional constraint;
- (ii)  $\text{spt } f' \subset [2, 4]$ ;
- (iii)  $f' \leq \theta \mathbb{1}_{[2,4]}$ .

Since  $f_0 \leq f_1$ , it is easy to see that in the minimization above, one can always assume that  $f_0 \leq f \leq f_1$  and then remove the absolute values and minimize under the constraint that  $f$  is non-decreasing and  $f_0 \leq f \leq f_1$ . We then have:

- (i) In the absence of constraints, this becomes the problem of finding the Wasserstein median between  $\nu_0$  and  $\nu_1$  (see [29] for more on Wasserstein medians). In particular, the optimal solutions  $\rho$  are characterized as follows:
  - if  $t > 1/2$  (respectively  $t < 1/2$ ), the unique solution is given by  $\rho = \nu_1$  (respectively  $\rho = \nu_0$ );
  - if  $t = 1/2$ , any probability  $\rho$  whose distribution function  $f$  is between the two distribution functions  $f_0$  and  $f_1$  of  $\nu_0$  and  $\nu_1$ , in the sense that

$$f_0(x) \leq f(x) \leq f_1(x) \quad \text{for all } x \in \mathbb{R},$$

is a minimizer.

- (ii) In the case of the location constraint  $K = [2, 4]$ , we observe a similar threshold effect:
  - if  $t > 1/2$  (respectively  $t < 1/2$ ), the unique solution is given by  $\rho = \delta_4$  (respectively  $\rho = \delta_2$ );
  - if  $t = 1/2$ , then any probability measure supported on  $K$  is a solution.
- (iii) In the case of density constraint  $\phi(x) := \theta \mathbb{1}_{[2,4]}(x)$  with  $\theta > 1/2$  we have:
  - if  $t > 1/2$  (respectively  $t < 1/2$ ), the unique solution is given by  $\rho = \theta \mathbb{1}_{[4-1/\theta, 4]}$  (respectively  $\rho = \theta \mathbb{1}_{[2, 2+1/\theta]}$ );

- if  $t = 1/2$  any probability measure satisfying the constraint is a solution.

The example above relies on the fact that for distance-like costs, optimality somehow forces the triangular inequality to be saturated in dimension 1. We will investigate this phenomenon further in Section 5.4.

We consider now strictly convex cost functions: as a prototype we take, with the same measures  $\nu_0$  and  $\nu_1$  above,

$$c_0(x, y) = (1 - t)|x - y|^2, \quad c_1(x, y) = t|x - y|^2 \quad \text{with } t \in (0, 1).$$

Also this case can be rephrased in terms of the so-called *pseudo-inverse*  $g, g_0, g_1$  of the distribution functions  $f, f_0, f_1$  as:

$$\inf \left\{ \int_0^1 (1 - t)(g - g_0)^2 + t(g_1 - g)^2 ds : g \text{ non-decreasing} \right\}$$

with the constraints

- (i) no additional constraint;
- (ii)  $g([0, 1]) \subset [2, 4]$ ;
- (iii)  $g' \geq 1/\theta$  and  $g([0, 1]) \subset [2, 4]$ .

This implies:

- (i) In the unconstrained case the solution simply corresponds to the Wasserstein-geodesic from  $\nu_0$  to  $\nu_1$  at time  $t \in (0, 1)$ , or equivalently the weighted barycenter. It is given by

$$\nu_t(x) := \mathbf{1}_{[5t, 1+5t]}(x).$$

- (ii) Take the constraint  $K = [2, 4]$ , as above. Here the solution depends on the location of the unconstrained geodesic  $\nu_t$ . We present a few cases (the other ones are clear by symmetry)

- if  $t \leq \frac{1}{5}$  the support of  $\nu_t$  is contained in  $[0, 2]$ , hence the optimal solution is  $\delta_2$ ;
- if  $\frac{1}{5} < t < \frac{2}{5}$  the optimal solution is  $\rho = (2 - 5t)\delta_2 + \mathbf{1}_{[2, 1+5t]}$ ;
- if  $\frac{2}{5} \leq t \leq \frac{3}{5}$  the support of  $\nu_t$  is contained in  $[2, 4]$ , hence the solution is simply  $\nu_t$ .

- (iii) Take the function  $\phi(x) := \theta \mathbf{1}_{[2, 4]}(x)$  with  $1 > \theta > \frac{1}{2}$ . The solution depends again on the location of the unconstrained geodesic  $\nu_t$ . We have the following cases (remaining cases are again obtained by symmetry)

- if  $t \leq \frac{1}{5}$  the support of  $\nu_t$  is contained in  $[0, 2]$ , hence the optimal solution is  $\theta \mathbf{1}_{[2, 2+1/\theta]}$ ;
- if  $\frac{1}{5} < t < \frac{2}{5}$  the optimal solution is still  $\rho = \theta \mathbf{1}_{[2, 2+1/\theta]}$ ;
- if  $\frac{2}{5} \leq t \leq \frac{3}{5}$  the support of  $\nu_t$  is contained in  $[2, 4]$ , but by the density constraint  $\nu_t$  is not even feasible this time. So the solution is of the form  $\theta \mathbf{1}_{[a, b]}$  with  $2 \leq a < b \leq 4$  and  $b - a = 1/\theta$ .

### 5.2.2 Reformulation, existence, uniqueness

Let us now come back to the constrained Wasserstein interpolation problem (WI) assuming that the measures  $\nu_0$  and  $\nu_1$  are compactly supported and the costs  $c_0$  and  $c_1$  are continuous and non-negative, then by the direct method one directly gets

**Lemma 5.2.2.** *Assume either the case (ii):  $\mathcal{A} = \mathcal{P}(K)$  with  $K \subset \mathbb{R}^d$  compact or the case (iii)  $\mathcal{A} := \{\rho \in \mathcal{P}(\mathbb{R}^d) : \rho \leq \phi\}$  with  $\phi \in L^1(\mathbb{R}^d)$  compactly supported and  $\int_{\mathbb{R}^d} \phi \, dx \geq 1$ . Then problem (WI) admits a solution.*

*Proof.* In both cases, one is left to optimize over probabilities over a fixed compact set, the sum of two Wasserstein terms which are weakly\* lower semicontinuous.  $\square$

In the unconstrained case where  $\mathcal{A} := \mathcal{P}(\mathbb{R}^d)$ , one of course needs some coercivity in the problem. We shall therefore assume that there exists a compact subset of  $\mathbb{R}^d$ , denoted (again) by  $K$ , such that for every  $(x_0, x_1) \in \text{spt}(\nu_0) \times \text{spt}(\nu_1)$  one has

$$\arg \min_{x \in \mathbb{R}^d} \{c_0(x_0, x) + c_1(x, x_1)\} \text{ is non-empty and included in } K. \quad (5.2.1)$$

We then define, for  $(x_0, x_1) \in \text{spt}(\nu_0) \times \text{spt}(\nu_1)$

$$c(x_0, x_1) := \inf_{x \in \mathbb{R}^d} \{c_0(x_0, x) + c_1(x, x_1)\} = \min_{x \in K} \{c_0(x_0, x) + c_1(x, x_1)\}.$$

In the following proposition, we show that the optimization problem (WI), with  $\mathcal{A} = \mathcal{P}(\mathbb{R}^d)$ , is equivalent to the standard transport problem with cost  $c$

$$\inf_{\gamma \in \Pi(\nu_0, \nu_1)} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x_0, x_1) \, d\gamma(x_0, x_1), \quad (5.2.2)$$

which clearly admits a solution, since  $c \in C(\text{spt}(\nu_0) \times \text{spt}(\nu_1))$ . We easily deduce the existence of a solution to (WI) when  $\mathcal{A} = \mathcal{P}(\mathbb{R}^d)$  as well as the fact that all solutions are supported by  $K$ .

We will denote by  $\Pi(\nu_0, \rho, \nu_1)$  the set of transport plans in the variables  $(x_0, x, x_1)$  with marginals  $\nu_0, \rho, \nu_1$ , and we denote by  $\pi_{0,\text{piv}}, \pi_{\text{piv},1}, \pi_{0,1}$  the projections on the first and second, second and third, first and third factors respectively.

**Proposition 5.2.3.** *Assume the coercivity condition (5.2.1). Let  $\gamma \in \Pi(\nu_0, \nu_1)$  solve (5.2.2) and let  $T : \text{spt}(\nu_0) \times \text{spt}(\nu_1) \rightarrow \mathbb{R}^d$  be measurable and such that*

$$T(x_0, x_1) \in \arg \min_{x \in K} \{c_0(x_0, x) + c_1(x, x_1)\} \quad \forall (x_0, x_1) \in \text{spt}(\nu_0) \times \text{spt}(\nu_1).$$

Then

- $T\#\gamma$  is a solution of (WI) with  $\mathcal{A} = \mathcal{P}(\mathbb{R}^d)$  and the optimal values of (WI) and (5.2.2) coincide;
- conversely, for any optimal solution  $\rho$  of (WI), consider optimal transport plans  $\gamma_0 \in \Pi(\nu_0, \rho)$  with respect to the cost  $c_0$  and  $\gamma_1 \in \Pi(\rho, \nu_1)$  with respect to the cost  $c_1$ . Then there exists a plan  $\tilde{\gamma} \in \Pi(\nu_0, \rho, \nu_1)$  with  $\pi_{0,\text{piv}}^\#\tilde{\gamma} = \gamma_0$  and  $\pi_{\text{piv},1}^\#\tilde{\gamma} = \gamma_1$  such that  $\pi_{0,1}^\#\tilde{\gamma}$  is optimal for (5.2.2) and  $c_0(x_0, x) + c_1(x, x_1) = c(x_0, x_1)$  on  $\text{spt}(\tilde{\gamma})$  so that  $\rho$  is supported by  $K$ .

The previous equivalence also holds between (WI) with  $\mathcal{A} = \mathcal{P}(K)$  (with  $K$  a given compact subset of  $\mathbb{R}^d$ ) and (5.2.2) with  $c$  given by  $c(x_0, x_1) = \min_{x \in K} \{c_0(x_0, x) + c_1(x, x_1)\}$ .

*Proof.* Let  $\rho \in \mathcal{P}(\mathbb{R}^d)$ ,  $\gamma_0 \in \Pi(\nu_0, \rho)$  and  $\gamma_1 \in \Pi(\rho, \nu_1)$ ; by the gluing Lemma (see Lemma 7.6 in [112]), there is a plan  $\tilde{\gamma} \in \Pi(\nu_0, \rho, \nu_1)$  with  $\pi_{0, \text{piv}}^\# \tilde{\gamma} = \gamma_0$  and  $\pi_{\text{piv}, 1}^\# \tilde{\gamma} = \gamma_1$ . Hence, since  $\gamma$  solves (5.2.2) and  $\pi_{0,1}^\# \tilde{\gamma} \in \Pi(\nu_0, \nu_1)$ , we have

$$\begin{aligned} \int_{\mathbb{R}^d \times \mathbb{R}^d} c_0 \, d\gamma_0 + \int_{\mathbb{R}^d \times \mathbb{R}^d} c_1 \, d\gamma_1 &= \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \{c_0(x_0, x) + c_1(x, x_1)\} \, d\tilde{\gamma}(x_0, x, x_1) \\ &\geq \int_{\mathbb{R}^d \times \mathbb{R}^d} c \, d\pi_{0,1}^\# \tilde{\gamma} \geq \int_{\mathbb{R}^d \times \mathbb{R}^d} c \, d\gamma \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^d} \{c_0(x_0, T(x_0, x_1)) + c_1(T(x_0, x_1), x_1)\} \, d\gamma(x_0, x_1) \\ &\geq W_{c_0}(\nu_0, T^\# \gamma) + W_{c_1}(T^\# \gamma, \nu_1) \end{aligned}$$

which, taking the infimum with respect to  $\gamma_0 \in \Pi(\nu_0, \rho)$  and  $\gamma_1 \in \Pi(\rho, \nu_1)$ , enable us to deduce that  $T^\# \gamma$  solves (WI) as well as the equality of the optimal values of (WI) and (5.2.2).

Assume now that  $\rho$  solves (WI) and consider optimal transport plans  $\gamma_0 \in \Pi(\nu_0, \rho)$  with respect to the cost  $c_0$  and  $\gamma_1 \in \Pi(\rho, \nu_1)$  with respect to the cost  $c_1$ . Using again the gluing lemma we find  $\tilde{\gamma} \in \Pi(\nu_0, \rho, \nu_1)$  with  $\pi_{0, \text{piv}}^\# \tilde{\gamma} = \gamma_0$  and  $\pi_{\text{piv}, 1}^\# \tilde{\gamma} = \gamma_1$ , and we then have

$$\begin{aligned} \inf (5.2.2) &= \inf (\text{WI}) = \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \{c_0(x_0, x) + c_1(x, x_1)\} \, d\tilde{\gamma}(x_0, x, x_1) \\ &\geq \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} c(x_0, x_1) \, d\tilde{\gamma}(x_0, x, x_1) = \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} c \, d\pi_{0,1}^\# \tilde{\gamma}. \end{aligned}$$

Therefore  $\pi_{0,1}^\# \tilde{\gamma}$  is optimal for (5.2.2) and  $c_0(x_0, x) + c_1(x, x_1) = c(x_0, x_1)$  on  $\text{spt}(\tilde{\gamma})$ .  $\square$

In other words, the coercivity condition (5.2.1) ensures that we can replace  $\mathcal{A} = \mathcal{P}(\mathbb{R}^d)$  by  $\mathcal{A} = \mathcal{P}(K)$  in (WI) and therefore always optimize over probabilities over a fixed compact subset of  $\mathbb{R}^d$ .

*Remark 5.2.4.* If  $\nu_0$  is absolutely continuous and  $c_0$  is locally Lipschitz and satisfies the twist condition, i.e. it is differentiable in the first coordinate and for every  $x_0 \in \text{spt}(\nu_0)$

$$y \mapsto \nabla_{x_0} c_0(x_0, y) \quad \text{is injective,}$$

then (WI) has a unique minimizer. Indeed, the conditions above imply that

$$\rho \mapsto W_{c_0}(\rho, \nu_0) \quad \text{is strictly convex.}$$

The proof follows along the lines of Proposition 7.19 of [104] once one observes that, thanks to the twist condition and the regularity assumptions on  $c_0$  and  $\nu_0$ , the optimal transport problem between  $\nu_0$  and  $\rho$  has a unique transport plan induced by a map, see Proposition 1.15 [104] and discussion after. This gives uniqueness for smooth and strictly convex costs. Note that this also gives uniqueness for (ii) and (iii) in the case of concave costs, i.e. when  $c_0(x, y) = l(|x - y|)$  for  $l : \mathbb{R}_+ \rightarrow \mathbb{R}_+$  strictly concave, increasing and differentiable on  $(0, +\infty)$ , if we assume  $\nu_0$  absolutely continuous and for (ii)  $K \cap \text{spt} \nu_0 = \emptyset$ , or for (iii)  $\text{spt}(\phi) \cap \text{spt} \nu_0 = \emptyset$  (see [59] or [97] for refinements and weaker conditions). All these arguments for uniqueness of course remain true if we replace the assumptions on  $\nu_0$  and  $c_0$  by similar assumptions on  $\nu_1$  and  $c_1$ .

## 5.3 Dual formulations

### 5.3.1 Location constraints

Thanks to the coercivity condition (5.2.1) any solution  $\rho$  to (WI) with  $\mathcal{A} = \mathcal{P}(\mathbb{R}^d)$  is necessarily concentrated on the compact set  $K$ , hence both cases (i) and (ii) (without the coercivity condition) can be formulated over  $\mathcal{P}(K)$ . In this case, it can be convenient, to characterize solutions of the convex minimization problem (WI) by duality as follows.

**Proposition 5.3.1.** *In the cases (i) together with (5.2.1), and (ii) problem (WI) admits the dual formulation*

$$\sup \left\{ \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 : \varphi_0, \varphi_1 \in C(K), \varphi_0 + \varphi_1 = 0 \right\}, \quad (5.3.1)$$

where for a function  $\varphi \in C(K)$  the  $c_0$ -transform of  $\varphi$ ,  $\varphi^{c_0} \in C(\text{spt}(\nu_0))$  is defined by

$$\varphi_0^{c_0}(x_0) := \min_{x \in K} \{c_0(x_0, x) - \varphi(x)\} \quad \forall x_0 \in \text{spt}(\nu_0), \quad (5.3.2)$$

and similarly the  $c_1$ -transform of  $\varphi$ ,  $\varphi^{c_1} \in C(\text{spt}(\nu_1))$  is given by

$$\varphi_1^{c_1}(x_1) := \min_{x \in K} \{c_1(x, x_1) - \varphi(x)\} \quad \forall x_1 \in \text{spt}(\nu_1). \quad (5.3.3)$$

Furthermore, the dual problem (5.3.1) has an optimizer and it is also equivalent to the problem

$$\sup \left\{ \int_{\mathbb{R}^d} u_0 d\nu_0 + \int_{\mathbb{R}^d} u_1 d\nu_1 : u_0(x_0) + u_1(x_1) \leq c(x_0, x_1) \right\}, \quad (5.3.4)$$

where the cost function  $c$  is given by

$$c(x_0, x_1) = \min \{c_0(x_0, x) + c_1(x, x_1) : x \in K\}.$$

*Proof.* We start by showing the duality formula (5.3.1). Since  $K$  is compact, this follows immediately by applying Fenchel-Rockafellar theorem. Indeed, defining for  $\varphi \in C(K)$

$$G(\varphi) := \int_{\mathbb{R}^d} \varphi^{c_0} d\nu_0, \quad H(\varphi) := \int_{\mathbb{R}^d} (-\varphi)^{c_1} d\nu_1,$$

we have

$$(5.3.1) = - \inf_{\varphi \in C(K)} \{-G(\varphi) - H(\varphi)\}.$$

Note that the functionals  $G$  and  $H$  are convex, continuous with respect to the  $L^\infty$ -norm and finite around, say,  $0 \in C(K)$ . This implies by Fenchel-Rockafellar theorem

$$(5.3.1) = - \max_{\rho \in (C(K))^*} -G^*(\rho) - H^*(-\rho) = \min_{\rho \in (C(K))^*} G^*(\rho) + H^*(-\rho).$$

Now note that by Kantorovich duality we have

$$G^*(\rho) = \begin{cases} W_{c_0}(\rho, \nu_0) & \text{if } \rho \in \mathcal{P}(K) \\ +\infty & \text{if } \rho \in (C(K))^* \setminus \mathcal{P}(K), \end{cases}$$

$$H^*(-\rho) = \begin{cases} W_{c_1}(\rho, \nu_1) & \text{if } \rho \in \mathcal{P}(K) \\ +\infty & \text{if } \rho \in (C(K))^* \setminus \mathcal{P}(K). \end{cases}$$

This implies that indeed

$$(5.3.1) = (\text{WI}).$$

The proof of existence of a minimizer of (5.3.1) follows by standard arguments. We give the main steps for completeness. Note that for any admissible pair  $(\varphi_0, -\varphi_0) \in (C(K))^2$  we can replace  $\varphi_0$  by its  $c_0$ -concave envelope, i.e. setting

$$\begin{aligned} \tilde{\varphi}_0(x) &:= \inf_{x_0 \in \text{spt}(\nu_0)} \{c_0(x_0, x) - \varphi_0^{c_0}(x_0)\}, \\ \tilde{\varphi}_1(x) &:= -\tilde{\varphi}_0(x). \end{aligned} \quad (5.3.5)$$

Then we obtain  $\tilde{\varphi}_0^{c_0} = \varphi_0^{c_0}$  and  $\tilde{\varphi}_0 \geq \varphi_0$  which also implies  $\tilde{\varphi}_1^{c_1} \geq \varphi_1^{c_1}$  (see for instance Proposition 1.34 of [104]). Furthermore, for any  $\lambda \in \mathbb{R}$  the transformation given by  $(\tilde{\varphi}_0, \tilde{\varphi}_1) \mapsto (\tilde{\varphi}_0 + \lambda, \tilde{\varphi}_1 - \lambda)$  does not change the value of the objective in (5.3.1) and keeps  $\tilde{\varphi}_0$   $c_0$ -concave, i.e. like in (5.3.5) up to a constant.

