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Inside and around Wasserstein barycenters

Aleksei Kroshnin

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Résumé

Le problème du transport optimal, initialement introduit par G. Monge en 1781 et redécouvert par L. Kantorovich en 1942, consiste à transformer une distribution de masse μ en une autre ν avec le minimum de travail :

$$\int c(x, y) d\gamma(x, y) \rightarrow \min_{\gamma},$$

où la minimisation se fait parmi les couplages de μ et ν (plans de transport) et $c(x, y)$ est le coût de transport d'une unité de masse de x à y . Dans cette thèse, on considère quelques problèmes variationnels impliquant un transport optimal. On est principalement motivé par le problème du barycentre de Wasserstein introduit par M. Agueh et G. Carlier en 2011 :

$$\sum_{i=1}^n w_i W_2^2(\mu_i, \nu) \rightarrow \min_{\nu},$$

où ν_1, \dots, ν_n sont des mesures de probabilité, w_1, \dots, w_n sont des poids positifs, et W_2 est la distance de 2-Wasserstein entre mesures, définie par transport optimal. On traite les problèmes suivants :

- les barycentres par rapport à un coût général de transport, leur existence et leur stabilité ;
- concentration et théorème central limite pour les barycentres empiriques de Wasserstein des mesures gaussiennes ;
- caractérisation, propriétés et théorème central limite pour les barycentres de Wasserstein pénalisés par l'entropie ;
- le problème de transport optimal, pénalisé en l'énergie de Dirichlet d'un plan de transport.

Une autre partie de la thèse est consacrée à l'analyse de la complexité de l'algorithme des projections itératives de Bregman [Ben+15]. Il s'agit d'une généralisation de l'algorithme bien connu de Sinkhorn, qui nous permet de trouver une solution approximative du problème de transport optimal ainsi que du problème du barycentre de Wasserstein.

Mots clés : transport optimal, espace de Wasserstein, barycentre de Wasserstein, moyenne de Fréchet, théorème central limite, espace de Sobolev, algorithme de Sinkhorn, projections itératives de Bregman, complexité des algorithmes.

Abstract

Inside and around Wasserstein barycenters

The optimal transportation problem originally introduced by G. Monge in 1781 and rediscovered by L. Kantorovich in 1942 consists in transformation of one mass distribution μ to another ν with the minimal amount of work:

$$\int c(x, y) d\gamma(x, y) \rightarrow \min_{\gamma}$$

over the couplings of μ and ν (transport plans), where $c(x, y)$ is the cost of transportation of unit mass from x to y . In this thesis, we consider some variational problems involving optimal transport. We are mainly motivated by the Wasserstein barycenter problem introduced by M. Agueh and G. Carlier in 2011:

$$\sum_{i=1}^n w_i W_2^2(\mu_i, \nu) \rightarrow \min_{\nu}$$

where ν_1, \dots, ν_n are probability measures, w_1, \dots, w_n are positive weights, and W_2 is the 2-Wasserstein distance between measures, defined via optimal transport. We deal with the following problems:

- barycenters w.r.t. a general transportation cost, their existence and stability;
- concentration and central limit theorem for empirical Wasserstein barycenters of Gaussian measures;
- characterization, properties, and central limit theorem for entropy-penalized Wasserstein barycenters;
- optimal transportation problem, regularized with the Dirichlet energy of a transport plan.

Another part of the thesis is devoted to the complexity analysis of the iterative Bregman projections algorithm [Ben+15]. This is a generalization of the well-known Sinkhorn algorithm, which allows us to find an approximate solution of the optimal transportation problem and the Wasserstein barycenter problem as well.

Keywords: optimal transport, Wasserstein space, Wasserstein barycenter, Fréchet mean, central limit theorem, Sobolev space, Sinkhorn algorithm, iterative Bregman projections, algorithmic complexity.

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Contents

1	Introduction	1
1.1	Optimal transport	1
1.2	Variational problems involving Wasserstein distance	1
1.3	Iterative Bregman Projections	3
1.4	Related works	4
1.4.1	Wasserstein barycenters	4
1.4.2	Sobolev spaces of measure-valued maps	5
1.4.3	Numerical methods	6
1.5	Main results	7
1.6	Organisation of manuscript	8
2	Preliminaries	11
2.1	Measure theory	11
2.2	Monge–Kantorovich problem	13
2.3	Wasserstein space	17
3	Fréchet barycenters	19
3.1	Introduction	19
3.2	Properties of Monge–Kantorovich distance	20
3.3	Transportation topology	27
3.3.1	Class E_0	27
3.3.2	Topological properties	29
3.3.3	Locally compact X	31
3.4	Case of \mathbb{R}^d	32
3.5	Fréchet barycenters	33
3.5.1	Generalized averaging in $\mathcal{P}(X)$	34
3.5.2	Stability of barycenters	35
4	Bures–Wasserstein barycenters	37
4.1	Introduction	37
4.1.1	Bures–Wasserstein barycenters	38
4.2	Properties of Bures–Wasserstein distance and OT maps	40
4.2.1	Properties of T_Q^S	41
4.2.2	Properties of $d_{BW}(Q, S)$	47
4.3	Existence and uniqueness of barycenters	48
4.4	Central limit theorems	50
4.5	Concentrations	54
4.5.1	Concentration of Q_n	54
4.5.2	Concentration of V_n	57
4.6	Slow rate of convergence: example	58
4.A	Auxiliary results	62

5	Entropic-regularized barycenters	65
5.1	Introduction	65
5.2	Setting, assumptions and preliminaries	66
5.3	Characterization	69
5.4	Properties of the entropic barycenter	76
5.4.1	Global bounds	76
5.4.2	Stability	80
5.4.3	Maximum principle	82
5.5	Higher regularity	83
5.6	Statistical properties	85
5.6.1	Stochastic setting and law of large numbers	85
5.6.2	Central limit theorem	86
5.A	Linearization of Monge–Ampère equations	89
5.B	Auxiliary probability results	91
6	Dirichlet energy and Sobolev spaces of measure-valued maps	93
6.1	Introduction	93
6.2	Sobolev maps valued in metric space	94
6.3	Integral mappings and precise representatives	95
6.4	Convergence	99
6.5	Regularized Monge–Kantorovich problem	107
6.5.1	Open questions	108
7	Analysis of iterative Bregman projections	111
7.1	Introduction	111
7.2	Problem statement and preliminaries	112
7.3	Convergence of dual IBP	113
7.3.1	Greedy strategy	114
7.3.2	Randomized strategy	116
7.4	Multimarginal OT problem	118
7.5	Barycenter problem	121
7.6	Numerical experiments	125
8	Résumé des résultats de la thèse	129
8.1	Transport optimal	129
8.2	Topologie des transports	129
8.3	Barycentres	130
8.4	Espaces de Sobolev de fonctions à valeur mesures et problème de Monge–Kantorovich régularisé	132
8.5	Analyse des projections itératives de Bregman	132
	Bibliography	133

Chapter 1

Introduction

1.1 Optimal transport

The *optimal transportation theory* can be dated back to G. Monge [Mon81], while its modern formulation is due to L. Kantorovich [Kan42]. The central object is the optimal transportation problem consisting in transformation of one mass distribution μ to another ν with the minimal amount of work. Namely, given measures μ and ν of the same mass (e.g. equal to 1) we want to minimize the total transportation cost of μ to ν . The cost is measured via a *cost function* $c(x, y)$ that gives the price to move unit mass from x to y . In the Kantorovich formulation, this leads to the *Monge–Kantorovich problem*:

$$\int c(x, y) d\gamma(x, y) \rightarrow \min_{\gamma},$$

where the minimization is among measures γ with marginals μ and ν (i.e. the couplings of μ and ν). Of particular interest is the case where μ and ν are probability measures on the same metric space (X, ρ) and $c := \rho^p$ for some $1 \leq p < \infty$. This leads to so-called *p-Wasserstein distance*¹:

$$W_p(\mu, \nu) := \left(\inf \left\{ \int_{X \times X} \rho^p(x, y) d\gamma(x, y) : \gamma \text{ is a coupling of } \mu \text{ and } \nu \right\} \right)^{1/p}.$$

The space $\mathcal{P}_p(X)$ of probability measures on X with finite p -th moment endowed with W_p is called the *p-Wasserstein space* over X . An important property of the Wasserstein distance is that it captures the geometry of the underlying space X . The Wasserstein metric — especially of order 1 or 2 — is used in a wide range of areas, such as probability theory and statistics [LT13; BFS12; Zha18; Fla+18; PZ19], stochastic processes, PDE, kinetic theory, and dynamical systems [CT04; MM13; HI17; QH18; LZZ19], image processing [RTG00; PKD07], data analysis and machine learning [Kus+15; Cou+16; Kol+17; MMC16; ACB17]. In the same time, the optimal transportation theory itself remains an active area of research [DF14; Moa16; Lot17; KK17; CF19; DL+19].

1.2 Variational problems involving Wasserstein distance

Now let us discuss some variational problems in the Wasserstein space considered in the current study.

Wasserstein barycenters. In 2011 M. Agueh and G. Carlier introduced a “typical element” of a family of probability measures μ_1, \dots, μ_n on the Euclidean space \mathbb{R}^d , called the *2-Wasserstein*

¹Although this is the common name for this object nowadays, it is quite questionable from the historical point of view, and some authors suggest to use the name transportation or Kantorovich metric instead [Ver06]. Moreover, in the image processing community it is known as the earth mover’s distance (EMD) due to the seminal work of Monge, which makes this question even more confusing [RTG00].

barycenter [AC11]:

$$\nu^* := \operatorname{argmin}_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} \sum_{i=1}^n w_i W_2^2(\mu_i, \nu), \quad (1.1)$$

where w_1, \dots, w_n are positive weights. This is a special case of the *Fréchet mean* in the 2-Wasserstein space [Fré48]. It turns out that the barycenter to some extent captures the shape of the averaged measures μ_1, \dots, μ_n (see Figure 1.1), which makes it favorable compared to the linear averaging of measures. This brings a lot of attention to barycenters: there are attempts to use it in the image processing [Rab+11; BPC16], data analysis [Del+17; Álv+18; Ho+17; SJ17; GPC15] etc. The works [BK12; KP17; LL17] generalize the concept of the Wasserstein barycenter to the case of a probability distribution P on $\mathcal{P}_p(X)$ and an exponent $p \geq 1$:

$$\nu^* := \operatorname{argmin}_{\nu \in \mathcal{P}_p(X)} \int W_p^p(\mu, \nu) dP(\mu). \quad (1.2)$$

This setting brings up the question of stability of the barycenter. In particular, in [BK18] the authors consider a stochastic setting where measures μ_1, μ_2, \dots are drawn independently from P , and define the *empirical barycenters*

$$\nu_n := \operatorname{argmin}_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} \frac{1}{n} \sum_{i=1}^n W_2^2(\mu_i, \nu). \quad (1.3)$$

Under suitable assumptions on P the *population barycenter* ν^* is unique and ν_n converge to it: $W_2(\nu_n, \nu^*) \rightarrow 0$, i.e. the law of large numbers (LLN) holds true. Having this LLN in mind, it is natural to look for an asymptotic normality and a concentration of the empirical barycenters around the population one, but this appears to be a much more subtle problems (see [AC17; ALP19] for some results in this direction). In this work, we deal with these questions in two special cases: for barycenters of Gaussian measures and general Wasserstein barycenters penalized with the entropy. Of note, this work naturally extends the Gaussian case to the case of barycenters of positive semi-definite Hermitian operators.