Now consider a maximizing sequence  $(\varphi_0^n, \varphi_1^n)_{n \in \mathbb{N}}$  which without loss of generality satisfies  $\min \varphi_0^n = 0$  and (5.3.5) for every  $n \in \mathbb{N}$ . This implies that  $\varphi_0^n$  have the same modulus of continuity inherited from  $c_0$  (see Box 1.8 Memo in [104]). The uniform modulus of continuity on  $K$  together with  $\min \varphi_0^n = 0$  also give a uniform upper bound on  $\varphi_0^n$ . Since  $\varphi_1^n = -\varphi_0^n$  equicontinuity and boundedness hold for the sequence  $(\varphi_1^n)_{n \in \mathbb{N}}$  as well. By the Arzelà-Ascoli theorem we can then extract a uniformly convergent subsequence and conclude on the optimality of the limit by continuity of the integral operator with respect to uniform convergence.

For the equivalence between (5.3.1) and (5.3.4) let  $\varphi_0, \varphi_1 \in C(K)$  be optimal for (5.3.1) and define  $u_i := \varphi_i^{c_i}$ . They are feasible for (5.3.4) since for any  $x \in K$

$$\begin{aligned} u_0(x_0) + u_1(x_1) &\leq c_0(x_0, x) - \varphi_0(x) + c_1(x, x_1) - \varphi_1(x) \\ &= c_0(x_0, x) + c_1(x, x_1). \end{aligned}$$

This implies

$$\sup (5.3.4) \geq \int_{\mathbb{R}^d} u_0 \, d\nu_0 + \int_{\mathbb{R}^d} u_1 \, d\nu_1 \geq \sup (5.3.1).$$

On the other hand, for  $u_0, u_1$  admissible for (5.3.4) such that

$$\int_{\mathbb{R}^d} u_0 \, d\nu_0 + \int_{\mathbb{R}^d} u_1 \, d\nu_1 \geq \sup (5.3.4) - \varepsilon,$$

define  $\varphi_0 := u_0^{c_0}$ ,  $\varphi_1 := -\varphi_0$ , where for a function  $u$

$$u^{\bar{c}_0}(x) := \inf_{y \in \text{spt} \nu_0} \{c_0(y, x) - u(y)\}.$$

Now we have for  $x_0 \in \text{spt} \nu_0$ ,  $x_1 \in \text{spt} \nu_1$ , by construction

$$\varphi_0^{c_0}(x_0) \geq u(x_0)$$

and

$$\begin{aligned} \varphi_1^{c_1}(x_1) &= \inf_{x \in K} \{c_1(x, x_1) + u_0^{\bar{c}_0}(x)\} \\ &\geq \inf_{x \in K} \left\{ -c_0(x_0, x) + u_0(x_0) + u_1(x_1) + \inf_{y \in \text{spt} \nu_0} \{c_0(y, x) - u_0(y)\} \right\}. \end{aligned}$$

Choosing  $x_0 \in \text{spt } \nu_0$  such that for  $n \in \mathbb{N}$

$$c_0(x_0, x) - u_0(x_0) \geq \inf_{y \in \text{spt } \nu_0} \{c_0(y, x) - u_0(y)\} - \frac{1}{n},$$

we obtain as  $n \rightarrow \infty$

$$\varphi_1^{c_1}(x_1) \geq u_1(x_1).$$

This altogether yields

$$\sup (5.3.1) \geq \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 \geq \sup (5.3.4) - \varepsilon.$$

Letting  $\varepsilon \rightarrow 0$  concludes the desired equality.  $\square$

*Remark 5.3.2.* Note that (5.3.4) is the dual of the standard OT problem (5.2.2). Hence, with Proposition 5.2.3 it would have been enough to prove duality of one of the formulations.

Proposition 5.3.1 gives the following primal dual optimality conditions. If the functions  $\varphi_0$  and  $\varphi_1$  solve (5.3.1), then  $\rho \in \mathcal{P}(K)$  solves (WI) if and only if  $\varphi_0$  is a Kantorovich potential between  $\nu_0$  and  $\rho$  and  $\varphi_1$  is a Kantorovich potential (see Theorem 2.1.13) between  $\rho$  and  $\nu_1$  i.e. there exist  $(\gamma_0, \gamma_1) \in \Pi(\nu_0, \rho) \times \Pi(\rho, \nu_1)$  such that

$$\begin{aligned} \varphi_0(x) + \varphi_0^{c_0}(x_0) &= c_0(x_0, x) & \forall (x_0, x) \in \text{spt}(\gamma_0), \\ \varphi_1(x) + \varphi_1^{c_1}(x_1) &= c_1(x, x_1) & \forall (x, x_1) \in \text{spt}(\gamma_1). \end{aligned}$$

Defining the  $c_0$ -concave envelope of  $\varphi_0$  and the  $c_1$ -concave envelope of  $\varphi_1$  by

$$\begin{aligned} \tilde{\varphi}_0(x) &:= \min_{x_0 \in \text{spt}(\nu_0)} \{c_0(x_0, x) - \varphi_0^{c_0}(x_0)\}, \\ \tilde{\varphi}_1(x) &:= \min_{x_1 \in \text{spt}(\nu_1)} \{c_1(x, x_1) - \varphi_1^{c_1}(x_1)\}, \end{aligned}$$

one has  $\tilde{\varphi}_0 \geq \varphi_0$  and  $\tilde{\varphi}_1 \geq \varphi_1$  with an equality on  $\text{spt}(\rho)$  so that  $\tilde{\varphi}_0 + \tilde{\varphi}_1 \geq 0$  with an equality on  $\text{spt}(\rho)$ .

### 5.3.2 Density constraint

We now consider case (iii) where there is a constraint on the density  $\rho \leq \phi$ , one can characterize minimizers by duality as follows:

**Proposition 5.3.3.** *Consider (WI) in the case (iii) where there is a constraint on the density  $\rho \leq \phi$  with  $\phi \in L^1(\mathbb{R}^d)$ ,  $\phi \geq 0$ ,  $\int_{\mathbb{R}^d} \phi dx > 1$  and  $\text{spt}(\phi)$  compact (as well as  $\text{spt}(\nu_0)$  and  $\text{spt}(\nu_1)$ ). Then the value of (WI) coincides with the value of its (pre-)dual formulation*

$$\sup_{\varphi_0, \varphi_1 \in C(\text{spt}(\phi))^2} \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 + \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0) \phi dx \quad (5.3.6)$$

(where  $\varphi_i^{c_i}$  are as in formulae (5.3.2)-(5.3.3) with  $K$  replaced by  $\text{spt}(\phi)$ ). Moreover, the supremum in (5.3.6) is attained. If  $(\varphi_0, \varphi_1)$  solves (5.3.6), then  $\rho$  solves (WI) under the constraint  $\rho \leq \phi$  if and only if there exist  $\gamma_0 \in \Pi(\rho, \nu_0)$  and  $\gamma_1 \in \Pi(\rho, \nu_1)$  such that

$$\varphi_0(x) + \varphi_0^{c_0}(x_0) = c_0(x_0, x), \quad \forall (x_0, x) \in \text{spt}(\gamma_0), \quad (5.3.7)$$

$$\varphi_1(x) + \varphi_1^{c_1}(x_1) = c_1(x, x_1), \quad \forall (x, x_1) \in \text{spt}(\gamma_1) \quad (5.3.8)$$

(so that  $\gamma_0$  and  $\gamma_1$  are optimal plans and  $\varphi_0$  and  $\varphi_1$  are Kantorovich potentials) and

$$\varphi_0 + \varphi_1 \geq 0 \text{ on } \text{spt}(\phi - \rho), \quad \varphi_0 + \varphi_1 \leq 0 \text{ on } \text{spt}(\rho). \quad (5.3.9)$$

*Proof.* The fact that the concave maximization problem (5.3.6) is the dual of (WI) under the constraint  $\rho \leq \phi$  follows directly from the Fenchel-Rockafellar duality theorem and the Kantorovich duality formula, similarly to the proof of Proposition 5.3.1.

Let us prove now that (5.3.6) admits a solution. To see this we remark that the objective is unchanged when one replaces  $(\varphi_0, \varphi_1)$  by  $(\varphi_0 + \lambda, \varphi_1 - \lambda)$  where  $\lambda$  is a constant. Moreover, replacing  $\varphi_0$  and  $\varphi_1$  by their  $c_0/c_1$ -concaves envelopes defined for every  $x \in \text{spt}(\phi)$  by

$$\begin{aligned} \tilde{\varphi}_0(x) &:= \min_{x_0 \in \text{spt}(\nu_0)} \{c_0(x_0, x) - \varphi_0^{c_0}(x_0)\}, \\ \tilde{\varphi}_1(x) &:= \min_{x_1 \in \text{spt}(\nu_1)} \{c_1(x, x_1) - \varphi_1^{c_1}(x_1)\} \end{aligned} \quad (5.3.10)$$

it is well-known that  $\tilde{\varphi}_i \geq \varphi_i$  and  $\tilde{\varphi}_i^{c_i} = \varphi_i^{c_i}$  for  $i = 0, 1$  so that replacing  $\varphi_i$  by  $\tilde{\varphi}_i$  is an improvement in the objective of (5.3.6), moreover the functions  $\tilde{\varphi}_i$  have a uniform modulus of continuity inherited from the uniform continuity of  $c_i$ . From these observations, we can find a uniformly equicontinuous maximizing sequence  $(\varphi_0^n, \varphi_1^n)_n$  for which  $\min_{\text{spt}(\phi)} \varphi_0^n = 0$  so that  $\varphi_0^n$  is also uniformly bounded. Since  $\min(\varphi_1^n + \varphi_0^n, 0) \leq 0$ , the fact that  $(\varphi_0^n, \varphi_1^n)_{n \in \mathbb{N}}$  is a maximizing sequence together with the uniform bounds on  $\varphi_0^n$  we get a uniform lower bound on  $\int_{\mathbb{R}^d} (\varphi_1^n)^{c_1} d\nu_1$  from which we easily derive a uniform upper bound on  $\varphi_1^n$  thanks to (5.3.10). To show that  $\varphi_1^n$  is also uniformly bounded from below, we observe that the quantity

$$\int_{\mathbb{R}^d} (\varphi_1^n)^{c_1} d\nu_1 + \int_{\mathbb{R}^d} \min(\varphi_1^n + \varphi_0^n, 0) \phi dx$$

is bounded from below and bounded from above by  $C + (\int \phi dx - 1) \min_{\text{spt}(\phi)} \varphi_1^n$  for some constant  $C$ . Since  $\int \phi dx > 1$  this gives the desired lower bound. Having thus found a uniformly bounded and equicontinuous maximizing sequence, we deduce the existence of a solution to (5.3.6) from Arzelà-Ascoli theorem.

Let us now look at the optimality conditions which follow from the above duality. If  $(\varphi_0, \varphi_1)$  solves (5.3.6), then  $\rho$  solves (WI) under the constraint  $\rho \leq \phi$  if and only if

$$W_{c_0}(\nu_0, \rho) + W_{c_1}(\rho, \nu_1) = \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 + \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0) \phi.$$

If  $\gamma_0$  (respectively  $\gamma_1$ ) is an optimal plan for  $c_0$  (resp.  $c_1$ ) between  $\nu_0$  and  $\rho$  (resp.  $\rho$  and  $\nu_1$ ), we thus have

$$\begin{aligned} & \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 + \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0) \phi = \int_{\mathbb{R}^d} c_0 d\gamma_0 + \int_{\mathbb{R}^d} c_1 d\gamma_1 \\ & \geq \int_{\mathbb{R}^d} (\varphi_0^{c_0}(x_0) + \varphi_0(x)) d\gamma_0(x_0, x) + \int_{\mathbb{R}^d} (\varphi_1^{c_1}(x_1) + \varphi_1(x)) d\gamma_1(x, x_1) \\ & = \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_0 + \int_{\mathbb{R}^d} (\varphi_0 + \varphi_1) d\rho \\ & \geq \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_0 + \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0) d\rho \\ & \geq \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_0 + \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0) \phi dx \end{aligned}$$

where we have used that  $\rho \leq \phi$  in the last line. All the inequalities above should therefore be equalities which together with the continuity of  $\varphi_0$  and  $\varphi_1$  is easily seen to imply (5.3.7)-(5.3.8)-(5.3.9). This shows the necessity of these conditions.

For the proof of sufficiency first note that weak duality holds, i.e. for any  $\rho \in \mathcal{P}_{\text{ac}}(\text{spt}(\phi))$  with  $\rho \leq \phi$  and  $\varphi_0, \varphi_1 \in C(\text{spt}(\phi))^2$  we have

$$\begin{aligned} & W_{c_0}(\nu_0, \rho) + W_{c_1}(\rho, \nu_1) \\ & \geq \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 + \int_{\mathbb{R}^d} (\varphi_0 + \varphi_1)\rho dx \\ & \geq \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 + \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0)\rho dx \\ & \geq \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 + \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0)\phi dx \end{aligned}$$

Assume now that  $\rho \in \mathcal{P}_{\text{ac}}(\text{spt}(\phi))$  and  $\varphi_0, \varphi_1 \in C(\text{spt}(\phi))^2$  satisfy (5.3.7)-(5.3.8)-(5.3.9), then

$$\begin{aligned} & W_{c_0}(\nu_0, \rho) + W_{c_1}(\rho, \nu_1) \\ & \stackrel{(5.3.7), (5.3.8)}{=} \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 + \int_{\mathbb{R}^d} (\varphi_0 + \varphi_1)\rho dx \\ & \stackrel{(5.3.9)}{=} \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 + \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0)\phi dx - \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0)(\phi - \rho) dx \\ & \stackrel{(5.3.9)}{=} \int_{\mathbb{R}^d} \varphi_0^{c_0} d\nu_0 + \int_{\mathbb{R}^d} \varphi_1^{c_1} d\nu_1 + \int_{\mathbb{R}^d} \min(\varphi_0 + \varphi_1, 0)\phi dx. \end{aligned}$$

□

**Corollary 5.3.4.** *Under the same assumptions as in Proposition 5.3.3, assume that  $\rho$  is optimal for (WI) under the constraint  $\rho \leq \phi$  and let  $\gamma_0$  and  $\gamma_1$  be optimal transport plans. Then, whenever  $x_0, x, x_1$  are such that  $(x_0, x) \in \text{spt}(\gamma_0)$ ,  $(x, x_1) \in \text{spt}(\gamma_1)$ ,  $x \in \text{spt}(\phi - \rho)$ , we have*

$$c_0(x_0, x) + c_1(x, x_1) = \min_{y \in \text{spt}(\phi - \rho)} \{c_0(x_0, y) + c_1(y, x_1)\}.$$

*Proof.* Let  $(\varphi_0, \varphi_1)$  solve (5.3.6). By definition of the  $c_i$ -transforms ((5.3.2), (5.3.3)), for every  $(x_0, x_1, y) \in \text{spt}(\nu_0) \times \text{spt}(\nu_1) \times \text{spt}(\phi)$  one has

$$c_0(x_0, y) + c_1(y, x_1) \geq \varphi_0^{c_0}(x_0) + \varphi_1^{c_1}(x_1) + (\varphi_0 + \varphi_1)(y).$$

Together with (5.3.9) this implies that for every  $(x_0, x_1) \in \text{spt}(\nu_0) \times \text{spt}(\nu_1)$

$$\min_{y \in \text{spt}(\phi - \rho)} \{c_0(x_0, y) + c_1(y, x_1)\} \geq \varphi_0^{c_0}(x_0) + \varphi_1^{c_1}(x_1).$$

But now if  $x \in \text{spt}(\rho) \cap \text{spt}(\phi - \rho)$ , by (5.3.9) again we have  $\varphi_0(x) + \varphi_1(x) = 0$ . Hence by (5.3.7)-(5.3.8) whenever  $(x_0, x) \in \text{spt}(\gamma_0)$ ,  $(x, x_1) \in \text{spt}(\gamma_1)$  and  $x \in \text{spt}(\phi - \rho)$  we have

$$\varphi_0^{c_0}(x_0) + \varphi_1^{c_1}(x_1) = c_0(x_0, x) + c_1(x, x_1) \geq \min_{y \in \text{spt}(\phi - \rho)} \{c_0(x_0, y) + c_1(y, x_1)\},$$

which yields the desired result. □

In the discrete case, we can deduce a bang-bang result stating that the constraint  $\rho \leq \phi$  is always binding when  $\rho > 0$  under mild conditions on the cost. We will give similar bang-bang results for distance-like costs in Section 5.4.

**Corollary 5.3.5.** *Assume that  $\nu_0$  and  $\nu_1$  are discrete, for every  $(x_0, x_1) \in \text{spt}(\nu_0) \times \text{spt}(\nu_1)$ ,  $c_0(x_0, \cdot)$  and  $c_1(\cdot, x_1)$  are  $C^1$  and  $M$ -Lipschitz on  $\text{spt}(\phi)$  (for some  $M$  that does not depend on  $x_0$  and  $x_1$ ) and that the set*

$$\{x \in \text{spt}(\phi) : \nabla_x c_0(x_0, x) + \nabla_x c_1(x, x_1) = 0\}, \quad (5.3.11)$$

*is Lebesgue negligible. Then if  $\rho$  is optimal for (WI) under the constraint  $\rho \leq \phi$ , there exists a measurable subset  $E$  of  $\text{spt}(\phi)$  such that  $\rho = \phi \mathbf{1}_E$ .*

*Proof.* Let  $(\varphi_0, \varphi_1)$  solve (5.3.6), As seen in the proof of Proposition 5.3.3, we may assume that, for every  $x \in \text{spt}(\phi)$

$$\begin{aligned} \varphi_0(x) &:= \min_{x_0 \in \text{spt}(\nu_0)} \{c_0(x_0, x) - \varphi_0^{c_0}(x_0)\}, \\ \varphi_1(x) &:= \min_{x_1 \in \text{spt}(\nu_1)} \{c_1(x, x_1) - \varphi_1^{c_1}(x_1)\}, \end{aligned}$$

so that  $\varphi_0$  and  $\varphi_1$  are Lipschitz hence differentiable a.e. on  $\text{spt}(\phi)$ . Since  $\varphi_0 + \varphi_1 = 0$  on  $\text{spt}(\rho) \cap \text{spt}(\phi - \rho)$ , we then have

$$\nabla \varphi_0 + \nabla \varphi_1 = 0 \quad \text{a.e. on } \{0 < \rho < \phi\},$$

but if  $\varphi_0$  (resp.  $\varphi_1$ ) is differentiable at  $x$  and  $(x_0, x) \in \text{spt}(\gamma_0)$  (resp.  $(x, x_1) \in \text{spt}(\gamma_1)$ ), where  $\gamma_0$  and  $\gamma_1$  are optimal plans, then

$$\nabla \varphi_0(x) = \nabla_x c_0(x_0, x), \quad \nabla \varphi_1(x) = \nabla_x c_1(x, x_1).$$

Hence, denoting by  $A_i$  the countable concentration set of  $\nu_i$  ( $i = 0, 1$ ), a.e.  $x$  such that  $0 < \rho(x) < \phi(x)$  belongs to

$$\bigcup_{(x_0, x_1) \in A_0 \times A_1} \{x \in \text{spt}(\phi) : \nabla_x c_0(x_0, x) + \nabla_x c_1(x, x_1) = 0\},$$

which is negligible by assumption. The desired bang-bang conclusion then readily follows.  $\square$

*Remark 5.3.6.* In some cases, for instance when the costs  $c_0$  and  $c_1$  depend quadratically or more generally as a  $p$ -th power of the distance (with  $p > 1$ ), the set in (5.3.11) reduces to a single point which depends in a Lipschitz way on  $x_0$  and  $x_1$ . The conclusion of Corollary 5.3.5 then still holds under the weaker assumption that one between  $\nu_0$  and  $\nu_1$  is discrete and the other one is singular with respect to the Lebesgue measure. More precisely, this still holds if the Hausdorff dimension of the support of  $\nu_0$  is  $h_0$ , and the Hausdorff dimension of the support of  $\nu_1$  is  $h_1$ , with  $h_0 + h_1 < d$ .

## 5.4 Distance like costs

In this section, we pay special attention to the case of distance-like costs:

$$c_0(x_0, x) := |x_0 - x|^\alpha, \quad c_1(x, x_1) := \lambda |x - x_1|^\alpha, \quad (5.4.1)$$

with  $0 < \alpha \leq 1$  and  $\lambda > 0$ .

### 5.4.1 Location constraint, concentration and integrability on the boundary

Let us start with the case of a location constraint of type (ii):  $\rho \in \mathcal{P}(K)$  for some non-empty compact subset  $K$  of  $\mathbb{R}^d$ .

**Lemma 5.4.1.** *Assume  $K$  is a compact subset of  $\mathbb{R}^d$  and that one of the following assumption holds:*

- $\alpha = 1$ ,  $\lambda > 1$  and the interior of  $K$  is disjoint from  $\text{spt}(\nu_1)$ ,
- $\alpha \in (0, 1)$  and the interior of  $K$  is disjoint from  $\text{spt}(\nu_0) \cup \text{spt}(\nu_1)$ .

Then any solution  $\rho$  of (WI) under the constraint  $\rho \in \mathcal{P}(K)$  is supported by  $\partial K$ .

*Proof.* For  $(x_0, x_1) \in \text{spt}(\nu_0) \times \text{spt}(\nu_1)$ , set

$$c(x_0, x_1) := \min_{x \in K} \{|x_0 - x|^\alpha + \lambda|x - x_1|^\alpha\},$$

$$T(x_0, x_1) := \arg \min_{x \in K} \{|x_0 - x|^\alpha + \lambda|x - x_1|^\alpha\}.$$

We know from Proposition 5.2.3 that  $\rho$  is supported by  $T(\text{spt}(\nu_0) \times \text{spt}(\nu_1))$ . In particular, if  $x \in \text{spt}(\rho)$  is an interior point of  $K$  then it is a local minimizer of  $c_0(x_0, \cdot) + c_1(\cdot, x_1)$  for some  $(x_0, x_1) \in \text{spt}(\nu_0) \times \text{spt}(\nu_1)$ . In the case  $\alpha = 1$ ,  $\lambda > 1$ , by the triangular inequality there is one unique global minimizer (without constraint  $x \in K$ ) which equal to  $x_1$ , and no other local minimizer, but since  $x \neq x_1$ , this is clearly impossible.

In the case  $\alpha < 1$ , our assumption implies that  $x \notin \{x_0, x_1\}$ , so that  $x$  has to be a critical point of  $c_0(x_0, \cdot) + c_1(\cdot, x_1)$ . One should have

$$\alpha|x - x_0|^{\alpha-2}(x - x_0) + \lambda\alpha|x - x_1|^{\alpha-2}(x - x_1) = 0,$$

so that  $x_0 \neq x_1$  and  $x \in [x_0, x_1]$ . But  $c_0(x_0, \cdot) + c_1(\cdot, x_1)$  is strictly concave on  $[x_0, x_1]$  which contradicts  $x$  being a local minimizer.  $\square$

*Remark 5.4.2.* If  $\alpha = \lambda = 1$  the previous result is false: if  $d = 1$ ,  $\nu_0 = \delta_0$  and  $\nu_1 = \delta_1$ , and  $K = [1/4, 3/4]$ , then it follows from the triangle inequality that any probability supported by  $K$  is actually optimal.

Now that we know that minimizers are supported by  $\partial K$ , one may wonder, if  $K$  and  $\nu_1$  are regular enough, whether these minimizers are absolutely continuous with respect to the  $(d - 1)$ -Hausdorff measure on  $\partial K$ , the answer is positive if  $\nu_0$  is discrete, i.e. is concentrated on a countable set,  $\nu_0(K) = 0$  and  $\nu_1$  is absolutely continuous with support disjoint from  $\text{int}(K)$  (see Proposition 5.4.4 below). A first step consists in the following result.

**Lemma 5.4.3.** *Assume that  $c_0$  and  $c_1$  are as in (5.4.1) (with  $\alpha \in (0, 1]$  and  $\lambda > 1$  if  $\alpha = 1$ ), and that  $K$  is compact. Then for every  $x_0$  and (Lebesgue-)almost every  $x_1 \in \mathbb{R}^d \setminus K$ , the set*

$$T_{x_0}(x_1) := \arg \min_{x \in K} \{|x_0 - x|^\alpha + \lambda|x - x_1|^\alpha\}$$

*is a singleton.*

*Proof.* Fix  $x_0$ , set

$$c_{x_0}(x_1) := \min_{x \in K} \{|x_0 - x|^\alpha + \lambda|x - x_1|^\alpha\},$$

and observe that  $c_{x_0}$  is locally Lipschitz on  $\mathbb{R}^d \setminus K$ . It thus follows from Rademacher's theorem that almost every  $x_1 \in \mathbb{R}^d \setminus K$  is a point of differentiability of  $c_{x_0}$ , and for such a point, if  $x \in T_{x_0}(x_1)$ , we have

$$\nabla c_{x_0}(x_1) = \lambda\alpha|x_1 - x|^{\alpha-2}(x_1 - x) \neq 0.$$

If  $\alpha \in (0, 1)$  this immediately gives the claim with

$$T_{x_0}(x_1) = \{x_1 + (\lambda\alpha)^{\frac{1}{1-\alpha}} |\nabla c_{x_0}(x_1)|^{\frac{2-\alpha}{\alpha-1}} \nabla c_{x_0}(x_1)\}.$$

If  $\alpha = 1$  and  $\lambda > 1$ , if both  $x$  and  $x'$  belong to  $T_{x_0}(x_1)$  then  $x_1, x$  and  $x'$  are aligned, so that the triangle inequality between their differences is saturated. But if  $x \in [x_1, x']$ , by the definition of  $T_{x_0}(x_1)$  and  $\lambda > 1$ , we should also have

$$\begin{aligned} c_{x_0}(x_1) &= |x - x_0| + \lambda|x - x_1| = |x' - x_0| + \lambda|x' - x_1| \\ &= |x' - x_0| + \lambda(|x - x_1| + |x' - x|) \\ &> |x' - x_0| + |x' - x| + \lambda|x - x_1|, \end{aligned}$$

which is impossible by the triangle inequality, yielding the a.e. single-valuedness of  $T_{x_0}$  in this case as well.  $\square$

**Proposition 5.4.4.** *Assume that either  $\alpha = 1$ ,  $\lambda > 1$  or  $\alpha \in (0, 1)$  and*

- $K$  is the closure of an open, bounded set in  $\mathbb{R}^d$  with a boundary of class  $C^{1,1}$ ,
- $\nu_0$  is discrete and  $\nu_0(K) = 0$ ,
- $\nu_1$  is absolutely continuous and  $\text{int}(K) \cap \text{spt } \nu_1 = \emptyset$ .

*Then, any solution  $\rho$  of (WI) under the constraint  $\rho \in \mathcal{P}(K)$  is absolutely continuous with respect to the  $(d-1)$ -Hausdorff measure on  $\partial K$ .*

*Proof.* Since  $\nu_0$  is discrete, we can write  $\nu_0 = \sum_{x_0 \in A_0} p_{x_0} \delta_{x_0}$ , with  $A_0$  at most countable, disjoint from  $K$  and  $p_{x_0} > 0$  for every  $x_0 \in A_0$ . It follows from Proposition 5.2.3 and Lemma 5.4.3 that there exists a transport plan  $\gamma$  between  $\nu_0$  and  $\nu_1$ , which can be written as

$$\gamma = \sum_{x_0 \in A_0} p_{x_0} \delta_{x_0} \otimes \nu_1^{x_0},$$

such that defining  $T_{x_0}$  as in Lemma 5.4.3 and  $T(x_0, x_1) = T_{x_0}(x_1)$  one has

$$\rho = T^\# \gamma = \sum_{x_0 \in A_0} p_{x_0} T_{x_0}^\# \nu_1^{x_0}.$$

Since the second marginal of  $\gamma$  is  $\nu_1$ , we also have

$$\nu_1 = \sum_{x_0 \in A_0} p_{x_0} \nu_1^{x_0},$$

so that all the measures  $\nu_1^{x_0}$  are dominated by  $1/p_{x_0}\nu_1$  hence absolutely continuous. We are thus left to show that for each fixed  $x_0$  in the countable set  $A_0$ , the measure  $T_{x_0}^\#\nu_1^{x_0}$  (which is supported by  $\partial K$  by Lemma 5.4.1) is absolutely continuous with respect to the  $(d-1)$ -Hausdorff measure on  $\partial K$  which from now on we denote by  $\sigma_{(d-1),\partial K}$ . We now fix  $x_0 \in A_0$  and a Borel subset  $A$  of  $\partial K$  and our aim is to bound

$$(T_{x_0}^\#\nu_1^{x_0})(A) = \nu_1^{x_0}(T_{x_0}^{-1}(A)).$$

To this end, let us distinguish the two cases  $\alpha = 1, \lambda > 1$  and  $\alpha \in (0, 1)$ .

Assume  $\alpha = 1$  and  $\lambda > 1$ . Since  $\nu_1(K) = 0$  (because  $\partial K$  being a smooth hypersurface, it is Lebesgue negligible and  $\nu_1(\text{int}(K)) = 0$ ), we have

$$\nu_1^{x_0}(T_{x_0}^{-1}(A) \setminus K) = \nu_1^{x_0}(T_{x_0}^{-1}(A)).$$

Now take  $x = T_{x_0}(x_1) \in \partial K$  with  $x_1 \notin K$  which is  $\nu_1$ -a.e. the case (so that  $x \notin \{x_0, x_1\}$ ). By optimality, there exists  $\beta \geq 0$  such that

$$\widehat{x - x_0} + \lambda \widehat{x - x_1} + \beta n(x) = 0,$$

where for  $\xi \in \mathbb{R}^d \setminus \{0\}$ , we have set  $\widehat{\xi} = \xi/|\xi|$ , and where  $n(x)$  is the outward normal to  $\partial K$  at  $x$ . Using the fact that  $\lambda \widehat{x - x_1}$  has norm  $\lambda$  yields

$$\lambda^2 = \beta^2 + 1 + 2\beta n(x) \cdot \widehat{x - x_0},$$

whose only non-negative root is

$$\beta = \beta_{x_0}(x) := -n(x) \cdot \widehat{x - x_0} + \sqrt{\lambda^2 - 1 + (n(x) \cdot \widehat{x - x_0})^2},$$

so that

$$\lambda \widehat{x_1 - x} = \beta_{x_0}(x)n(x) + \widehat{x - x_0},$$

and the right hand side is a Lipschitz function of  $x$  thanks to our assumptions ( $\partial K$  being  $C^{1,1}$  and  $x_0$  being at a positive distance from  $K$ , hence from  $x$ ). Using again that  $\lambda \widehat{x_1 - x}$  has norm  $\lambda$ , this shows that if  $x = T_{x_0}(x_1)$  then for some  $r \in [0, R]$  with  $R = \lambda^{-1} \text{diam}(\text{spt } \nu_1 - K)$  there holds

$$x_1 = F_{x_0}(r, x) := x + r[\beta_{x_0}(x)n(x) + \widehat{x - x_0}].$$

Hence

$$\nu_1^{x_0}(T_{x_0}^{-1}(A)) \leq \nu_1^{x_0}(F_{x_0}([0, R] \times A)).$$

If  $\sigma_{(d-1),\partial K}(A) = 0$ , the smoothness of  $K$  and the fact that  $F_{x_0}$  is Lipschitz on  $[0, R] \times \partial K$ , readily imply that  $F_{x_0}([0, R] \times A)$  is Lebesgue negligible. Hence  $\nu_1^{x_0}(T_{x_0}^{-1}(A)) = 0$  and since this holds for any  $x_0 \in A_0$ , we also have  $\rho(A) = 0$ , which implies the absolute continuity of  $\rho$  with respect to  $\sigma_{(d-1),\partial K}$ .

Let us now assume that  $\alpha \in (0, 1)$ . To cope with the fact that  $c_1(x, x_1)$  is not differentiable if  $x = x_1$ , it will be convenient to fix  $\varepsilon > 0$  and to consider  $x_1 \in A_1^\varepsilon$ , where

$$A_1^\varepsilon := \{x_1 \in \text{spt}(\nu_1) ; d(K, x_1) \geq \varepsilon\},$$

and

$$d(K, x) := \min_{y \in K} |x - y|,$$

is the Euclidean distance to  $K$ . If  $x_1 \in A_1^\varepsilon \cap T_{x_0}^{-1}(x)$  with  $x \in A$ , it follows from the first-order optimality condition, there is some  $r \geq 0$  such that

$$x_1 = G_{x_0}(r, x) := x + |H_{x_0}(r, x)|^{\frac{2-\alpha}{\alpha-1}} H_{x_0}(r, x),$$

where

$$H_{x_0}(r, x) = rn(x) + \lambda^{-1}|x - x_0|^{\alpha-2}(x - x_0).$$

Now, note that

$$|H_{x_0}(r, x)| = |x_1 - x|^{\alpha-1}.$$

This shows that

$$\begin{aligned} |r| &\leq |x_1 - x|^{\alpha-1} + \lambda^{-1}|x - x_0|^{\alpha-1} \\ &\leq \varepsilon^{\alpha-1} + \lambda^{-1} \max_{x \in K} |x - x_0|^{\alpha-1} =: R_\varepsilon(x_0). \end{aligned}$$

Hence,  $A_1^\varepsilon \cap T_{x_0}^{-1}(x)$  is included in the image by  $G_{x_0}$  of the set  $\{(r, x), x \in A, r \in [0, R_\varepsilon(x_0)]\}$ . Since  $G_{x_0}$  is Lipschitz (with a Lipschitz constant depending on  $\varepsilon$ ) on this set we obtain as soon as  $\sigma_{(d-1), \partial K}(A) = 0$

$$\begin{aligned} \nu_1^{x_0}(T_{x_0}^{-1}(A)) &= \nu_1^{x_0}(T_{x_0}^{-1}(A) \setminus K) = \lim_{\varepsilon \searrow 0} \nu_1^{x_0}(T_{x_0}^{-1}(A) \cap A_1^\varepsilon) \\ &\leq \lim_{\varepsilon \searrow 0} \nu_1^{x_0}(G_{x_0}([0, R_\varepsilon(x_0)] \times A)) = 0. \end{aligned}$$

Thus we can conclude as before that  $\rho$  is absolutely continuous.  $\square$

**Proposition 5.4.5.** *Suppose in addition to the assumptions of Proposition 5.4.4 that  $\nu_0$  has finite support,  $\nu_1$  has a bounded density with respect to the  $d$ -dimensional Lebesgue measure. If  $\alpha \in (0, 1)$ , further assume that  $K \cap \text{spt } \nu_1 = \emptyset$ . Then  $\rho$  has a bounded density with respect to the  $(d-1)$ -Hausdorff measure on  $\partial K$ .*

*Proof.* In the case  $\alpha = 1$ ,  $\lambda > 1$  we can continue using the same notation and Lipschitz mapping  $F_{x_0}$  and  $R$  as in the proof of Proposition 5.4.4 to conclude for any Borel subset  $A$  of  $\partial K$

$$\begin{aligned} \rho(A) &= \sum_{x_0 \in \text{spt}(\nu_0)} p_{x_0} \nu_1^{x_0}(T_{x_0}^{-1}(A)) \\ &\leq \sum_{x_0 \in \text{spt}(\nu_0)} p_{x_0} \nu_1^{x_0}(F_{x_0}([0, R] \times A)) \\ &\leq \sum_{x_0 \in \text{spt}(\nu_0)} \|\nu_1\|_{L^\infty} \mathcal{L}^d(F_{x_0}([0, R] \times A)) \\ &\leq C \text{card}(\text{spt } \nu_0) \|\nu_1\|_{L^\infty} R \sigma_{(d-1), \partial K}(A) \end{aligned}$$

where  $C$  is a constant that only depends on the  $C^{1,1}$  smoothness of  $\partial K$  and the maximal Lipschitz constant of  $F_{x_0}$  over  $[0, R] \times \partial K$ , with respect to  $x_0 \in \text{spt}(\nu_0)$ , and  $\text{card}(\text{spt } \nu_0)$  denotes the cardinality of the support of  $\nu_0$ . This way we deduce that  $\rho \in L^\infty(\partial K, \sigma_{(d-1), \partial K})$ .