Harmonic maps and regularized Monge–Kantorovich problem. Let Δ^{k-1} be the k -dimensional probability simplex. When we fix k points x_1, \dots, x_k in \mathbb{R}^d , the barycenter map

$$x(\lambda) := \operatorname{argmin}_{x \in \mathbb{R}^d} \sum_{i=1}^k \lambda_i \|x - x_i\|^2 = \sum_{i=1}^k \lambda_i x_i, \quad \lambda \in \delta^{k-1},$$

is affine — in particular, it is harmonic. This is not the case anymore for a Fréchet mean in a general metric space (i.e. for $\operatorname{argmin}_x \sum_{i=1}^k \lambda_i d(x, x_i)^2$), so barycenters and harmonic extensions are different, but related notions (both define a nonlinear interpolation in a metric space). The latter are introduced in [KS93] in the following way: let $\Omega \subset \mathbb{R}^m$ be a domain with Lipschitz boundary, (X, ρ) be a non-positively curved metric space; given $f: \partial\Omega \rightarrow X$, its harmonic extension is a minimizer of the Dirichlet energy

$$\operatorname{Dir}(u) := \int_{\Omega} |Du(x)|^2 dx,$$

among Sobolev maps $u: \Omega \rightarrow X$ such that $\operatorname{tr} u = f$. Of course, one has to define the Sobolev space $H^1(\Omega; X)$ and the “metric gradient” $|Du(x)|$. In [Lav19b; Lav19a] H. Lavenant studies harmonic maps valued in the 2-Wasserstein space. He defines the H^1 Sobolev space of measure-valued maps on Ω (and the corresponding Dirichlet energy) using an analogue of the Benamou–Brenier formula for absolutely continuous curves in the Wasserstein space proposed by [Bre03] and shows that this definition is equivalent to the ones from [KS93] and [Res97].

Another application of Sobolev spaces is using the Dirichlet energy as a penalization. Similar approaches are of interest in applied mathematics, e.g. image and data processing [Sol+14;

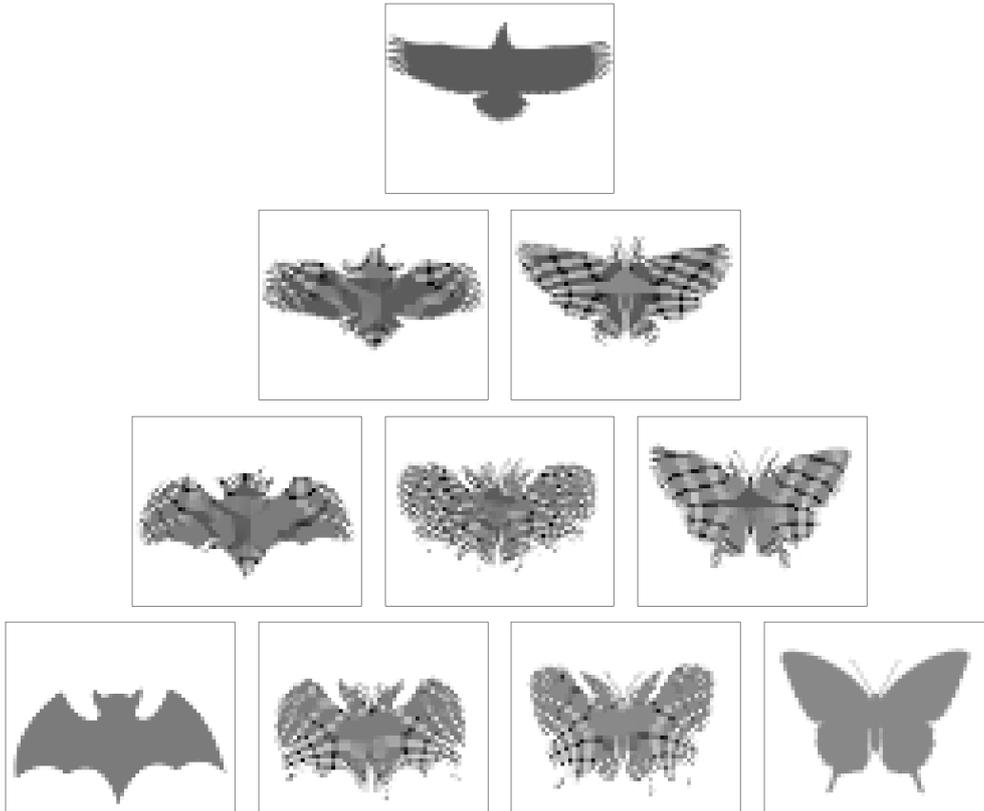


Figure 1.1: Wasserstein barycenters of three images considered as probability measures on the regular grid of size 60×50 . One can see the change of the barycenter as the weights vary. The intensity oscillations are discretization artefacts.

[Fer+14](#); [GM14](#); [VL18](#)]. J. Louet in [\[Lou14\]](#) applies this to the optimal transport considering the regularized Monge problem

$$\int_{\Omega} c(x, T(x)) d\mu(x) + \int_{\Omega} \|DT(x)\|^2 dx \rightarrow \min_{T \in H^1(\Omega; \mathbb{R}^d): T_{\#}\mu = \nu}$$

with $\mu \in \mathcal{P}(\Omega)$ and $\nu \in \mathcal{P}(\mathbb{R}^d)$. He also proposes a Kantorovich-like formulation in terms of transport plans. The discrete version of this problem was also considered in [\[Fer+14\]](#). Instead, here we will consider the Monge–Kantorovich problem penalized with the Dirichlet energy of a coupling γ between μ and ν (which can be viewed as a measure-valued map $x \mapsto \gamma_x \in \mathcal{P}(\mathbb{R}^d)$ due to the disintegration theorem) to ensure the smoothness of the optimal transport.

1.3 Iterative Bregman Projections

Now let us briefly recall the computational aspects of the optimal transport. If μ and ν are discrete measures, then the Monge–Kantorovich problem is an LP problem of special form:

$$\inf \left\{ \sum_{i,j=1}^{n,m} C_{i,j} X_{i,j} : X_{i,j} \geq 0, \sum_{j=1}^m X_{i,j} = \mu_i, \sum_{i=1}^n X_{i,j} = \nu_j \right\}, \quad (1.4)$$

where $\mu = \sum_{i=1}^n \mu_i \delta_{x_i}$, $\nu = \sum_{j=1}^m \nu_j \delta_{y_j}$, and $C_{i,j} := c(x_i, y_j)$. Thus, it can be numerically solved by standard methods for LP problems, e.g. the simplex method. Moreover, one can show that it can be written in the form of the minimum-cost flow problem, which also admits efficient numerical solution [\[PC+19\]](#).