For the case  $\alpha \in (0, 1)$  we need in addition  $K \cap \text{spt } \nu_1 = \emptyset$  to ensure that, again using the same arguments and notation as in the proof of Proposition 5.4.4, there is an  $\varepsilon_0 > 0$

such that  $A_1^{\varepsilon_0} = \text{spt}(\nu_1)$ . In this way, all the analysis from the previous proof can be carried through on  $A_1^{\varepsilon_0}$  and we obtain

$$\begin{aligned}
 \rho(A) &= \sum_{x_0 \in \text{spt}(\nu_0)} p_{x_0} \nu_1^{x_0}(T_{x_0}^{-1}(A) \cap A_1^{\varepsilon_0}) \\
 &\leq \sum_{x_0 \in \text{spt}(\nu_0)} p_{x_0} \nu_1^{x_0}(G_{x_0}([0, R_{\varepsilon_0}(x_0)] \times A)) \\
 &\leq \sum_{x_0 \in \text{spt}(\nu_0)} \|\nu_1\|_{L^\infty} \mathcal{L}^d(G_{x_0}([0, R_{\varepsilon_0}(x_0)] \times A)) \\
 &\leq C \text{card}(\text{spt} \nu_0) \|\nu_1\|_{L^\infty} R_{\varepsilon_0}(x_0) \sigma_{(d-1), \partial K}(A),
 \end{aligned}$$

where  $C$  is a constant that only depends on the  $C^{1,1}$  smoothness of  $\partial K$  and the maximal with respect to  $x_0 \in \text{spt}(\nu_0)$  Lipschitz constant of  $G_{x_0}$  over  $[0, R_{\varepsilon_0}(x_0)] \times \partial K$ .  $\square$

One might also be interested in the case that the distribution of residents represented by  $\nu_0$  is absolutely continuous and  $\nu_1$  is discrete. The case  $\alpha \in (0, 1)$  is completely symmetric as we have not assumed  $\lambda > 1$  in the previous proofs. However for the case  $\alpha = 1, \lambda > 1$ , the proof slightly differs as we shall see below. Arguing as for the proof of Lemma 5.4.3, we have:

**Lemma 5.4.6.** *Assume that  $c_0$  and  $c_1$  are as in (5.4.1) (with  $\alpha \in (0, 1]$  and  $\lambda > 1$  if  $\alpha = 1$ ), and that  $K$  is compact. Then for (Lebesgue-)almost every  $x_0 \in \mathbb{R}^d \setminus K$  and every  $x_1$ , the set*

$$T_{x_1}(x_0) := \arg \min_{x \in K} \{|x_0 - x|^\alpha + \lambda|x - x_1|^\alpha\}$$

is a singleton.

The analogue of Proposition 5.4.4, then reads

**Proposition 5.4.7.** *Assume that either  $\alpha = 1, \lambda > 1$  or  $\alpha \in (0, 1)$  and*

- $K$  is the closure of an open, bounded set in  $\mathbb{R}^d$  with a boundary of class  $C^{1,1}$ ,
- $\nu_0$  is absolutely continuous and  $\text{int}(K) \cap \text{spt} \nu_0 = \emptyset$ ,
- $\nu_1$  is discrete and  $\nu_1(K) = 0$ .

Then, any solution  $\rho$  of (WI) under the constraint  $\rho \in \mathcal{P}(K)$  is absolutely continuous with respect to the  $(d-1)$ -Hausdorff measure on  $\partial K$ .

*Proof.* As already explained, the case  $\alpha > 1$  can be handled exactly as for Proposition 5.4.4, we shall therefore assume that  $\alpha = 1$  and  $\lambda > 1$ . We write  $\nu_1 = \sum_{x_1 \in A_1} p_{x_1} \delta_{x_1}$ , with  $A_1$  countable and  $p_{x_1} > 0$ . It follows from Proposition 5.2.3 and Lemma 5.4.6 that there exists a transport plan  $\gamma$  between  $\nu_0$  and  $\nu_1$ , which can be written as

$$\gamma = \sum_{x_1 \in A_1} \nu_0^{x_1} \otimes p_{x_1} \delta_{x_1},$$

such that defining  $T_{x_1}$  as in Lemma 5.4.3 and  $T(x_0, x_1) = T_{x_1}(x_0)$  one has

$$\rho = T^\# \gamma = \sum_{x_1 \in A_1} p_{x_1} T_{x_1}^\# \nu_0^{x_1}.$$

Since the first marginal of  $\gamma$  is  $\nu_0$ ,  $\nu_0^{x_1}$  is absolutely continuous for every  $x_1 \in A_1$ . We are thus left to show that for each fixed  $x_1$  in the countable set  $A_1$ , the measure  $T_{x_1}^\# \nu_0^{x_1}$  is absolutely continuous with respect to the  $(d-1)$ -Hausdorff measure on  $\partial K$  which from now on we denote by  $\sigma_{(d-1), \partial K}$ . We now fix  $x_1 \in \text{spt}(\nu_1)$  and a Borel subset  $A$  of  $\partial K$  and our aim is to bound

$$(T_{x_1}^\# \nu_0^{x_1})(A) = \nu_0^{x_1}(T_{x_1}^{-1}(A)).$$

Since  $\nu_0(K) = 0$ , we have  $\nu_0^{x_1}(T_{x_1}^{-1}(A) \setminus K) = \nu_0^{x_1}(T_{x_1}^{-1}(A))$ . Now take  $x = T_{x_1}(x_0) \in \partial K$  with  $x_0 \notin K$ . By optimality, there exists  $\beta \geq 0$  such that

$$\widehat{x - x_0} + \lambda \widehat{x - x_1} + \beta n(x) = 0 \text{ where for } \xi \in \mathbb{R}^d \setminus \{0\}, \text{ we have set } \widehat{\xi} = \frac{\xi}{|\xi|}$$

where  $n(x)$  is the outward normal to  $\partial K$  at  $x$ . This time our aim is to write, for fixed  $x_1$ ,  $x_0$  as a Lipschitz function of  $x$  and a length factor, so we proceed as follows. Using the fact that  $\lambda \widehat{x - x_1}$  has norm  $\lambda$  yields

$$1 = \beta^2 + \lambda^2 + 2\beta\lambda n(x) \cdot \widehat{x - x_1}.$$

This time, it is possible that there are two positive solutions for  $\beta$ . We denote them

$$\begin{aligned} \beta_{x_1}^+(x) &:= -\lambda n(x) \cdot \widehat{x - x_1} + \sqrt{(\lambda n(x) \cdot \widehat{x - x_1})^2 + 1 - \lambda^2}, \\ \beta_{x_1}^-(x) &:= -\lambda n(x) \cdot \widehat{x - x_1} - \sqrt{(\lambda n(x) \cdot \widehat{x - x_1})^2 + 1 - \lambda^2}. \end{aligned}$$

Hence, we have one of the following equalities is satisfied by  $(x_0, x, x_1)$

$$\begin{aligned} x_0 &= x + r(\lambda \widehat{x - x_1} + \beta_{x_1}^+(x)n(x)) =: F_{x_1}^+(r, x), \\ x_0 &= x + r(\lambda \widehat{x - x_1} + \beta_{x_1}^-(x)n(x)) =: F_{x_1}^-(r, x), \end{aligned}$$

where  $r \in [0, R]$  and  $R = \text{diam}(\text{spt} \nu_0 - K)$ .

Consider now a Borel set  $A \subset \partial K$  with  $\sigma_{(d-1), \partial K}(A) = 0$ . We distinguish the cases where the discriminant  $(\lambda n(x) \cdot \widehat{x - x_1})^2 + 1 - \lambda^2$  is zero or positive

$$\begin{aligned} A_0 &:= \left\{ x \in A : (\lambda n(x) \cdot \widehat{x - x_1})^2 + 1 - \lambda^2 = 0 \right\}, \\ A_{>} &:= \left\{ x \in A : (\lambda n(x) \cdot \widehat{x - x_1})^2 + 1 - \lambda^2 > 0 \right\} \\ &= \bigcap_{\delta > 0} \underbrace{\left\{ x \in A : (\lambda n(x) \cdot \widehat{x - x_1})^2 + 1 - \lambda^2 \geq \delta \right\}}_{=: A_\delta}. \end{aligned}$$

Since  $F_{x_1}^+$  and  $F_{x_1}^-$  agree with Lipschitz functions on  $[0, R] \times A_0$  and  $[0, R] \times A_\delta$  for  $\delta > 0$  fixed, we obtain

$$\begin{aligned} \nu_0^{x_1}(T_{x_1}^{-1}(A)) &\leq \nu_0^{x_1}(T_{x_1}^{-1}(A_0)) + \lim_{\delta \searrow 0} \nu_0^{x_1}(T_{x_1}^{-1}(A_\delta)) \\ &\leq \nu_0^{x_1}(F_{x_1}^+([0, R] \times A_0)) + \lim_{\delta \searrow 0} (\nu_0^{x_1}(F_{x_1}^+([0, R] \times A_\delta)) + \nu_0^{x_1}(F_{x_1}^-([0, R] \times A_\delta))) \\ &= 0, \end{aligned}$$

as required.  $\square$

It is unclear whether an  $L^\infty$ -bound can be obtained with the same proof strategy since the Lipschitz constant of the maps  $F_{x_1}^+$  and  $F_{x_1}^-$  may blow up as  $\delta \rightarrow 0^+$ . In addition, in Proposition 5.4.4 the smoothness of  $K$  is crucial, as the example below shows.

*Example 5.4.8.* The regularity of  $K$  is essential for the conclusion of the previous propositions. Take for example in the two-dimensional case  $K = \{(x, y) \in \mathbb{R}^d : |x| + |y| \leq 1\}$  and consider the distance-like cost (5.4.1) for any  $\alpha \in (0, 1]$  and  $\lambda > 0$ . Let  $\nu_0 = \delta_{x_0}$  for  $x_0 = (-2, 0)$  and  $\nu_1$  the (normalized) Lebesgue measure on the disc  $B_1(-4)$ . We prove that an optimal pivot measure  $\rho$  is given by  $\delta_{(-1,0)}$ .

Indeed, since

$$\arg \min_{y \in K} \{|y - x_0|^\alpha\} = (-1, 0) = \arg \min_{y \in K} \{|y - x_1|^\alpha\} \quad \text{for all } x_1 \in B_1(-4),$$

we have  $(-1, 0) = \arg \min_{y \in K} \{|y - x_0|^\alpha + \lambda|x - x_1|^\alpha\}$  for all  $x_1 \in B_1(-4)$ . Hence, for the map  $T$  given by  $T(x_0, x_1) = (-1, 0)$  we have by Proposition 5.2.3 that for any optimal plan  $\gamma$  of the multi-marginal formulation (5.2.2) the measure  $T_{\#}\gamma = \delta_{(-1,0)}$  is optimal for (WI).

### 5.4.2 Density constrained solutions are bang-bang

We end this section by observing that in the case of a density constraint  $\rho \leq \phi$ , for distance-like costs minimizers are of bang bang type.

**Proposition 5.4.9.** *Assume that  $c_0$  and  $c_1$  are as in (5.4.1) with  $\lambda > 1$  if  $\alpha = 1$ , that  $\phi \in L^1(\mathbb{R}^d)$  is non-negative with compact support, that  $\int_{\mathbb{R}^d} \phi dx > 1$ , and that both  $\text{spt}(\phi) \cap \text{spt}(\nu_0)$  and  $\text{spt}(\phi) \cap \text{spt}(\nu_1)$  are Lebesgue negligible. Then any solution  $\rho$  of (WI) under the constraint  $\rho \leq \phi$  is of the form  $\rho = \phi \mathbb{1}_E$  for some measurable subset  $E$  of  $\text{spt}(\phi)$ .*

*Proof.* Let us start with the case  $\alpha = 1$ ,  $\lambda > 1$  and define  $A := \{0 < \rho < \phi\}$ , we then consider (Lipschitz) potentials  $\varphi_0$  and  $\varphi_1$  as in the proof of Corollary 5.3.5. A.e. point of  $A$  is a differentiability point of  $\varphi_0$  and  $\varphi_1$ , satisfies  $\nabla\varphi_0 + \nabla\varphi_1 = 0$  and lies in  $\mathbb{R}^d \setminus (\text{spt}(\nu_0) \cup \text{spt}(\nu_1))$ . Hence arguing as in the proof of corollary 5.3.5, for a.e.  $x$  in  $A$  one can find  $x_0 \in \text{spt}(\nu_0) \setminus \{x\}$  and  $x_1 \in \text{spt}(\nu_1) \setminus \{x\}$  such that

$$0 = \nabla\varphi_0(x) + \lambda\nabla\varphi_1(x) = \frac{x - x_0}{|x - x_0|} + \lambda \frac{x - x_1}{|x - x_1|}$$

which is impossible since  $\lambda > 1$ . This shows that  $A$  is negligible and ends the proof for this case.

Consider now the slightly more complicated case where  $\alpha \in (0, 1)$ , since  $x \mapsto |x - x_0|^\alpha$  is Lipschitz only away from  $x_0$ , it is convenient for  $\delta > 0$  to introduce the set

$$B_\delta := \{x \in \text{spt}(\phi) : d(x, \text{spt}(\nu_0) \cup \text{spt}(\nu_1)) \geq \delta\}$$

on  $B_\delta$  the potentials  $\varphi_0$  and  $\varphi_1$  are Lipschitz and we can find a subset  $\tilde{B}_\delta$  of  $B_\delta$  with  $B_\delta \setminus \tilde{B}_\delta$  negligible such that  $\varphi_0$  and  $\varphi_1$  are differentiable on  $\tilde{B}_\delta$ . Consider now for  $\varepsilon > 0$

$$A_\varepsilon := \{\varepsilon < \rho < \phi - \varepsilon\}$$

and let  $\tilde{A}_\varepsilon$  be the subset (of full Lebesgue measure) consisting of its points of density 1 (so that  $\tilde{A}_\varepsilon \subset \text{spt}(\phi - \rho)$ ). Arguing as before for a.e.  $x \in \tilde{A}_\varepsilon \cap \tilde{B}_\delta$ , we can find  $(x_0, x_1) \in \text{spt}(\nu_0) \times \text{spt}(\nu_1)$  such that

$$\nabla\varphi_0(x) + \nabla\varphi_1(x) = \nabla f_{x_0, x_1}(x) = 0,$$

where  $f_{x_0, x_1}(x) := |x - x_0|^\alpha + \lambda|x - x_1|^\alpha$ . Moreover we know from Corollary 5.3.4 that  $\text{spt}(\phi - \rho)$  (hence also  $\tilde{A}_\varepsilon$ ) is included in the level set  $f_{x_0, x_1} \geq f_{x_0, x_1}(x)$ . Since  $x \notin \{x_0, x_1\}$  is a critical point of  $f_{x_0, x_1}$  we have  $x_1 \neq x_0$  and  $x$  belongs to  $[x_0, x_1]$

$$e := \widehat{x - x_0} = \widehat{x_1 - x} = \widehat{x_1 - x_0}.$$

And then the Hessian  $D^2 f_{x_0, x_1}$  at  $x$  takes the form

$$D^2 f_{x_0, x_1}(x) = (\alpha|x - x_0|^{\alpha-2} + \lambda\alpha|x - x_1|^{\alpha-2})(\text{id} + (\alpha - 2)e \otimes e)$$

which shows that  $x$  is a saddle-point of  $f_{x_0, x_1}$ , its hessian having a negative eigenvalue with eigenvector  $e$  and being positive definite on  $e^\perp$ .

Hence for small  $r > 0$ ,  $\tilde{A}_\varepsilon$  should lie in the intersection of  $B(x, r)$  with a certain strict quadratic cone of  $\mathbb{R}^d$  contradicting the fact that  $x$  is a point of density 1 of  $\tilde{A}_\varepsilon$ . This shows that  $A_\varepsilon \cap B_\delta$  is negligible, letting  $\delta \rightarrow 0^+$  we find that  $A_\varepsilon$  is negligible and since this is true for every  $\varepsilon > 0$ , the desired conclusion follows.  $\square$

## 5.5 The case of strictly convex costs with a convex location constraint

We now consider (WI) in the case of the location constraint  $\mathcal{A} = \mathcal{P}(K)$  where  $K$  is a compact convex subset of  $\mathbb{R}^d$  with non-empty interior and  $c_0$  and  $c_1$  satisfy the strong convexity and smoothness assumptions

$$c_i(x, y) := F_i(y - x), \quad F_i \in C^2(\mathbb{R}^d), \quad \lambda \text{id} \leq D^2 F_i \leq \Lambda \text{id}, \quad i = 0, 1, \quad (5.5.1)$$

for some constants  $0 < \lambda \leq \Lambda$ . Since these costs are twisted, (WI) in the case of the location constraint  $\mathcal{A} = \mathcal{P}(K)$  admits a unique solution as soon as  $\nu_0$  (or  $\nu_1$ ) is absolutely continuous.

*Example 5.5.1.* Consider the two dimensional case with a location constraint given by the square  $K$  of Example 5.4.8; take  $\nu_0 = \delta_{(-2, 0)}$ ,  $\nu_1$  uniform on the ball of radius 1 centered at  $(3, 0)$ ,  $c_0(x, y) = |x - y|^2$  and  $c_1(x, y) = 2|x - y|^2$ . Then by a direct application of Proposition 5.2.3, the (unique) solution of (WI) is explicit: it is the image of the uniform measure on the ball  $B$  of radius  $2/3$  centered at  $(4/3, 0)$  by the projection onto  $K$ . It has an atom at  $(1, 0)$ , an absolutely continuous part, uniform on  $B \cap K$  and a one dimensional part corresponding to the points of  $B$  which project onto the segments  $[(0, 1), (1, 0)]$  and  $[(0, -1), (1, 0)]$ .