M. Cuturi in 2013 [\[Cut13\]](#) proposed to add the entropic penalization $\lambda \text{Ent}(X)$ with a small parameter $\lambda > 0$ and showed that the resulting problem is equivalent to finding $u \in \mathbb{R}_+^n$, $v \in \mathbb{R}_+^m$

such that for all i and j

$$\sum_{j=1}^m u_i \exp\left(-\frac{C_{i,j}}{\lambda}\right) v_j = \mu_i, \quad \sum_{i=1}^n u_i \exp\left(-\frac{C_{i,j}}{\lambda}\right) v_j = \nu_j.$$

This is the so-called *matrix scaling problem*, and one of the most famous methods for solving it is the *Sinkhorn algorithm*² [Sin74]. It consists in alternating scaling of rows and columns of a matrix X starting from $X := \left(-\frac{C_{i,j}}{\lambda}\right)_{i,j=1}^{n,m}$ such that it satisfies the first and the second equation, respectively. [Ben+15] proposed a generalization of the Sinkhorn algorithm called the iterative Bregman projections method (IBP). This is a particular case of Dykstra's algorithm with Bregman divergences [BL00], which in the case of affine constraints consists in alternating projections w.r.t. the Kullback–Leibler divergence.

It is well-known that the Sinkhorn algorithm for fixed λ converges geometrically [FL89], but the constant grows extremely fast as $\lambda \rightarrow 0$ and it makes this bound impractical for estimating the complexity of an approximate solution of the Monge–Kantorovich problem. The seminal work [AWR17] shows that to obtain an ε -solution \hat{X} of the optimal transportation problem, i.e. such that

$$\sum_{i,j=1}^{n,m} C_{i,j} \hat{X}_{i,j} \leq \sum_{i,j=1}^{n,m} C_{i,j} X_{i,j}^* + \varepsilon, \quad \text{where } X^* \text{ is a solution of (1.4),} \quad (1.5)$$

one should run the Sinkhorn algorithm for $O\left(\frac{\log(nm)}{\varepsilon^3}\right)$ iterations. In this work, we provide the improved bound $O\left(\frac{\log(nm)}{\varepsilon^2}\right)$ for IBP applied to some optimal transport problems.

1.4 Related works

1.4.1 Wasserstein barycenters

In the seminal paper [AC11], authors define barycenters of finitely many measures from the 2-Wasserstein space over \mathbb{R}^d , given by (1.1). They show the existence of a barycenter and its uniqueness under the assumption that at least one of the measures μ_i is absolutely continuous (Propositions 2.3 and 3.5). In the case $d = 1$ an explicit formula for barycenter is given via the inverse cumulative distribution functions of the measures. If all μ_i are Gaussian, it is shown that the barycenter is also Gaussian and satisfies some fixed-point equation (see Chapter 4 for details). The authors also obtain an equivalent multimarginal formulation for the barycenter problem:

$$\int c(x_1, \dots, x_n) d\gamma(x_1, \dots, x_n) \rightarrow \min_{\gamma \in \Pi(\mu_1, \dots, \mu_n)}, \quad (1.6)$$

where $\Pi(\mu_1, \dots, \mu_n)$ is the set of probability measures with marginals μ_1, \dots, μ_n , and

$$c(x_1, \dots, x_n) := \min_{x \in \mathbb{R}^d} \sum_{i=1}^n w_i \|x_i - x\|^2 = \sum_{i=1}^n w_i \|x_i\|^2 - \left\| \sum_{i=1}^n w_i x_i \right\|^2, \quad x_i \in \mathbb{R}^d$$

(we assume w.l.o.g. that $\sum_{i=1}^n w_i = 1$). If γ^* is a solution of the above problem, then $(f_w)_\# \gamma^*$ is a Wasserstein barycenter and vice versa, where $f_w(x_1, \dots, x_n) := \sum_{i=1}^n w_i x_i$. Finally, they show the regularity of the barycenter: once one of the measures (say, μ_1) has a bounded density, then (Theorem 5.1)

$$\|\nu^*\|_{L^\infty} \leq \frac{1}{w_1^d} \|\mu_1\|_{L^\infty}.$$

In [BK12] J. Bigot and T. Klein define for the first time the population barycenter in the 2-Wasserstein space over a compact set $\Omega \subset \mathbb{R}^d$ (recall formula (1.2)). They prove its existence and uniqueness under the assumption that the distribution P is concentrated on the set of a.c.

²also known as the Sinkhorn–Knopp, RAS, or balancing algorithms

measures. In the stochastic setting, they obtain the strong LLN for the empirical barycenters ν_n given by (1.3):

$$W_2(\nu_n, \nu^*) \rightarrow 0 \quad \text{a.s.}$$

The work [KP17] addresses the 2-Wasserstein population barycenters on a compact Riemannian manifold M . If $P(\mathcal{P}_{ac}(M)) > 0$, where $\mathcal{P}_{ac}(M)$ is the set of probability measures absolutely continuous w.r.t. the volume measure, then the barycenter of P exists and is unique (Theorem 3.1). The authors prove a regularity result similar to [AC11]: if the Ricci curvature is bounded from below and $P(\mathcal{P}_{ac}^\infty(M)) > 0$, then $\nu^* \in \mathcal{P}_{ac}^\infty(M)$, where $\mathcal{P}_{ac}^\infty(M)$ is the set of a.c. probability measures with bounded densities (Theorem 6.1). Moreover, they obtain so-called first and second order balance (Theorem 4.4), which is closely related to the characterization of entropic-Wasserstein barycenters that we consider in Chapter 5.

In [LL17] T. Le Gouic and J.-M. Loubes consider a more general setting of the p -Wasserstein space over an abstract Polish space X . They define the p -Wasserstein population barycenter and show its existence. They also prove that the barycenters are stable w.r.t. the change of the distribution: let \mathcal{W}_p be the p -Wasserstein distance between measures on $\mathcal{P}_p(X)$, $\nu_n := \text{bar}(P_n)$, and $\mathcal{W}_p(P_n, P) \rightarrow 0$; then, up to a subsequence, there is a barycenter ν^* of P such that $\mathcal{W}_p(\nu_n, \nu^*) \rightarrow 0$ (Theorem 3). In particular, this result immediately implies the strong LLN.

In the note [AC17] M. Agueh and G. Carlier suggest an approach to obtain the central limit theorem (CLT) for empirical 2-Wasserstein barycenters. In particular, they prove the CLT in the one-dimensional case if $P = \sum_{i=1}^n w_i \delta_{\mu_i}$ is a discrete distribution concentrated on the Gaussian measures. It is worth noting that the idea of the proof relies on the differentiability of optimal transportation maps, as in Chapter 4.

To the best of our knowledge, the most state-of-the-art result concerning the rates of convergence of empirical 2-Wasserstein barycenters is obtained as a particular case of a more general result by [Le +19]. This work establishes fast rates of convergence for empirical barycenters over a large class of geodesic spaces with curvature bounds in the sense of Alexandrov. For the 2-Wasserstein space over a Hilbert space it shows that $\mathbb{E} W_2^2(\nu_n, \nu^*) \leq \frac{C}{n}$, under the assumption of the strong convexity and smoothness of Brenier potentials between $\nu^* := \text{bar}(P)$ and P -a.e. μ (Corollary 16). This work extends and completes the results by [ALP19]. The latter paper provides the rates of convergence for empirical barycenters on a metric space either under the assumptions on weak curvature constraint on the underlying space or for the case of a nonnegatively curved space on which geodesics, emanating from a barycenter, can be extended.

J. Bigot, E. Cazelles, and N. Papadakis in [BCP19] observed that when one discretizes continuous measures the corresponding (discrete) barycenter exhibits strong oscillations and proposed to add a penalization to the Wasserstein variance functional to rule out such discretization artefacts. They show the existence, uniqueness, and stability (in the sense of [LL17]) of the regularized barycenters under suitable assumptions on the penalty functional (Section 3). Moreover, for a compact domain, they obtain the rate of convergence of the empirical barycenters in terms of Dudley's integral and the metric entropy (Theorem 4.6).

Finally, it is worth mentioning that there are some other works dealing with the central limit theorem for the Wasserstein distance, e.g. [RMS16; DL+19]. However, the setting in these works differs significantly from what is done in the present study. A result similar in spirit to Theorem 4.5.4 is obtained in [Del+19] for the case of the 2-Wasserstein space over the real line. We refer to the recent monograph [PZ20] for more details on statistical problems in the Wasserstein spaces including properties of empirical Wasserstein barycenters.

1.4.2 Sobolev spaces of measure-valued maps

There are several definitions of the Sobolev spaces of maps acting from $\Omega \subset \mathbb{R}^m$ to some metric space (X, ρ) . N. Korevaar and R. Schoen in [KS93] define it using approximate Dirichlet energies: $u \in W^{1,p}(\Omega; X)$ if there is $C < \infty$ such that

$$\limsup_{\varepsilon \rightarrow 0} \int_{\Omega'} \int_{B_\varepsilon(x)} \frac{\rho^p(u(x), u(y))}{\varepsilon^p} dy dx \leq C$$

for all compactly embedded $\Omega' \subset\subset \Omega$. Y. Reshetnyak in [Res97] gives another definition: $u \in W^{1,p}(\Omega; X)$ if there is a function $g \in L^p(\Omega)$ such that for any L -Lipschitz function $F: X \rightarrow \mathbb{R}$ it holds that $F \circ u \in W^{1,p}(\Omega)$ and

$$\|\nabla(F \circ u)\| \leq Lg \quad \text{a.e. in } \Omega.$$

In [Res04], he showed that the two definitions are equivalent. Y. Brenier in [Bre03] proposes a notion of Sobolev maps valued in the 2-Wasserstein space based on the Benamou–Brenier formula. Namely, a map $\mu: \Omega \rightarrow \mathcal{P}_2(\mathbb{R}^d)$ is Sobolev if there is a matrix field V satisfying (in a weak sense) the continuity equation

$$\nabla_{\Omega} \mu + \nabla_{\mathbb{R}^d}(V\mu) = 0$$

and such that $\int_{\Omega} \int_{\mathbb{R}^d} \|V\|^2 d\mu(x) dx < \infty$. In [Lav19b], H. Lavenant shows that in the 2-Wasserstein space all the above definitions coincide (Theorems 3.17 and 3.24). He studies harmonic maps valued in the Wasserstein space and their relations with convexity, geodesic curves, and Wasserstein barycenters.

1.4.3 Numerical methods

As we already mentioned, M. Cuturi in [Cut13] proposes to add the entropic penalty to the discrete Monge–Kantorovich problem (1.4) with a general cost matrix C and use the Sinkhorn method for solving the resulting problem. According to [FL89], the Sinkhorn iterations are contractive in the Hilbert projective metric, which leads to the geometric convergence. Namely, suppose for simplicity that all $C_{i,j} \in [0, 1]$ and consider the Sinkhorn algorithms' steps

$$u^{t+1} := \frac{Kv^t}{\mu}, \quad v^{t+1} := \frac{Cu^{t+1}}{\nu}$$

(here by $\frac{a}{b}$ we denote the coordinate-wise division), with $K_{i,j} := \exp\left(-\frac{C_{i,j}}{\lambda}\right)$, $u^0 := \mathbf{1} = (1, \dots, 1)$, $v^0 := \mathbf{1}$. Then

$$d(u^t, u^*) + d(v^t, v^*) \leq \frac{\gamma^{t-1}}{1 - \gamma} (d(u^1, u^*) + d(v^1, v^*)),$$

where (u^*, v^*) solve the matrix scaling problem and $\gamma := \left(\frac{e^{1/\lambda} - 1}{e^{1/\lambda} + 1}\right)^2 \approx 1 - 4e^{-1/\lambda}$ (Theorem 4). If λ is small (this is the case when we want to approximately solve the non-regularized problem (1.4)), then this bound becomes impractical. In [AWR17] J. Altschuler, J. Weed, and P. Rigollet obtained the first polynomial upper bound on the number of Sinkhorn iterations needed to obtain an ε -approximate solution of (1.4): $O\left(\frac{\log(nm)}{\varepsilon^3}\right)$ (Theorem 3). The key idea is that once we get u and v such that $\|\text{diag}(u)Kv - p\|_1 + \|\text{diag}(v)K^T u - q\|_1 \leq c\varepsilon$ we can obtain from them (by Algorithm 2) a feasible transport plan \hat{X} , which is an ε -solution, i.e. satisfies (1.5). They also proposed a greedy version of the Sinkhorn algorithm called Greenhorn.