This shows that, contrary to the case of distance like costs, one should expect that  $\rho$  in general decomposes into a (non-zero) interior part and a boundary part

$$\rho = \rho^{\text{int}} + \rho^{\text{bd}} \quad \text{where } \rho^{\text{int}}(A) := \rho(A \cap \text{int}(K)), \quad \rho^{\text{bd}}(A) := \rho(A \cap \partial K), \quad (5.5.2)$$

for every Borel subset  $A$  of  $\mathbb{R}^d$ . Regarding  $\rho^{\text{bd}}$ , arguing as in Proposition 5.4.5, one can show that if  $\nu_0$  is absolutely continuous,  $\nu_1$  is discrete and  $K$  is of class  $C^{1,1}$ ,  $\rho^{\text{bd}}$  is absolutely continuous with respect to the  $(d - 1)$ -Hausdorff measure on  $\partial K$  (and has a bounded density if in addition  $\nu_0 \in L^\infty$  and  $\nu_1$  is finitely supported). As for the regularity of  $\rho^{\text{int}}$ , we have:

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**Proposition 5.5.2.** *Assume  $c_0$  and  $c_1$  are of the form (5.5.1), that  $\nu_0$  and  $\nu_1$  are compactly supported, with  $\nu_0 \in \mathcal{P}_{\text{ac}}(\mathbb{R}^d)$ , having an bounded density, and that  $K$  is a compact convex subset of  $\mathbb{R}^d$  with non-empty interior. Decomposing the solution  $\rho$  of (WI) in the case of the location constraint  $\mathcal{A} := \mathcal{P}(K)$  as in (5.5.2), we have  $\rho^{\text{int}} \in L^\infty(K)$  and more precisely (identifying  $\rho^{\text{int}}$  with its density), we have*

$$\|\rho^{\text{int}}\|_{L^\infty(K)} \leq \|\nu_0\|_{L^\infty(\mathbb{R}^d)} 2^d \lambda^{-d} \Lambda^d \quad (5.5.3)$$

where  $\lambda$  and  $\Lambda$  are the positive constants appearing in (5.5.1).

To establish the  $L^\infty$  bound in (5.5.3), we shall use a penalization strategy, detailed in the next paragraph, the proof by a standard  $\Gamma$ -convergence argument is postponed to the end of this section.

### 5.5.1 Penalization

Given  $g \in C^2(\mathbb{R}^d)$ , with  $g$  convex and non-negative, let us consider

$$\inf_{\rho \in \mathcal{P}(\mathbb{R}^d)} T(\rho) + \int_{\mathbb{R}^d} g \, d\rho \quad \text{with } T(\rho) := W_{c_0}(\nu_0, \rho) + W_{c_1}(\nu_1, \rho) \quad (5.5.4)$$

then we have.

**Proposition 5.5.3.** *Assuming (5.5.1) and  $\nu_0 \in L^\infty(\mathbb{R}^d)$  compactly supported, (5.5.4) admits a unique solution  $\rho_g$ . Moreover  $\rho_g$  is absolutely continuous with respect to the Lebesgue measure and its density (still denoted  $\rho_g$ ) satisfies for a.e.  $x \in \mathbb{R}^d$ , the bound*

$$\rho_g(x) \leq \|\nu_0\|_{L^\infty} \lambda^{-d} \det(D^2g(x) + 2\Lambda \text{id}) \quad (5.5.5)$$

where  $\lambda$  and  $\Lambda$  are the positive constants appearing in (5.5.1).

*Proof.* The coercivity of  $c_0$ ,  $c_1$  and  $g \geq 0$  give the existence of a minimizer as in Proposition 5.2.3, whereas uniqueness is guaranteed by twistedness of the costs and the absolute continuity of  $\nu_0$ , see Remark 5.2.4. Also Proposition 5.2.3 ensures there is some ball  $B$  which contains a neighbourhood of  $\text{spt}(\rho_g)$ . Then, Theorem 3.3 [93] (incorporating  $g$  in one of the costs considered there), guarantees that the minimizer  $\rho_g$  is absolutely continuous. The optimality condition derived from the dual formulation of (5.5.4), (see (5.3.1)) gives the existence of potentials  $\varphi_0$  and  $\varphi_1$  such that

$$\varphi_0 + \varphi_1 + g = 0 \quad \text{on } B, \quad (5.5.6)$$

and

$$W_{c_0}(\nu_0, \rho_g) = \int_{\mathbb{R}^d} \varphi_0^{c_0} \, d\nu_0 + \int_{\mathbb{R}^d} \varphi_0 \, d\rho_g, \quad W_{c_1}(\rho_g, \nu_1) = \int_{\mathbb{R}^d} \varphi_1^{c_1} \, d\nu_1 + \int_{\mathbb{R}^d} \varphi_1 \, d\rho_g,$$

so that defining the  $c_i$ -concave potentials

$$\begin{aligned} \tilde{\varphi}_0(x) &:= \inf_{x_0 \in \text{spt}(\nu_0)} \{c_0(x_0, x) - \varphi_0^{c_0}(x_0)\}, \\ \tilde{\varphi}_1(x) &:= \inf_{x_1 \in \text{spt}(\nu_1)} \{c_1(x, x_1) - \varphi_1^{c_1}(x_1)\}, \end{aligned}$$

one should have

$$\varphi_i \leq \tilde{\varphi}_i \text{ on } B \quad \text{and} \quad \varphi_i = \tilde{\varphi}_i \text{ on } \text{spt}(\rho_g). \quad (5.5.7)$$

Now observe that thanks to (5.5.1),  $\tilde{\varphi}_0$  and  $\tilde{\varphi}_1$  are semi-concave and more precisely

$$D^2\tilde{\varphi}_i \leq \Lambda \text{id}, \quad i = 0, 1. \quad (5.5.8)$$

In particular  $\tilde{\varphi}_0$  and  $\tilde{\varphi}_1$  are everywhere superdifferentiable, but on  $\text{spt}(\rho_g)$ , thanks to (5.5.6) and (5.5.7),  $\tilde{\varphi}_0 + \tilde{\varphi}_1 + g$  is minimal and since  $g$  is differentiable this implies that  $\tilde{\varphi}_0 + \tilde{\varphi}_1$  is also subdifferentiable on  $\text{spt}(\rho_g)$ . This readily implies that  $\tilde{\varphi}_0$  and  $\tilde{\varphi}_1$  are differentiable on  $\text{spt}(\rho_g)$  and that

$$\nabla\tilde{\varphi}_0 + \nabla\tilde{\varphi}_1 + \nabla g = 0 \text{ on } \text{spt}(\rho_g).$$

By Alexandrov's Theorem (see Theorem 6.9 [53]),  $\tilde{\varphi}_0$  and  $\tilde{\varphi}_1$  are also twice differentiable  $\rho_g$ -a.e. and minimality of  $\tilde{\varphi}_0 + \tilde{\varphi}_1 + g$  on  $\text{spt}(\rho_g)$  also gives

$$D^2\tilde{\varphi}_0 + D^2\tilde{\varphi}_1 + D^2g \geq 0 \text{ } \rho_g\text{-a.e.} \quad (5.5.9)$$

The optimal transport  $S_0$  for the cost  $c_0$  between  $\rho_g$  and  $\nu_0$  (see Theorem 2.1.16) is then given by

$$S_0(x) = x - \nabla F_0^*(\nabla\tilde{\varphi}_0(x)), \quad x \in \text{spt}(\rho_g),$$

where  $F_0^*$  is the Legendre transform of  $F_0$ . The absolute continuity of  $\rho_g$  enables us to use Theorem 2.1.25 and the existence of a set of full measure for  $\rho_g$  for which one has the Jacobian equation

$$\rho_g = \nu_0 \circ S_0 \det(\text{id} - D^2F_0^*(\nabla\tilde{\varphi}_0)D^2\tilde{\varphi}_0), \quad (5.5.10)$$

where  $D^2\tilde{\varphi}_0(x)$  is to be understood in the sense of Alexandrov and  $\text{id} - D^2F_0^*(\nabla\tilde{\varphi}_0)D^2\tilde{\varphi}_0$ , which is diagonalizable with real and non-negative eigenvalues, can be rewritten as

$$\text{id} - D^2F_0^*(\nabla\tilde{\varphi}_0)D^2\tilde{\varphi}_0 = D^2F_0^*(\nabla\tilde{\varphi}_0)(D^2F_0(x - S_0(x)) - D^2\tilde{\varphi}_0(x)),$$

together with (5.5.10), since  $D^2F_0^* \leq \lambda^{-1} \text{id}$  and  $D^2F_0(x - S_0(x)) - D^2\tilde{\varphi}_0(x)$  is semidefinite positive, this gives for  $\rho_g$  a.e.  $x$

$$\rho_g(x) \leq \|\nu_0\| L^\infty \lambda^{-d} \det(D^2F_0(x - S_0(x)) - D^2\tilde{\varphi}_0(x)),$$

by (5.5.9) and (5.5.8), we then have

$$-D^2\tilde{\varphi}_0(x) \leq D^2g(x) + D^2\tilde{\varphi}_1(x) \leq D^2g(x) + \Lambda \text{id},$$

but since  $D^2F_0 \leq \Lambda \text{id}$ , the bound (5.5.5) follows.  $\square$

### 5.5.2 Proof of the bound by $\Gamma$ -convergence

Recall that we have assumed that  $K$  is a convex compact subset with non-empty interior. For  $\varepsilon > 0$ , setting  $K_\varepsilon := K + 2\varepsilon B$  (where  $B$  is the unit Euclidean ball of  $\mathbb{R}^d$ ); consider the mollifiers  $\eta_\varepsilon = \varepsilon^{-d} \eta(\frac{\cdot}{\varepsilon})$  with  $\eta$  a smooth probability density supported on  $B$ , consider the smooth and convex function

$$g_\varepsilon := \eta_\varepsilon \star \varepsilon^{-1} d_{K_\varepsilon}^2,$$

where  $d_{K_\varepsilon}$  is the distance to  $K_\varepsilon$ . Define  $T$  as in (5.5.4) and for every  $\rho \in \mathcal{P}(\mathbb{R}^d)$ :

$$J_\varepsilon(\rho) := T(\rho) + \int_{\mathbb{R}^d} g_\varepsilon d\rho, \quad J(\rho) := \begin{cases} T(\rho) & \text{if } \rho \in \mathcal{P}(K) \\ +\infty & \text{otherwise} \end{cases},$$

where by abuse of notation we write  $\rho \in \mathcal{P}(K)$  if  $\rho \in \mathcal{P}(\mathbb{R}^d)$  with  $\text{spt} \rho \subset K$ . We have.

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**Proposition 5.5.4.** *Suppose that  $K$  is a convex compact subset with non-empty interior. Then  $J_\varepsilon$   $\Gamma$ -converges to  $J$  as  $\varepsilon \rightarrow 0^+$  for the narrow topology.*

*Proof.* The  $\Gamma$ -limsup inequality follows directly by considering the constant recovery sequence. Indeed let  $\rho \in \mathcal{P}(\mathbb{R}^d)$ . If  $\rho \notin \mathcal{P}(K)$ , then clearly

$$\limsup_{\varepsilon \rightarrow 0^+} J_\varepsilon(\rho) \leq +\infty = J(\rho).$$

If  $\rho \in \mathcal{P}(K)$ , then  $\text{spt } \rho \cap \text{spt } g_\varepsilon = \emptyset$ , so that

$$\limsup_{\varepsilon \rightarrow 0^+} J_\varepsilon(\rho) = W_{c_0}(\nu_0, \rho) + W_{c_1}(\nu_1, \rho) = J(\rho).$$

For the  $\Gamma$ -liminf inequality let  $\rho \in \mathcal{P}(K)$  and  $(\rho_n)_{n \in \mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$  be a narrowly converging sequence and  $(\varepsilon_n)_n \in \mathbb{R}_+^{\mathbb{N}}$  a sequence s.t.  $\varepsilon_n \xrightarrow{n \rightarrow \infty} 0$ . If  $\rho \in \mathcal{P}(K)$ , then

$$\begin{aligned} \liminf_{n \rightarrow \infty} J_{\varepsilon_n}(\rho_n) &\geq \liminf_{n \rightarrow \infty} (W_{c_0}(\nu_0, \rho_n) + W_{c_1}(\nu_1, \rho_n)) \\ &\geq W_{c_0}(\nu_0, \rho) + W_{c_1}(\nu_1, \rho) = J(\rho), \end{aligned}$$

where we have used the lower semicontinuity of the Wasserstein functional w.r.t. the narrow topology.

Assume now  $\rho \notin \mathcal{P}(K)$ . For  $R > 0$  define

$$g_\varepsilon^R := \eta_\varepsilon \star (R \wedge \varepsilon^{-1} d_{K_\varepsilon}^2),$$

so that  $\|g_\varepsilon^R\|_{L^\infty(\mathbb{R}^d)} \leq R$ . Since  $g_\varepsilon \geq g_\varepsilon^R$  we have

$$\begin{aligned} \liminf_{n \rightarrow \infty} J_{\varepsilon_n}(\rho_n) &\geq \liminf_{n \rightarrow \infty} \left( W_{c_0}(\nu_0, \rho_n) + W_{c_1}(\nu_1, \rho_n) + \int_{\mathbb{R}^d} g_{\varepsilon_n}^R d\rho_n \right) \\ &\geq W_{c_0}(\nu_0, \rho) + W_{c_1}(\nu_1, \rho) + \liminf_{n \rightarrow \infty} \int_{\mathbb{R}^d} g_{\varepsilon_n}^R d\rho_n. \end{aligned}$$

Now since  $\rho \notin \mathcal{P}(K)$  there is  $\Omega \subset \mathbb{R}^d$  open such that  $\inf_{x \in \Omega} d_K(x) \geq \delta > 0$  and  $\rho(\Omega) = m > 0$ . Hence

$$\begin{aligned} \liminf_{n \rightarrow \infty} \int_{\mathbb{R}^d} g_{\varepsilon_n}^R d\rho_n &\geq \liminf_{n \rightarrow \infty} \int_{\Omega} g_{\varepsilon_n}^R d\rho_n \\ &\geq \liminf_{n \rightarrow \infty} \int_{\Omega} R d\rho_n = Rm, \end{aligned}$$

where in the last inequality we have used that for  $n$  large enough  $\varepsilon_n^{-1} d_{K_{\varepsilon_n}}^2 \geq R$ . We conclude by arbitrariness of  $R$ .  $\square$

Hence the tight sequence of minimizers of  $J_{\frac{1}{n}}$  for  $n \in \mathbb{N}^*$ ,  $(\rho_n)_{n \in \mathbb{N}^*}$  with  $\rho_n := \rho g_{\frac{1}{n}}$  converges narrowly to  $\rho$ , the minimizer of  $J$  i.e. the solution of (WI) with  $\mathcal{A} = \mathcal{P}(K)$ . Since  $D^2 g_{\frac{1}{n}} = 0$  on  $\text{int}(K)$ , we deduce from (5.5.5) that for every open  $\Omega$  such that  $\Omega \Subset \text{int}(K)$

$$\|\rho_n\|_{L^\infty(\Omega)} \leq \|\nu_0\|_{L^\infty} 2^d \lambda^{-d} \Lambda^d$$

from which one deduces (5.5.3) by letting  $n \rightarrow \infty$ .

## 5.6 Numerical simulations

For the numerical simulation of examples in the case of interpolation between measures (WI) and the parking problem (5.1.1) we replace the optimal transportation costs by their entropically regularized versions. This will enable us to apply some variants of the celebrated Sinkhorn's algorithm, popularized in the context of optimal transport and matching by [42] and [58]. For an introduction to this rapidly developing subject and convergence results, we refer to [96] and [89].

### 5.6.1 Description of the Sinkhorn-like algorithm

The general idea of the Sinkhorn algorithm applied to the entropic optimal transport problem has already been discussed in Section 2.4. Now, we are going to apply this idea to the minimization problems (WI) and (5.1.1), and more generally the minimization of several Wasserstein functionals, i.e. the multi-matching problem (2.2.1).

A Sinkhorn-like algorithm for the entropically regularized version of (2.2.1) in the discrete setting has been proposed in Section 3.2 [9]. The basic idea is to use Bregman alternate projections on affine subspaces, introduced by Bregman [16] and generalized by Dykstra's algorithm [49] to convex sets. A very general framework in the continuous setting is studied in [36]. In Section 1.1.3 [36] the authors comment that the Bregman projections, respectively Dykstra's algorithm, correspond actually to an alternate dual ascend method, as we have already seen for the Sinkhorn algorithm for the basic entropic OT problem in Remark 2.4.6.

Note that for the Wasserstein multi-matching problems (2.2.1) as well as for the Wasserstein interpolation (WI) and the parking location problem (5.1.1) (both with location constraint) there exist multi-marginal formulations, namely (2.2.3), (5.2.2) and (5.1.3). One could hence also apply entropic regularization to these multi-marginal formulations as proposed and studied in [9, 81, 28]. However, this would require to compute the multi-marginal cost-function, which in our case is an minimization in itself and usually does not have a simple closed form expression. This is why we entropically regularize each OT functional individually for our purposes.

For sake of completeness we compute the dual formulations of the entropically regularized variational problems we are interested in and deduce the (generalized) Sinkhorn iterates, the proofs are postponed to Section 5.5.2.

#### The Wasserstein interpolation problem

The entropic regularization of the interpolation problem (WI) becomes for two suitably chosen reference measures  $R_0, R_1$

$$\inf \left\{ H(\gamma_0|R_0) + H(\gamma_1|R_1) : \rho \in \mathcal{A}, \gamma_0 \in \Pi(\nu_0, \rho), \gamma_1 \in \Pi(\rho, \nu_1) \right\}.$$

Naturally, the cases (i) with no additional constraint and (ii) with location constraint  $K$  are treated by choosing the reference measures to enforce the support of  $\rho$  being included in  $K$ . Namely we choose

$$R_0 = e^{-c_0/\varepsilon} \nu_0 \otimes \mathbf{1}_K, \quad R_1 = e^{-c_1/\varepsilon} \mathbf{1}_K \otimes \nu_1,$$

where for case (i) we choose  $K$  large enough (yet still compact) as before. The resulting Sinkhorn iterations are given in Proposition 1 and 2 [9] in the discrete case. The case (iii)

of a density constraint  $\phi$  requires performing a suitable projection of the estimated interpolation, as specified in Proposition 4.1 in [95] in the case of  $\phi \equiv \kappa$ .

Since there is no additional technical effort, we consider the entropic regularization of the more general multi-matching problem (2.2.1), possibly with additional constraints. We are given  $\nu_i \in \mathcal{P}(\mathbb{R}^d)$  and cost functions  $c_i \in C(\mathbb{R}^d \times \mathbb{R}^d)$  for  $i = 1, \dots, N$ . For simplicity, as we are developing the following theory for numerical simulations, we assume that all the  $\nu_i$  have compact support. Note also that we switch the order of arguments, in order to have the unknown pivot measure in the second component.

The basic entropically regularized multi-matching problem reads as follows

$$\inf_{\rho \in \mathcal{P}(\mathbb{R}^d)} \left\{ \sum_{i=1}^N H(\gamma_i | R_i) : \gamma_i \in \Pi(\rho, \nu_i) \right\} \quad (\text{EMM})$$

where we choose  $R_i = \exp(-c_i(x_i, x))Q_i$  with  $Q_i = R_{\nu_i} \otimes \mu$  for  $R_{\nu_i} \in \mathcal{P}(\mathbb{R}^d)$ ,  $\nu_i \ll R_{\nu_i}$  and  $\mu \in \mathcal{P}(\mathbb{R}^d)$  is a suitable reference measure with compact support.

In what follows, we develop duality results for the regularized multi-matching problem with additional constraints and deduce the alternate ascent algorithm.

For the duality results, we work in the space of bounded real valued Radon measures  $\mathcal{M}(\mathbb{R}^M)$ , which is the topological dual of  $C_0(\mathbb{R}^M)$ , where  $M \in \mathbb{N}^*$  (typically equal to  $d$  or  $2d$ , we also use the  $\mathbb{R}^{2d} \simeq \mathbb{R}^d \times \mathbb{R}^d$  for readability). We postpone the proof strategies to Section 5.6.3.

**Proposition 5.6.1.** *Let  $\nu_i \in \mathcal{P}(\mathbb{R}^d)$  with compact support for  $i = 1, \dots, N$ . Suppose further that  $R_i \in \mathcal{M}(\mathbb{R}^d \times \mathbb{R}^d)$  is of the form  $R_i = e^{-c_i(x,y)/\varepsilon} R_{\nu_i} \otimes \mu$  with  $R_i \sim \nu_i \otimes \mu$ ,  $\log\left(\frac{d\nu_i}{dR_{\nu_i}}\right) \in L^1(\nu_i)$ ,  $c \in L^1(R_{\nu_i} \otimes \mu)$  for a fixed compactly supported measure  $\mu \in \mathcal{M}(\mathbb{R}^d)$ .*

*Then, the dual of (EMM) is given by*

$$\sup_{(\varphi_i, \psi_i) \in C_0(\mathbb{R}^d)^{2N}} \left\{ \sum_{i=1}^N \int_{\mathbb{R}^d} \varphi_i(x) d\nu_i(x) - \sum_{i=1}^N \int_{\mathbb{R}^{2d}} \exp(\varphi_i(x) + \psi_i(y)) dR_i(x, y) : \sum_{i=1}^N \psi_i = 0 \right\} \quad (\text{EMM}^*)$$

Thanks to this duality result we can now state Sinkhorn's algorithm in this case.

**Algorithm 2** (Sinkhorn's algorithm, adapted to multi-matching problem). Given  $\psi_0 = 0$ . Iterate for  $l \geq 0$  for each  $i = 1, \dots, N$

$$\begin{aligned} \varphi_i^{l+1}(x_i) &= \log \frac{d\nu_i}{dR_{\nu_i}}(x_i) - \log \left( \int_K \exp \left( -\frac{c_i(x_i, x)}{\varepsilon} + \psi_i^l(x) \right) d\mu(x) \right), \\ \psi_i^{l+1}(x) &= \log \frac{d\rho^l}{d\mu}(x) - \log \left( \int_{\mathbb{R}^d} \exp \left( -\frac{c_i(x_i, x)}{\varepsilon} + \varphi_i^{l+1}(x_i) \right) dR_{\nu_i}(x_i) \right), \end{aligned}$$

where  $\rho^l$  is the current approximate interpolation which is given by the geometric mean formula (see Proposition 2 of [9])

$$\rho^l(x) = \prod_{j=1}^N \left( \int_{\mathbb{R}^d} \exp \left( -\frac{c_j(x_j, x)}{\varepsilon} + \varphi_j^{l+1}(x_j) + \psi_j^l(x) \right) d\nu_j(x_j) \right)^{\frac{1}{N}}.$$

We now treat the case of an additional density constraint.

**Proposition 5.6.2.** *Let  $\nu_i \in \mathcal{P}(\mathbb{R}^d)$  with compact support for  $i = 1, \dots, N$  and  $\phi \in L^1(\mathbb{R}^d)$  compactly supported with  $\int_{\mathbb{R}^d} \phi \, dx \geq 1$ . Suppose further for a fixed compactly supported measure  $\mu \in \mathcal{M}(\mathbb{R}^d)$  that  $\text{spt } \varphi \subset \text{spt } \mu$ ,  $R_i \in \mathcal{M}(\mathbb{R}^d \times \mathbb{R}^d)$  with  $R_i \sim \nu_i \otimes \mu$ ,  $\log \left( \frac{d\nu_i}{dR_{\nu_i}} \right) \in L^1(\nu_i)$ ,  $c \in L^1(R_{\nu_i} \otimes \mu)$ .*

*Consider the problem with additional density constraint*

$$\inf_{\substack{\rho \in \mathcal{P}(\mathbb{R}^d), \\ \rho \leq \phi \mathcal{L}^d}} \left\{ \sum_{i=1}^N H(\gamma_i | R_i) : \gamma_i \in \Pi(\nu_i, \rho) \right\} \quad (\text{EMD})$$

*Then, its dual is given by*

$$\sup_{(\varphi_i, \psi_i)_{i=1}^N \in C(X)^{2N}} \left\{ - \sum_{i=1}^N \int_{\mathbb{R}^{2d}} \exp(\varphi_i(x) + \psi_i(y)) \, dR_i(x, y) \right. \\ \left. + \sum_{i=1}^N \int_{\mathbb{R}^d} \varphi_i(x) \, d\nu_i(x) + \int_{\mathbb{R}^d} \phi \sum_{i=1}^N \psi_i \, dx : \sum_{i=1}^N \psi_i \leq 0 \right\} \quad (\text{EMD}^*)$$

*for a compact set  $X$ .*

This gives the algorithm for the additional density constraint.

**Algorithm 3** (Sinkhorn's algorithm, adapted to density constraint). Given  $\psi_0 = 0$ . Iterate for  $l \geq 0$  for each  $i = 1, \dots, N$

$$\varphi_i^{l+1}(x_i) = \log \frac{d\nu_i}{dR_{\nu_i}}(x_i) - \log \left( \int_K \exp \left( -\frac{c_i(x_i, x)}{\varepsilon} + \psi_i^l(x) \right) \, d\mu(x) \right), \\ \psi_i^{l+1}(x) = \log \frac{d \min \{ \rho^l, \phi \}}{d\mu}(x) - \log \left( \int_{\mathbb{R}^d} \exp \left( -\frac{c_i(x_i, x)}{\varepsilon} + \varphi_i^{l+1}(x_i) \right) \, dR_{\nu_i}(x_i) \right),$$

where  $\rho^l$  is the current approximate interpolation which is given by the geometric mean formula (see Proposition 2 of [9])

$$\rho^l(x) = \prod_{j=1}^N \left( \int_{\mathbb{R}^d} \exp \left( -\frac{c_j(x_j, x)}{\varepsilon} + \varphi_j^{l+1}(x_j) + \psi_j^l(x) \right) \, d\nu_j(x_j) \right)^{\frac{1}{N}}.$$

### The parking location problem

Regularizing the parking problem (5.1.1) in a similar way leads to

$$\inf_{(\gamma, \tilde{\gamma}_0, \tilde{\gamma}_1) \in \mathcal{D}} \{ H(\gamma | R) + H(\tilde{\gamma}_0 | R_0) + H(\tilde{\gamma}_1 | R_1) \}, \quad (5.6.5)$$

where

$$\mathcal{D} = \left\{ (\gamma, \tilde{\gamma}_0, \tilde{\gamma}_1) \in \mathcal{M}_+(\mathbb{R}^d \times \mathbb{R}^d) : \pi_{0\#}(\gamma + \tilde{\gamma}_0) = \nu_0, \pi_{1\#}\gamma + \pi_{0\#}\tilde{\gamma}_1 = \nu_1, \pi_{1\#}\tilde{\gamma}_1 = \pi_{1\#}\tilde{\gamma}_0 \right\}.$$

Note that here we have switched the order of arguments in  $\tilde{\gamma}_1$  compared to the formulation (5.1.1) in order to simplify notation in the following.

As before, a location constraint on a given set  $K$  can be encoded in the choice of the reference measures

$$R = e^{-c_1/\varepsilon} \nu_0 \otimes \nu_1, \quad R_0 = e^{-c_0/\varepsilon} \nu_0 \otimes \mathbf{1}_K, \quad R_1 = e^{-c_1/\varepsilon} \nu_1 \otimes \mathbf{1}_K.$$

For the location constraint the primal-dual relation is given in the following proposition.

**Proposition 5.6.3.** *Let  $\nu_i \in \mathcal{P}(\mathbb{R}^d)$  with compact support for  $i = 0, 1$ . Suppose further that  $R_i \in \mathcal{M}(\mathbb{R}^d \times \mathbb{R}^d)$  is of the form  $R_i = e^{-c_i(x,y)/\varepsilon} R_{\nu_i} \otimes \mu$  with  $R_i \sim \nu_i \otimes \mu$ ,  $\log\left(\frac{d\nu_i}{dR_{\nu_i}}\right) \in L^1(\nu_i)$ ,  $c \in L^1(R_{\nu_i} \otimes \mu)$  for a fixed compactly supported measure  $\mu \in \mathcal{M}(\mathbb{R}^d)$ . Then, the dual of (5.6.5) is given by*

$$\sup_{(\varphi_i, \psi_i)_{i=0}^1 \in C(X)^4} \left\{ \sum_{i=0}^1 \int_{\mathbb{R}^d} \varphi_i d\nu_i - \int_{\mathbb{R}^d \times \mathbb{R}^d} \exp(\varphi_0(x_0) + \varphi_1(x_1)) dR(x_0, x_1) - \sum_{i=0}^1 \int_{\mathbb{R}^d \times \mathbb{R}^d} \exp(\varphi_i(x_i) + \psi_i(x)) dR(x_i, x) : \psi_0 + \psi_1 = 0 \right\},$$

for a compact set  $X \subset \mathbb{R}^d$ .

We also state the duality for the case of density constraint, the proof being analogous to the ones executed in Section 5.6.3.

$$\inf_{(\gamma, \tilde{\gamma}_0, \tilde{\gamma}_1) \in \mathcal{D}_\phi} \{H(\gamma|R) + H(\tilde{\gamma}_0|R_0) + H(\tilde{\gamma}_1|R_1)\}, \quad (5.6.6)$$

where

$$\mathcal{D}_\phi := \left\{ (\gamma, \tilde{\gamma}_0, \tilde{\gamma}_1) \in \mathcal{D} : \pi_{1\#} \tilde{\gamma}_0 = \pi_{1\#} \tilde{\gamma}_1 \leq \phi \mathcal{L}^d \right\}.$$

**Proposition 5.6.4.** *Let  $\nu_i \in \mathcal{P}(\mathbb{R}^d)$  with compact support for  $i = 0, 1$  and  $\phi \in L^1(\mathbb{R}^d)$  compactly supported and  $\int_{\mathbb{R}^d} \phi dx \geq 1$ . Suppose further for a fixed compactly supported measure  $\mu \in \mathcal{M}(\mathbb{R}^d)$  that  $\text{spt } \phi \subset \text{spt } \mu$ . Assume further that  $R_i \in \mathcal{M}(\mathbb{R}^d \times \mathbb{R}^d)$  is of the form  $R_i = e^{-c_i(x,y)/\varepsilon} R_{\nu_i} \otimes \mu$  with  $R_i \sim \nu_i \otimes \mu$ ,  $\log\left(\frac{d\nu_i}{dR_{\nu_i}}\right) \in L^1(\nu_i)$ ,  $c \in L^1(R_{\nu_i} \otimes \mu)$ . Then, the dual of (5.6.6) is given by*

$$\sup_{(\varphi_i, \psi_i)_{i=0}^1 \in C(X)^4} \left\{ \sum_{i=0}^1 \int_{\mathbb{R}^d} \varphi_i d\nu_i + \int_{\mathbb{R}^d} (\psi_0 + \psi_1) \phi dx - \int_{\mathbb{R}^d \times \mathbb{R}^d} \exp(\varphi_0(x_0) + \varphi_1(x_1)) dR(x_0, x_1) - \sum_{i=0}^1 \int_{\mathbb{R}^d \times \mathbb{R}^d} \exp(\varphi_i(x_i) + \psi_i(x)) dR(x_i, x) : \psi_0 + \psi_1 \leq 0 \right\},$$

for a compact set  $X \subset \mathbb{R}^d$ .

The Sinkhorn iterations (density constraint included) in the dual variables then become.

**Algorithm 4** (Sinkhorn's algorithm, adapted to parking density problem). Given  $\psi_0 = 0$ . Iterate for  $l \geq 0$  for  $i = 0, 1$

$$\begin{aligned} \varphi_i^{l+1}(x_i) &= \log \frac{d\nu_i}{dR_{\nu_i}}(x_i) - \log \left( \int_{\mathbb{R}^d} \exp\left(-\frac{c_1}{\varepsilon} + \varphi_{i+1}^l\right) dR_{\nu_{i+1}} + \int_{\mathbb{R}^d} \exp\left(-\frac{c_i}{\varepsilon} + \psi_i^l\right) d\mu \right), \\ \psi_i^{l+1}(x) &= \log \frac{d \min\{\rho^l, \phi\}}{d\mu}(x) - \log \left( \int_{\mathbb{R}^d} \exp\left(-\frac{c_i}{\varepsilon} + \varphi_i^{l+1}(x_i)\right) dR_{\nu_i}(x_i) \right), \end{aligned}$$

where the  $i+1$  is to be understood modulo 2 and  $\rho^l$  is the current approximate interpolation which is given by the geometric mean formula (see Proposition 2 of [9]):

$$\rho^l(x) = \prod_{j=0}^1 \left( \int_{\mathbb{R}^d} \exp \left( -\frac{c_j(x_j, x)}{\varepsilon} + \varphi_j^{l+1}(x_j) + \psi_j^l(x) \right) d\nu_j(x_j) \right)^{\frac{1}{2}}.$$

### 5.6.2 Numerical results: comparison of the optimal interpolation and the optimal parking

We now present some numerical results based on the iterative schemes described in the previous paragraph. In all our examples (presented in Figures 5.2 to 5.5), we compare the solutions of the interpolation and parking problems with a constant density constraint on the unit square  $K = [0, 1]^2$ . We always take as distribution of services  $\mu_1 = \nu_1 = \delta_{1/2, 1/2}$ , the Dirac measure at the center of the square and as distribution of residents, we take a symmetric sum of four Dirac measures

$$\mu_0 = \nu_0 = \frac{1}{4} \left( \delta_{(0.5, 0.1)} + \delta_{(0.5, 0.9)} + \delta_{(0.1, 0.5)} + \delta_{(0.9, 0.5)} \right),$$

and we denote the optimal pivot measure in the figures by  $\mu$ . We consider power-like costs

$$c_0(x, y) = |x - y|^p \text{ and } c_1(x, y) = 1.5 c_0(x, y),$$

for several values of  $p$  corresponding to concave, linear or convex costs and various constant threshold values for the density constraints  $\phi$ . In this setting, we know (Corollary 5.3.5 for  $p > 1$  and Proposition 5.4.9 for  $p \leq 1$ ) that the optimal interpolation and the optimal parking are of bang-bang type. Even with the entropic regularization (which has the effect of blurring the true solution) this is clearly what we observe in these figures with a small regularization  $\varepsilon = 5.10^{-4}$ . Since the optimal parking may have total mass less than 1 (it can even be 0, see Figure 5.2), we have indicated its total mass on each figure, of course if the total mass of the parking is 1 it coincides with the interpolation, a case which is more likely to occur when the threshold level is high. Finally, one can see the influence of the exponent  $p$  on the shape of the support of the optimal measure.

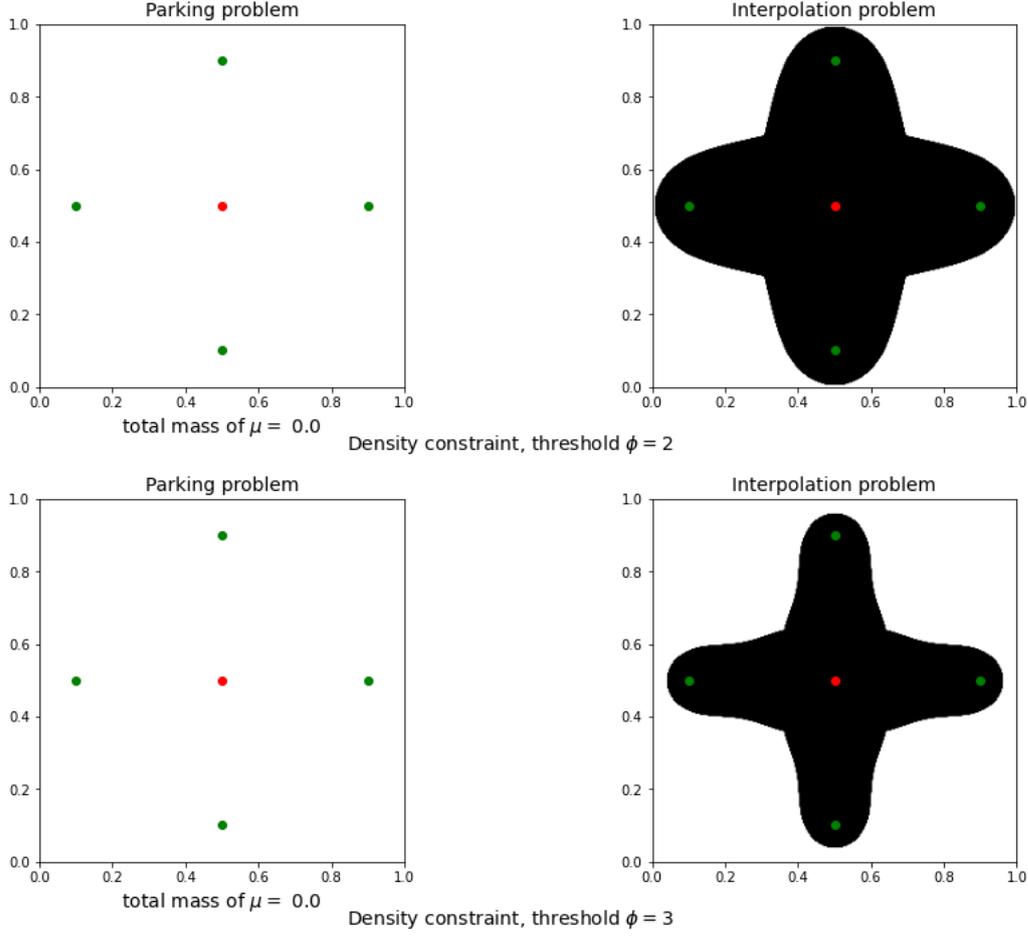
### 5.6.3 Proofs of duality

*Proof of Proposition 5.6.1.* Even though a proof using the Fenchel-Rockafellar Duality Theorem is possible here, we give a different proof based on infimal convolution inspired by the arguments in [1] to prove Proposition 2.2.

For  $i = 1, \dots, N$  define  $G_i : C_0(\mathbb{R}^d) \rightarrow \mathbb{R}$  by

$$G_i(\psi_i) := \inf_{\varphi_i \in C_0(\mathbb{R}^d)} \left\{ \int_{\mathbb{R}^{2d}} \exp(\varphi_i(x) + \psi_i(y)) dR_i(x, y) - \int_{\mathbb{R}^d} \varphi_i(x) d\nu_i(x) \right\}.$$

Note that for every  $1 \leq i \leq N$ ,  $G_i$  is a convex function because it is the (unconstrained) infimum of a jointly convex function in  $(\varphi_i, \psi_i)$ .