To the best of our knowledge, the first algorithms for solving Wasserstein barycenter problem (with fixed and non-fixed support) were proposed by M. Cuturi and A. Doucet in [CD14] based on the accelerated Nesterov method. In this regard, it is worth mentioning the recent work [AB21] where J. Altschuler and E. Boix-Adsera prove that computing a Wasserstein barycenter with non-fixed support is an NP-hard problem (essentially, it has the same complexity as solving the equivalent multimarginal optimal transport).

The iterative Bregman projections method proposed in [Ben+15] is a generalization of the Sinkhorn algorithm that solves an entropy-penalized LP problem of the form

$$\langle c, x \rangle + \lambda \text{Ent}(x) \rightarrow \min_{x \in \mathcal{C}_1, \dots, \mathcal{C}_m},$$

where $\mathcal{C}_1, \dots, \mathcal{C}_m$ are convex subsets of \mathbb{R}_+^d . In the case of affine constraints, the method consists of alternating projections w.r.t. the Kullback–Leibler divergence, and in a general setting, this

is nothing but Dykstra’s algorithm with Bregman divergences [BL00]. The authors consider the IBP application to the Wasserstein barycenters problem, the multimarginal optimal transport, the partial and capacity constrained optimal transport, etc. The recent works [Car21] and [Lin+19] study the convergence of IBP for the multimarginal optimal transport. The first one establishes a geometric convergence (but suffering from the same problem as in the case of the Sinkhorn algorithm). The second one obtains the iteration complexity $O\left(\frac{\log n}{\varepsilon^2}\right)$ with the use of the technique from our paper [DGK18], where n is the size of the support of a marginal. We independently obtained the last result in the current thesis.

There are also a lot of works applying gradient and second-order methods of convex optimization to various optimal transportation-related problems, e.g. [COO15; CP16; Gen+16; Dvu+17; DGK18; Dvu+18; Kro+19; LHJ19; Lin+20; PRV20]. For further reading, we refer to the recent monograph [PC+19] and theses [Tup20; Dvi21].

1.5 Main results

Transportation topology. First of all, we consider an abstract setting with a metric space X and a continuous cost function $c: X \times X \rightarrow \mathbb{R}_+$ and define the transportation functional

$$J(\mu, \nu) := \inf \left\{ \int_{X \times X} c(x, y) d\gamma(x, y) : \gamma \text{ is a coupling of } \mu \text{ and } \nu \right\}.$$

Imposing suitable assumptions on X and c (a weak triangle inequality and a “consistency” of c with the topology on X) we show that J inherits a lot of properties of the cost function c and induces a topology τ_J on $\mathcal{P}(X)$ with the basis of “balls” $B_r^J(\mu) := \{\nu \in \mathcal{P}(X) : J(\mu, \nu) < r\}$ (thus, it can be considered as a generalization of the Wasserstein metric). Moreover, any set $E(\mu) := \{\nu \in \mathcal{P}(X) : J(\mu, \nu) < \infty\}$ endowed with τ_J is a Polish space.

Fréchet barycenters. We define an average in $\mathcal{P}(X)$ w.r.t. J in the spirit of the Wasserstein barycenter, which we call the regularized *Fréchet barycenter*: given a distribution P on $\mathcal{P}(X)$ and a penalty G ,

$$\nu^* := \operatorname{argmin}_{\nu \in \mathcal{P}(X)} \left[\int J(\mu, \nu) dP(\mu) + G(\nu) \right].$$

We show that these barycenters exist and are stable w.r.t. P . Namely, let

$$\mathcal{J}(P, Q) := \inf \left\{ \int J(\mu, \nu) d\Gamma(\mu, \nu) : \Gamma \text{ is a coupling of } P \text{ and } Q \right\}, \quad P, Q \in \mathcal{P}(X),$$

and $\mathcal{J}(P_n, P) \rightarrow 0$. If ν_n is a barycenter of P_n , then there is a subsequence converging to some barycenter of P in the transportation topology. In particular, in the stochastic setting mentioned above the law of large numbers holds true.

Wasserstein barycenters of Gaussian measures. In the case of the 2-Wasserstein space over \mathbb{R}^d and a distribution concentrated on the Gaussian measures we prove the central limit theorem and concentration results for empirical Wasserstein barycenters. It is known that in this case the population and the empirical barycenters are also Gaussian, say $\nu_* = \mathcal{N}(0, Q_*)$ and $\nu_n = \mathcal{N}(0, Q_n)$ (w.l.o.g. we can assume they have zero-mean). We show the asymptotic normality of their covariance matrices:

$$\sqrt{n}(Q_n - Q_*) \xrightarrow{d} \mathcal{N}(0, \Xi),$$

and non-asymptotic bounds on $\|Q_n - Q_*\|$ and $W_2(\nu_n, \nu_*)$. Moreover, the results are obtained in a bit more general setting of *Bures–Wasserstein barycenters*. For the case of a scale-location family we also provide an example of slower than $\frac{1}{\sqrt{n}}$ rate of convergence.

Entropic-Wasserstein barycenters. Consider a distribution P on the 2-Wasserstein space over \mathbb{R}^d and define its entropy-regularized barycenter

$$\nu^* := \operatorname{argmin}_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} \left[\int W_2^2(\mu, \nu) dP(\mu) + \lambda \operatorname{Ent}(\nu) \right].$$

We prove existence and uniqueness of this object, and characterize it in terms of dual Kantorovich potentials. Using this characterization, we study the properties of the entropic-Wasserstein barycenters: moment bounds, a maximum principle, higher regularity, and stability. Moreover, in the stochastic setting we obtain the central limit theorem in H^2 for empirical barycenters under additional regularity assumptions on the measures.

Sobolev spaces and regularized Monge–Kantorovich problem. We consider the Sobolev spaces $W^{1,p}$ of maps from an open domain $\Omega \subset \mathbb{R}^m$ to $\mathcal{P}_p(\mathbb{R}^d)$ defined in the sense of Reshetnyak [Res97] and admitting an equivalent definition through the continuity equation as shown by Lavenant [Lav19b]. We study the fine properties of these maps [EG15], namely, we show the existence of precise representatives up to a small set. We also give two notions of convergence in the Sobolev space of measure-valued functions. Finally, we apply this theory to the Monge–Kantorovich problem regularized with the Dirichlet energy:

$$\int_{\Omega} \int_{\mathbb{R}^d} c(x, y) d\gamma_x^*(y) d\mu(x) + \int_{\Omega} \|D\gamma_x\|^p dx \rightarrow \min_{\gamma_x \in W^{1,p}: \int \gamma_x^* d\mu(x) = \nu},$$

where γ_x^* is the precise representative of the map $x \mapsto \gamma_x \in \mathcal{P}_p(\mathbb{R}^d)$ and show existence of a solution under mild assumptions.