 Figure 5.2 – concave cost  $p = 0.25$ 

By Proposition 2.4.5 we have for  $\rho \in \mathcal{M}(\mathbb{R}^d)$

$$G_i^*(\rho) = \sup_{(\psi_i, \varphi_i) \in C_0(\mathbb{R}^d)^2} \left\{ \int_{\mathbb{R}^d} \psi_i(y) d\rho(y) + \int_{\mathbb{R}^d} \varphi_i(x) d\nu_i(x) - \int_{\mathbb{R}^{2d}} \exp(\varphi_i(x) + \psi_i(y)) dR_i(x, y) \right\}$$

$$= \begin{cases} \inf_{\gamma \in \Pi(\nu_i, \rho)} H(\gamma | R_i) & \text{if } \rho \in \mathcal{P}(\mathbb{R}^d), \\ +\infty & \text{otherwise.} \end{cases}$$

Indeed, if  $\rho \notin \mathcal{M}_+(\mathbb{R}^d)$ , then there is  $f \in C_0(\mathbb{R}^d)$  with  $f \leq 0$  and  $\int_{\mathbb{R}^d} f d\rho > 0$ . Taking  $\psi_i^n = nf$ ,  $\varphi_i \in C_0(\mathbb{R}^d)$  fix and letting  $n \rightarrow \infty$  yields  $G_i^*(\rho) = +\infty$ . Now suppose that  $\rho \in \mathcal{M}_+(\mathbb{R}^d)$  but  $\rho(\mathbb{R}^d) \neq 1$ . W.l.o.g. suppose  $\rho(\mathbb{R}^d) > 1$ . Then for every  $n \in \mathbb{N}^*$  there is  $k_n > 0$  such that

$$R_i(\mathbb{R}^{2d} \setminus [-n, n]^{2d}) \leq k_n \text{ and } |\rho - \nu_i|(\mathbb{R}^d \setminus [-n, n]^d) \leq k_n, \quad (5.6.9)$$

and  $\lim_{n \rightarrow \infty} k_n = 0$ . Here  $|\rho - \nu_i| = (\rho - \nu_i)^+ + (\rho - \nu_i)^-$  where  $\rho - \nu_i = (\rho - \nu_i)^+ - (\rho - \nu_i)^-$  is the Hahn-Jordan decomposition. Now take  $\psi_i^n \in C_0(\mathbb{R}^d)$  with  $\|\psi_i^n\|_{L^\infty(\mathbb{R}^d)} = \log(1/\sqrt{k_n})$  and

$$\psi_i^n(y) = \begin{cases} \log\left(\frac{1}{\sqrt{k_n}}\right) & \text{if } |y| \leq n \\ 0 & \text{if } |y| \geq n+1. \end{cases}$$

Taking  $\varphi_i^n = -\psi_i^n$  we have

$$\begin{aligned} & \int_{\mathbb{R}^d} \psi_i^n(y) \, d\rho(y) + \int_{\mathbb{R}^d} \varphi_i^n(x) \, d\nu_i(x) - \int_{\mathbb{R}^{2d}} \exp(\varphi_i^n(x) + \psi_i^n(y)) \, dR_i(x, y) \\ & \geq \log\left(\frac{1}{\sqrt{k_n}}\right) (\bar{\rho} - \nu_i)([-n, n]^d) - \log\left(\frac{1}{\sqrt{k_n}}\right) |\rho - \nu_i|(\mathbb{R}^d \setminus [-n, n]^d) \\ & \quad - k_n - \frac{1}{\sqrt{k_n}} R_i(\mathbb{R}^{2d} \setminus [-n, n]^{2d}) \\ & \longrightarrow +\infty \quad \text{as } n \rightarrow \infty, \end{aligned}$$

thanks to (5.6.9).

This means that

$$(\text{EMM}) = \inf_{\rho \in \mathcal{P}(\mathbb{R}^d)} \sum_{i=1}^N G_i^*(\rho) = - \left( \sum_{i=1}^N G_i^* \right)^*(0).$$

To rewrite the last expression, define the infimal convolution for  $\psi \in C_0(\mathbb{R}^d)$

$$G(\psi) = \left( \bigsqcup_{i=1}^N G_i \right) (\psi) := \inf_{(\psi_i)_{i=1}^N \in C_0(\mathbb{R}^d)^N} \left\{ \sum_{i=1}^N G_i(\psi_i) : \sum_{i=1}^N \psi_i = \psi \right\}.$$

Then by iteratively applying Lemma 3.7 [27] we have  $G^* = \sum_{i=1}^N G_i^*$ , so that

$$\begin{aligned} (\text{EMM}) &= -(G^*)^*(0) \\ &\geq -G(0) = (\text{EMM}^*). \end{aligned}$$

This establishes weak duality.

For strong duality, it is sufficient by the Fenchel-Moreau Theorem (see e.g. Proposition 4.1 [50]) to prove that  $G$  is a proper (i.e. not identically  $\pm\infty$ ), lower semicontinuous and convex function in a neighborhood of 0. Since  $G$  is convex it is sufficient to prove that  $0 \in \text{int}(\text{dom } G)$  thanks to Corollary 2.3 [50]. For this note that  $\bigcap_{i=1}^N \text{dom } G_i^* \neq \emptyset$  which implies  $G > -\infty$  (see (3.24) in [27]). For the upper bound take  $\psi_i \in C_0(\mathbb{R}^d)$ , then

$$G_i(\psi_i) \leq \exp\left(\|\psi_i\|_{L^\infty(\mathbb{R}^d)}\right) R_i(\mathbb{R}^{2d}),$$

so that for  $\psi \in C_0(\mathbb{R}^d)$

$$G(\psi) \leq \exp\left(\|\psi\|_{L^\infty(\mathbb{R}^d)}/N\right) \sum_{i=1}^N R_i(\mathbb{R}^{2d}).$$

□

*Proof of Proposition 5.6.2.* Since all of the given quantities are compactly supported, choose a compact set  $X \subset \mathbb{R}^d$  which contains all of the supports.

Define  $F : C(X)^{2N} \rightarrow \mathbb{R} \cup \{-\infty, +\infty\}$  and  $G : C(X \times X)^N \rightarrow \mathbb{R} \cup \{-\infty, +\infty\}$  as follows

$$\begin{aligned} F(\varphi_1, \psi_1, \dots, \varphi_N, \psi_N) &:= - \sum_{i=1}^N \int_{\mathbb{R}^d} \varphi_i(x) \, d\nu_i(x) - \int_{\mathbb{R}^d} \phi(x) \sum_{i=1}^N \psi_i(x) \, dx \\ &\quad + \chi_{(-\infty, 0]} \left( \sum_{i=1}^N \psi_i \right), \\ G(u_1, \dots, u_N) &:= \sum_{i=1}^N \int_{\mathbb{R}^{2d}} \exp(u_i(x)) \, dR_i(x), \end{aligned}$$

where  $\chi_A$  for some set  $A$  denotes the indicator function

$$\chi_A(x) = \begin{cases} 0 & \text{if } x \in A, \\ +\infty & \text{otherwise.} \end{cases}$$

Define furthermore the linear operator  $\Lambda : C(X)^{2N} \rightarrow C(X \times X)^N$  by

$$\Lambda(\varphi_1, \psi_1, \dots, \varphi_N, \psi_N) = (\varphi_i + \psi_i)_{i=1}^N.$$

Since  $F, G$  are proper, l.s.c. and convex functions,  $F(0) = 0 < +\infty$ ,  $G(\Lambda(0)) \in (-\infty, +\infty)$  and  $G$  is continuous on  $\Lambda(0)$ , we can apply the Fenchel-Rockafellar duality theorem

$$\begin{aligned} (\text{EMD}^*) &= - \inf_{(\varphi_i, \psi_i)_{i=1}^N \in C(X)^{2N}} \{F(\varphi_i, \psi_i) + G(\Lambda(\varphi_i, \psi_i))\} \\ &= - \sup_{(\gamma_i)_{i=1}^N \in \mathcal{M}(X \times X)^N} \{-F^*(\Lambda^*(\gamma_i)) - G^*(-\gamma_i)\} \end{aligned} \quad (5.6.10)$$

We have that

$$G^*(\gamma_1, \dots, \gamma_N) = \sup_{(u_i)_{i=1}^N \in C(X \times X)^N} \left\{ \sum_{i=1}^N \int_{\mathbb{R}^{2d}} u_i \, d\gamma_i - \sum_{i=1}^N \int_{\mathbb{R}^{2d}} \exp(u_i(x)) \, dR_i(x) \right\} \quad (5.6.11)$$

is a supremum of (strictly) concave functions (of the  $u_i$ ). So that every maximal  $u_i$  if it exists satisfies the first order optimality condition given by, for all functions  $f_i \in C(X \times X)$

$$\int_{\mathbb{R}^{2d}} f_i \, d\gamma_i - \int_{\mathbb{R}^{2d}} f_i(x) \exp(u_i(x)) \, dR_i(x) = 0.$$

This implies that if all  $\gamma_i \ll R_i$  then  $u_i = \log(\frac{d\gamma_i}{dR_i})$  attains the maximum in (5.6.11). If there is one  $\gamma_i \not\ll R_i$ , then the supremum is equal to  $+\infty$ .

This can be seen as follows. If  $\gamma_i \not\ll R_i$ , there is a (Borel) measurable set  $A \subset X$  such that  $\gamma_i(A) > 0$  and  $R_i(A) = 0$ . Now, the short version is to note that the supremum (5.6.11) can be taken over all bounded measurable functions since for each bounded measurable function  $u_i$  and  $\epsilon > 0$  one can find a continuous function  $\bar{u}_i$  such that  $(\gamma_i + R_i)(u_i \neq \bar{u}_i) < \epsilon$  by (the strong version of) Lusin's theorem, see e.g. Theorem 1.15 [53]. Then choose the sequence defined by  $u_i^n = n\mathbb{1}_A$  to conclude.

More precisely, by Lusin's theorem there is a sequence of sets  $(E_n)_{n \in \mathbb{N}}$  and a sequence of continuous functions  $(u_i^n)_{n \in \mathbb{N}}$  such that

- $u_i^n = n\mathbb{1}_A$  on  $E_n$ ,
- $0 \leq u_i^n \leq n$  on  $\mathbb{R}^{2d}$ ,
- $(\gamma_i + R_i)(u_i^n \neq n\mathbb{1}_A) \leq (\gamma_i + R_i)(\mathbb{R}^{2d} \setminus E_n) \leq e^{-2n}$ .

With these properties we obtain

$$\begin{aligned} & \int_{\mathbb{R}^{2d}} u_i^n d\gamma_i - \int_{\mathbb{R}^{2d}} \exp(u_i^n(x)) dR_i(x) \\ & \geq \int_{E_n \cap A} u_i^n d\gamma_i - \int_E \exp(u_i^n(x)) dR_i(x) - \int_{\mathbb{R}^{2d} \setminus E} \exp(u_i^n(x)) dR_i(x) \\ & \geq n\gamma_i(E_n \cap A) - R_i(E_n \setminus A) - e^{-n} \end{aligned}$$

which converges to  $+\infty$  as  $n \rightarrow \infty$  because  $\gamma_i(E_n \cap A) \rightarrow \gamma_i(A) > 0$ .

In total we get

$$G^*(\gamma_1, \dots, \gamma_N) = \begin{cases} +\infty & \text{if there is } i \text{ s.t. } \gamma_i \not\ll R_i, \\ \sum_{i=1}^N H(\gamma_i | R_i) & \text{otherwise.} \end{cases}$$

Now

$$\begin{aligned} & F^*(\mu_1, \rho_1, \dots, \mu_N, \rho_N) \\ & = \sup_{(\varphi_i, \psi_i)_{i=1}^N \in C(X)^{2N}} \left\{ \sum_{i=1}^N \int \varphi_i d\mu_i + \int \psi_i d\rho_i - F(\varphi_1, \psi_1, \dots, \varphi_N, \psi_N) \right\} \\ & = \sup_{\substack{(\varphi_i, \psi_i)_{i=1}^N \in C(X)^{2N} \\ \sum_{i=1}^N \psi_i \leq 0}} \left\{ \sum_{i=1}^N \int \varphi_i d(\mu_i + \nu_i) + \int \psi_i d\rho_i + \int_{\mathbb{R}^d} \phi(x) \sum_{i=1}^N \psi_i(x) dx \right\} \\ & = \begin{cases} +\infty & \text{if there is } i \text{ s.t. } \nu_i \neq -\mu_i, \\ \sup_{\substack{\psi_i \in C(X)^N \\ \sum_{i=1}^N \psi_i \leq 0}} \left\{ \sum_{i=1}^N \int \psi_i d\rho_i + \int_{\mathbb{R}^{2d}} \phi(x) \sum_{i=1}^N \psi_i(x) dx \right\} & \text{otherwise.} \end{cases} \end{aligned}$$

Indeed, suppose that there is an  $1 \leq i \leq N$  such that  $\nu_i \neq -\mu_i$ . Then there is  $A \subset X$  Borel measurable such that  $(\nu_i + \mu_i)(A) \neq 0$ . W.l.o.g.  $(\nu_i + \mu_i)(A) > 0$ . Then choosing  $\varphi_i^n = n$ ,  $\varphi_j = 0$  for  $j \neq i$  and  $\psi_j = 0$  for  $1 \leq j \leq N$  and letting  $n \rightarrow \infty$  yields the result.

Now assume that there are  $i \neq j$  such that  $\rho_i \neq \rho_j$ . This means that there is  $A \subset X$  Borel measurable such that  $\rho_i(A) > \rho_j(A)$ . By a similar argument with Lusin's theorem we can hence choose  $\psi_i^n = n$ ,  $\psi_j^n = -n$  and  $\psi_k = 0$  for the remaining  $k$  and let  $n \rightarrow \infty$  to conclude that  $F^*(\mu_1, \rho_1, \dots, \mu_N, \rho_N) = +\infty$ . This yields

$$\begin{aligned} & F^*(\mu_1, \rho_1, \dots, \mu_N, \rho_N) \\ & = \begin{cases} +\infty & \text{if there is } i \text{ s.t. } \nu_i \neq -\mu_i, \text{ or if there are } i \neq j \text{ s.t. } \rho_i \neq \rho_j \\ \sup_{\substack{\psi_i \in C(X)^N \\ \sum_{i=1}^N \psi_i \leq 0}} \left\{ \sum_{i=1}^N \int \psi_i d\rho_i + \int_{\mathbb{R}^{2d}} \phi(x) \sum_{i=1}^N \psi_i(x) dx \right\} & \text{otherwise.} \end{cases} \\ & = \begin{cases} 0 & \text{if for all } i \text{ s.t. } \nu_i = -\mu_i, \text{ for all } i, j \text{ } \rho_i = \rho_j \text{ and } -\rho_1 \leq \phi \\ +\infty & \text{otherwise.} \end{cases} \end{aligned}$$

where the last equality follows by a similar argument as before.

To compute  $\Lambda^* : \mathcal{M}(X \times X)^N \rightarrow \mathcal{M}(X)^{2N}$  let  $(\varphi_i, \psi_i)_{i=1}^N \in C(X)^{2N}$ ,  $(\gamma_i)_{i=1}^N \in \mathcal{M}(X \times X)^N$ . We have

$$\begin{aligned} & \langle \Lambda((\varphi_i, \psi_i)_{i=1}^N), (\gamma_i)_{i=1}^N \rangle \\ &= \sum_{i=1}^N \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi_i(x) + \psi_i(y) \, d\gamma_i(x, y) \\ &= \sum_{i=1}^N \int_{\mathbb{R}^d} \varphi_i(x) \, d\gamma_i(x, y) + \int_{\mathbb{R}^d} \psi_i(y) \, d\gamma_i(x, y). \end{aligned}$$

This concludes  $\Lambda^*(\gamma_1, \dots, \gamma_N) = (\pi_{1\#}\gamma_i, \pi_{2\#}\gamma_i)_{i=1}^N$ , so that (5.6.10) becomes

$$\begin{aligned} (\text{EMD}^*) &= \inf_{\gamma_i} \left\{ \sum_{i=1}^N H(-\gamma_i | R_i) : \gamma_i \in \Pi(-\nu_i, \rho), -\rho \leq \phi \right\} \\ &= (\text{EMD}). \end{aligned}$$

□

*Proof idea of Proposition 5.6.3.* This follows again by the Fenchel-Rockafellar theorem with

$$\begin{aligned} F(\varphi_0, \psi_0, \varphi_1, \psi_1) &= - \sum_{i=0}^1 \int_{\mathbb{R}^d} \varphi_i \, d\nu_i + \chi_{\{0\}}(\psi_0 + \psi_1) \\ G(u, v_0, v_1) &= \int_{\mathbb{R}^{2d}} \exp(u) \, dR + \sum_{i=0}^1 \int_{\mathbb{R}^{2d}} \exp(v_i) \, dR_i \end{aligned}$$

The details of the proof are similar to the proof of Proposition 5.6.2.

□

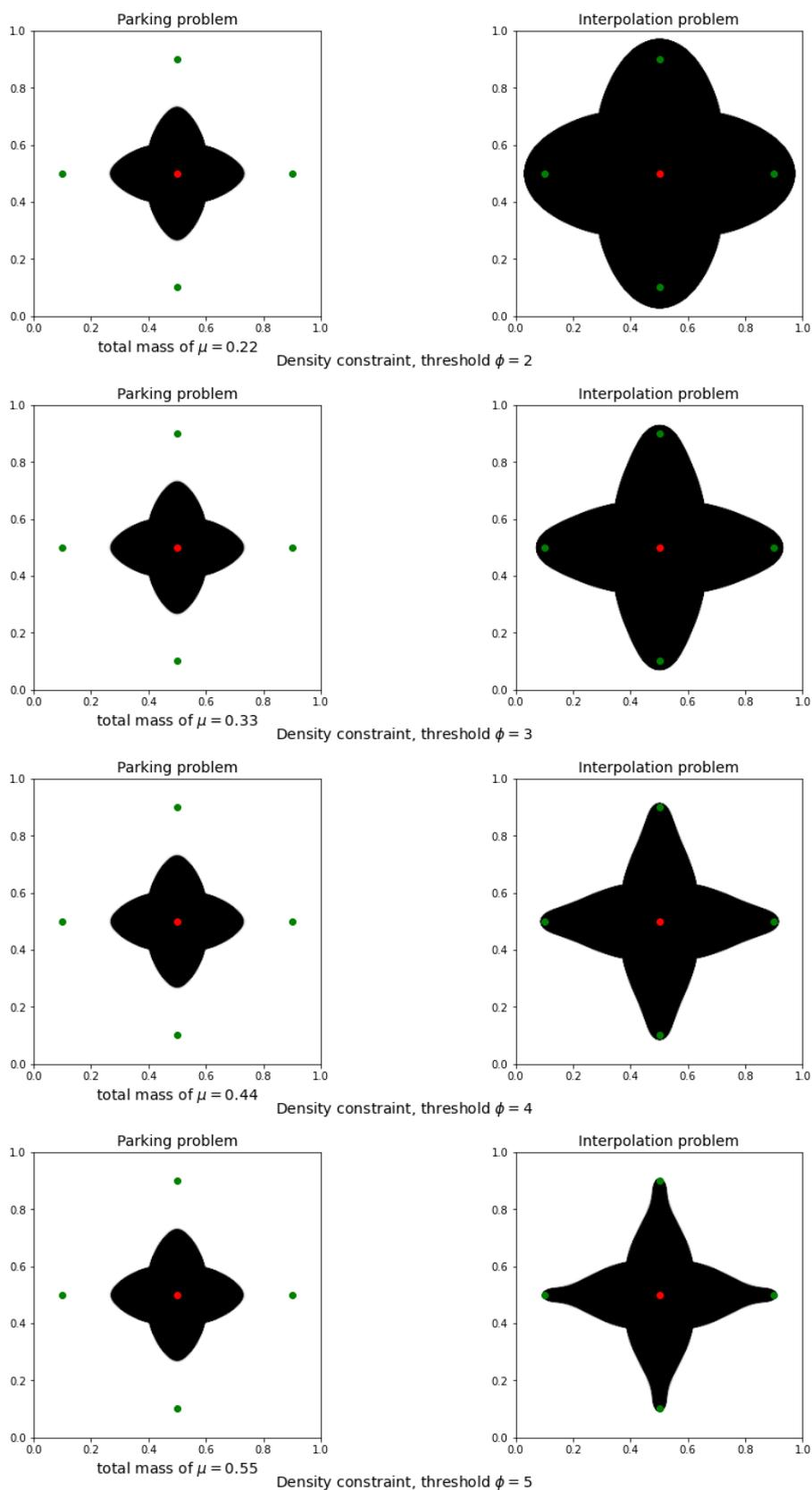


Figure 5.3 – concave cost  $p = 0.75$

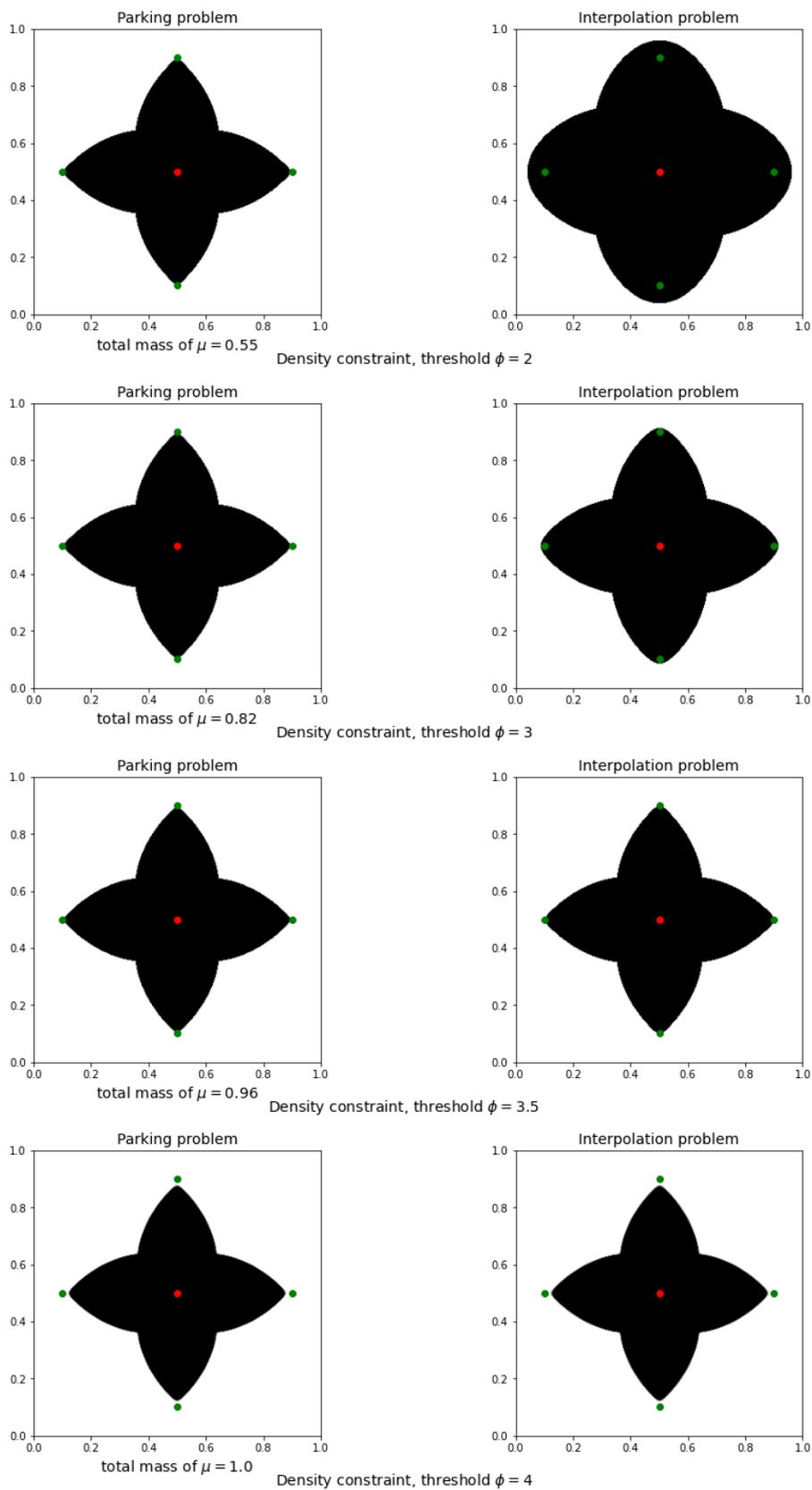


Figure 5.4 – Linear cost  $p = 1$

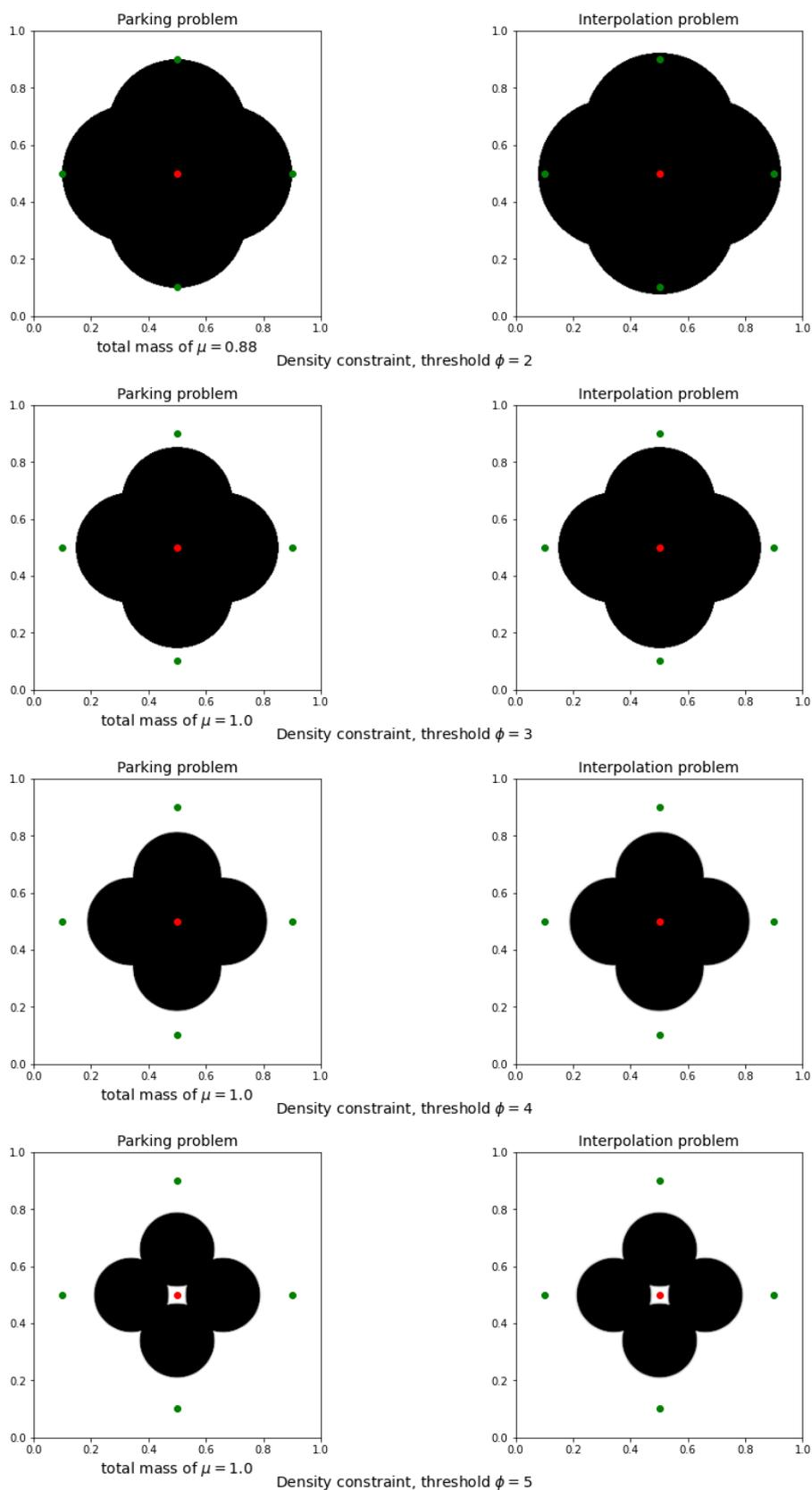


Figure 5.5 – Convex cost  $p = 2$

# Outlook

In this thesis, we studied interpolation problems involving several optimal transport functionals, which can also be seen as multi-matching problems or even means and medians in metric spaces. In addition to the results shown in this thesis, there are a lot of possible research directions for the problems discussed, which we elaborate in the following.

The Wasserstein barycenter problem has been a very active area of research ever since its introduction in 2011. Nevertheless, it is still an open problem to deduce higher regularity properties. The results on its entropically regularized version studied in Chapter 3 is a step in this direction. Moreover, having established a central limit theorem for empirical regularized Wasserstein barycenters, it could be interesting to study further probabilistic properties such as a large deviations principle. The regularity of the map  $\Phi_\nu$  defined in Theorem 3.5.2, which maps for a fixed target measure a source measure toward the corresponding Brenier potential, should enable to prove such a result. Finally, let us remark that further research can be done in finding efficient numerical methods to compute an entropically regularized Wasserstein barycenter.

The Wasserstein median studied in Chapter 4 turns out to be a promising statistical estimator thanks to its robustness to outliers. Still, in general uniqueness of this estimator cannot be guaranteed, so it would be interesting to study certain selections of Wasserstein medians and their properties, as it is done in this thesis in the case of the real line. Contrary to the case of the Wasserstein barycenter, the Wasserstein median does not allow for a linear  $L^\infty$ -bound when the given measures have  $L^\infty$ -densities, see Example 4.4.9. Maybe it is at least possible to prove that a non-linear  $L^\infty$ -bound holds true in certain cases or that absolute continuity of the given measures carries over. By imposing additional geometric conditions and using its multimarginal formulation, one can also hope to retrieve further properties. Of course, it is also interesting to extend the results from discrete to more general probability measures on the Wasserstein space  $(\mathcal{P}_1(X), W_1)$ . Finally, the reason the majority of this chapter has been kept in the framework of general metric spaces, is that we believe that the Wasserstein median could be of particular interest when studied on discrete structures such as graphs.

The constrained Wasserstein interpolation problem studied in Chapter 5 has issued several possible further research directions. First, note that in the case of location constraint, we believe the absolute continuity (w.r.t. the  $(d - 1)$ -Hausdorff measure) of the pivot measure on the boundary as announced in e.g. Proposition 5.4.4 should hold true without one of the measures assumed to be discrete. It seems that this is an artifact of our proof strategy. Next, the simulations in Figure 5.2, 5.3, 5.4 and 5.5 give rise to the question of its relation to shape optimization problems. For example, in the case  $p = 2$  the pivot measure appears to be the union of balls, which is indeed an exact solution if the threshold function is constant and both given measures are given by Dirac measures.

From this it is reasonable to conjecture that also other solutions take the form of unions of optimal shapes.

# Notation

$\mathbb{N}, \mathbb{N}^*$	set of non-negative integers, set of strictly positive integers
$\mathbb{R}^d$	$d$ -dimensional space of real numbers with $d \in \mathbb{N}^*$
$ \cdot $	Euclidean norm
$x \cdot y$	Euclidean scalar product between $x, y \in \mathbb{R}^d$
$ \cdot _\infty$	$l^\infty$ norm on space of real numbers
$\mathcal{L}^d$	Lebesgue measure on $\mathbb{R}^d$
$\mathcal{M}(X)$	space of finite Radon measures on $X$
$\mathcal{M}_+(X)$	set of non-negative finite Radon measures on $X$
$\mathcal{P}(X)$	space of Borel probability measures on $X$
$\mathcal{P}_p(X)$	space of Borel probability measures on $X$ with finite $p$ th moment, $p \geq 1$
$\mathcal{P}_{ac}(X)$	space of absolutely continuous Borel probability measures on $X \subset \mathbb{R}^d$
$\mathcal{M}_{div}(X, \mathbb{R}^d)$	space of vector-valued finite Radon measures whose weak divergence is a scalar Radon measure
$C(X)$	space of continuous functions on $X$
$C^k(X)$	space of $k$ times continuously differentiable functions on $X$ , $k \in \mathbb{N}^*$
$C^{k,\alpha}(X)$	space of $k$ times continuously differentiable functions on $X$ whose $k$ th derivative is Hölder continuous with exponent $\alpha \in (0, 1]$ , $k \in \mathbb{N}^*$
$\text{Lip}_M(X)$	set of Lipschitz continuous functions with maximal Lipschitz constant $M > 0$
$L^p(X)$	space of measurable functions for which $p$ th power of absolute value is integrable
$L^p(X, \rho), L^p(\rho)$	$L^p$ space w.r.t. measure $\rho$ , $p \geq 1$
$W^{k,p}(X)$	Sobolev of order $k \in \mathbb{N}^*$ and integrability $p \geq 1$
$H^k(X)$	Sobolev space $W^{2,p}(X)$
$\mathcal{F}_\diamond$	subset of functions with zero mean of the integrable function space $\mathcal{F}$
$\ \cdot\ _{\mathcal{F}}$	norm of Banach space $\mathcal{F}$



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## RÉSUMÉ

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Cette thèse étudie des problèmes variationnels comprenant plusieurs fonctionnelles de transport optimal. Un exemple populaire est le barycentre Wasserstein qui peut être vu en tant que moyenne dans l'espace de Wasserstein d'ordre 2. Depuis son introduction en 2011 de Agueh et Carlier, il est devenu très populaire en statistiques, machine learning et traitement des images. Bien que la consistance du barycentre Wasserstein soit désormais bien connue, une étude plus précise des taux de convergences nécessite encore une analyse supplémentaire. Nous faisons un pas dans cette direction en montrant un théorème central limite pour une version régularisée du barycentre Wasserstein qui a été introduite par Bigot, Cazelles et Papadakis en 2019. Même si le barycentre Wasserstein fournit déjà un bon estimateur statistique, ce n'est pas toujours un estimateur robuste car son breakdown point est bas. Cela nous a motivé d'étudier la médiane Wasserstein, la solution du problème de minimisation des sommes des distances de Wasserstein d'ordre 1. En effet, le breakdown point de la médiane Wasserstein s'avère être plus grand. Cependant, des propriétés de régularité de cet estimateur sont plus subtiles. Néanmoins, nous fournissons une caractérisation détaillée et des estimations d'intégrabilité dans le cas où les mesures sont supportées sur la droite réelle. Dans le cadre général des espaces métriques, des formulations duales et multimarginales équivalentes sont présentées. Nous donnons aussi une caractérisation d'EDP des médianes Wasserstein sur des espaces euclidiens. Motivé par un contexte différent, pourtant donnant une classe similaire des problèmes d'optimisation, est le problème d'emplacement de stationnement optimal. Ceci consiste de trouver une mesure optimale sous des contraintes supplémentaires, comme l'emplacement ou une contrainte de capacité, entre deux mesures, prenant en compte des différents types de coûts de transport. Dans ce cadre, nous démontrons des propriétés de régularité pour plusieurs classes du coût de transport. Finalement, nous fournissons un algorithme numérique afin de simuler des distributions de stationnement optimal en introduisant un terme de régularisation entropique et en déduisant une variante du célèbre algorithme du Sinkhorn.

## MOTS CLÉS

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Transport optimal, équation de Monge-Ampère, moyenne de Fréchet, médiane Fréchet, régularisation entropique

## ABSTRACT

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This thesis studies variational problems involving several optimal transport functionals. A popular example is the Wasserstein barycenter, which can be seen as a mean in the Wasserstein space of order 2. Since its introduction in 2011 by Agueh and Carlier, it has gained a lot of popularity in fields like statistics, machine learning and image processing. While consistency of the Wasserstein barycenter is by now well known, a deeper study of rates of convergence still requires further research. We give a step in this direction by proving a central limit theorem for a regularized version of the Wasserstein barycenter, which has been introduced by Bigot, Cazelles and Papadakis in 2019. While the Wasserstein barycenter already provides a good statistical estimator, it is not always a very robust estimator, as it has a low breakdown point. This motivates the study of the Wasserstein median, the solution to minimizing a sum of Wasserstein distances of order 1. Indeed, the breakdown point of the Wasserstein median turns out to be higher. However, regularity properties of this estimator are more subtle. Nevertheless, we provide a detailed characterization and integrability estimates in the case where the measures are supported on the real line. In the general setting of metric spaces, equivalent dual and multimarginal formulations are given. We also introduce a PDE characterization for Wasserstein medians on Euclidean spaces. Motivated by a different context, yet yielding a similar class of optimization problems, is the optimal parking location problem. It consists of finding an optimal measure under additional constraints, such as a location or a capacity constraint, between two distributions, taking into account different kind of transportation costs. In this case, we prove regularity properties for several classes of transport costs. Finally, we provide a numerical algorithm to simulate optimal parking distributions by introducing an entropic regularization term and deducing a variant of the celebrated Sinkhorn algorithm.

## KEYWORDS

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Optimal transport, Monge-Ampère equation, Fréchet mean, Fréchet median, Entropic regularization