Complexity of Iterative Bregman Projections. For IBP method we suggest two different strategies of projections: greedy and random. We provide a general scheme of the proof of complexity bounds and apply it to two optimal transport-related problems: multimarginal optimal transport and Fréchet barycenter, which in both cases gives the iteration complexity $O(\frac{1}{\varepsilon^2})$ to achieve accuracy ε , compared to the previous best-known bound $O(\frac{1}{\varepsilon^3})$ for the Sinkhorn algorithm [AWR17].

1.6 Organisation of manuscript

The thesis is organized as follows. In Chapter 2, we remind some facts from the measure theory and the theory of optimal transport and provide a survey of related works. In Chapter 3, we study some topological properties of the space of measures on an abstract metric space X endowed with the transportation functional. We also define regularized Fréchet barycenters, show their existence and stability. The chapter is mainly based on the work [Kro18]. In Chapter 4, we consider 2-Wasserstein barycenters of Gaussian measures, and, more generally, Bures–Wasserstein barycenters. We study some differential properties of the optimal transport maps and use them to prove the CLT and the concentration of empirical barycenters. We also provide an example of a slower than $\frac{1}{\sqrt{n}}$ rate of convergence. This chapter is based on the joint work with V. Spokoiny and A. Suvorikova [KSS21]. In Chapter 5, we consider the 2-Wasserstein barycenters penalized with the entropy. We obtain a formula for the density of a barycenter and some corollaries, e.g. regularity and moment bounds. In the stochastic setting, we derive the central limit theorem in H^2 . This chapter is based on the joint work with G. Carlier and K. Eichinger [CEK20]. Chapter 6 concerns the Sobolev spaces of measure-valued maps, their fine properties, and convergence. We further apply the obtained results to the regularized Monge–Kantorovich problem. This chapter will be transformed into a research paper and submitted to a scientific journal later on. Finally, Chapter 7 is devoted to the analysis of IBP. We provide new complexity bounds for the multimarginal optimal transport and the barycenter problems based on a general scheme — also obtained here — and illustrate them with numerical experiments.

This is based on and generalizes results from the joint works with A. Gasnikov, P. Dvurechensky et al. [DGK18; Kro+19; Sto+19].

Chapter 2

Preliminaries

2.1 Measure theory

Let X be a topological metrizable space endowed with the Borel σ -algebra $\mathcal{B}(X)$. Then $\mathcal{M}(X)$ denotes the space of finite signed measures on X . Respectively, $\mathcal{M}_+(X)$ is the space of nonnegative finite measures and $\mathcal{P}(X)$ is the space of probability measures on X . We suppose that a metric on X is fixed, though a specific choice is often not important.

We will often drop the argument of a function and a measure and the symbol of domain of integration if there is no risk of confusion, i.e. instead of $\int_X f(x) d\mu(x)$ we will write $\int f d\mu$. We denote the Lebesgue measure on \mathbb{R}^d by \mathcal{L} , $\mathcal{L}(A) = |A|$, and

$$\int_A f(x) d\mathcal{L}(x) = \int_A f(x) dx = \int_A f.$$

For two spaces X, Y , a Borel map $T: X \rightarrow Y$ induces a *push-forward map* $T_\#: \mathcal{M}(X) \rightarrow \mathcal{M}(Y)$ given by

$$T_\#\mu(A) := \mu(T^{-1}(A)) \text{ for any measurable } A \subset Y.$$

Recall that for any integrable function $f \in L^1(Y, T_\#\mu)$ it holds that

$$\int_Y f d(T_\#\mu) = \int_X f \circ T d\mu.$$

For a measure μ on X and a μ -integrable function $f: X \rightarrow \mathbb{R}$ the measure $f\mu$ is defined as

$$(f\mu)(A) := \int_A f d\mu \text{ for any measurable } A \subset Y.$$

Moreover, for any Borel set B define $\mu|_B := \mathbb{1}_B \mu$, where $\mathbb{1}_B$ is the indicator function of B .

Narrow convergence of measures.

Definition 2.1 (Polish space). A separable topological space X is a *Polish space* if it is homeomorphic to a complete metric space.

Definition 2.2 (Radon space; Definition 5.1.4 in [AGS08]). A separable topological metrizable space X is a *Radon space* if any measure $\mu \in \mathcal{M}_+(X)$ is a Radon one [AGS08, def. 5.1.4], i.e. for any $\varepsilon > 0$ there exists a compact set K_ε such that $\mu(X \setminus K_\varepsilon) < \varepsilon$.

E.g. any Polish space is also Radon [Bog07, Theorem 7.1.7].

Definition 2.3 (Narrow convergence; Definition 8.1.1 in [Bog07]). A sequence $\{\mu_n\}_{n \in \mathbb{N}} \subset \mathcal{M}(X)$ *narrowly converges* to $\mu \in \mathcal{M}(X)$ ($\mu_n \rightarrow \mu$) if

$$\int f d\mu_n \rightarrow \int f d\mu \text{ for all } f \in C_b(X),$$

where $C_b(X)$ is the space of continuous bounded functions over X . A corresponding topology τ_w on $\mathcal{M}(X)$ is generated by basis sets of form

$$\left\{ \nu \in \mathcal{M}(X) : \left| \int f_i d\mu - \int f_i d\nu \right| < \varepsilon, i = 1, \dots, n \right\}, \quad \mu \in \mathcal{M}(X), f_i \in C_b(X), n \in \mathbb{N}.$$

We sometimes refer to the narrow convergence as the weak one, meaning that it is defined by duality with test functions.

Note that when we consider only the space of probability measures $\mathcal{P}(X)$, it is enough to test against functions vanishing at infinity, $C_0(X)$. Moreover, if any closed ball in X is compact (e.g. in \mathbb{R}^d), then one can replace $C_0(X)$ with $C_c(X)$. Furthermore, in \mathbb{R}^d it is enough to consider $C_c^\infty(\mathbb{R}^d)$.

A useful property of the narrow convergence is that once $\{\mu_n\}_{n \in \mathbb{N}} \subset \mathcal{M}_+(X)$, $\mu_n \rightharpoonup \mu$, and $f \geq 0$ is a lower semicontinuous (l.s.c.) function over X , then

$$\int f d\mu \leq \liminf \int f d\mu_n.$$

Proposition 2.1.1 (Theorem 8.2.3 in [Bog07]). *Let $\{\mu_n\}_{n \in \mathbb{N}} \subset \mathcal{M}_+(X)$, $\mu \in \mathcal{M}_+(X)$. The following assertions are equivalent:*

1. $\mu_n \rightharpoonup \mu$;
2. $\mu_n(X) \rightarrow \mu(X)$ and $\mu(U) \leq \liminf \mu_n(U)$ for any open set $U \subset X$;
3. $\mu_n(X) \rightarrow \mu(X)$ and $\mu(F) \geq \limsup \mu_n(F)$ for any closed set $F \subset X$.

Combining Theorem 8.9.3 in [Bog07] and Section 5.1 in [AGS08] we obtain the following result.

Proposition 2.1.2. *Let X be a separable metrizable space. Then $(\mathcal{M}_+(X), \tau_w)$ also is separable and metrizable. We denote a metric inducing τ_w by d_w . Moreover, there exists a countable family $\{f_k\}_{k \in \mathbb{N}} \subset C_b(X)$ such that $\mu_n \rightharpoonup \mu$ iff $\mu_n(X)$ are bounded and $\int f_k d\mu_n \rightarrow \int f_k d\mu$ for all $k \in \mathbb{N}$. If X is Polish, then $(\mathcal{M}_+(X), \tau_w)$ is also Polish.*

One can take d_w induced by the *Kantorovich–Rubinstein norm* [Bog07, Theorem 8.3.1]: $d_w(\mu, \nu) := \|\mu - \nu\|_{KR}$, where

$$\|\lambda\|_{KR} := \sup \left\{ \int f d\lambda : f \in C(X), \sup_{x \in X} |f(x)| \leq 1, \text{Lip}(f) \leq 1 \right\}, \quad \lambda \in \mathcal{M}(X). \quad (2.1)$$

If X is complete, then $(\mathcal{M}_+(X), d_w)$ is also complete.

Definition 2.4 (Tightness). A set of measures $S \subset \mathcal{M}_+(X)$ on a topological space X is *tight*, if for any $\varepsilon > 0$ there exists a compact set $K_\varepsilon \subset X$ such that

$$\mu(X \setminus K_\varepsilon) \leq \varepsilon \quad \forall \mu \in S.$$

The next result concerning compactness w.r.t. τ_w follows from Theorems 8.6.2, 8.6.4, and 8.6.7 in [Bog07].

Proposition 2.1.3 (Prokhorov’s theorem). *Let X be a Radon space. If a set $S \subset \mathcal{M}_+(X)$ is uniformly bounded in variation and tight, then it is precompact in τ_w . On contrary, any narrowly convergent sequence $\{\mu_n\}_{n \in \mathbb{N}} \subset \mathcal{M}_+(X)$ is tight. Moreover, if X is Polish, then any subset of $\mathcal{M}_+(X)$ precompact in τ_w is tight and uniformly bounded in variation.*

Remark 2.1.4. We say a subset of a topological space is precompact if its closure is compact. Note that if the space is metric but non-complete, the total-boundedness is in general not enough for the set to be precompact.

Disintegration and gluing.

Proposition 2.1.5 (Disintegration theorem). *Let X, Y be Radon spaces and $\pi: X \rightarrow Y$ be a Borel map. Then for any $\mu \in \mathcal{P}(X)$ with $\nu := \pi_{\#}\mu \in \mathcal{P}(Y)$ there is a ν -a.e. uniquely defined family of measures $\{\mu_y\}_{y \in Y} \subset \mathcal{P}(X)$ such that*

$$\mu_y(\pi^{-1}(y)) = 1 \quad \text{for } \nu\text{-a.e. } y,$$

for any Borel set $A \subset X$ the function $y \mapsto \mu_y(A)$ is Borel, and

$$\int_X f \, d\mu = \int_Y \left(\int_X f \, d\mu_y \right) \, d\nu(y)$$

for any Borel $f: X \rightarrow \mathbb{R}_+$.

The next result shows that the disintegration theorem can be used to “glue” together several couplings sharing the same marginal. It is a trivial generalization of Lemmata 5.3.2 and 5.3.4 in [AGS08].

Proposition 2.1.6 (Gluing lemma). *Let $T = (V, E)$ be a (possibly infinite) tree with at most countable set of vertices V and $\{X_v\}_{v \in V}$ be a family of Radon spaces. If $\mu_v \in \mathcal{P}(X_v)$ for all $v \in V$, $\gamma_{u,v} \in \mathcal{P}(X_u \times X_v)$ has marginals μ_u and μ_v for all $(u, v) \in E$, and $\gamma_{u,v}$ transposed coincides with $\gamma_{v,u}$, then there is a probability measure ν on $\prod_{v \in V} X_v$ such that*

$$(\pi^u, \pi^v)_{\#}\nu = \gamma_{u,v} \quad \text{for all } (u, v) \in E,$$

where π^v is the projection to X_v .

2.2 Monge–Kantorovich problem

In this section we consider an optimal transportation problem, which is a key concept of this work, and recall some of its properties. For more details on the subject we refer to monographs [Vil03; AGS08; Vil09; San15].

Consider two Radon spaces X, Y and measures $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$. We define the set of *transport plans* (the term is specific for the optimal transportation theory; usually they are called couplings) taking μ to ν as

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

where π^1 and π^2 are the projections to the first and the second factor, respectively. Note that $\Pi(\mu, \nu)$ is always nonempty because it contains at least the product measure $\mu \otimes \nu$. Sometimes we also use a notation $\Pi(\mu_1, \dots, \mu_n)$ to denote the set of probability measures on $\prod_{i=1}^n X_i$ with marginals $\mu_1 \in \mathcal{P}(X_1), \dots, \mu_n \in \mathcal{P}(X_n)$.

Now fix a Borel nonnegative *cost function* $c: X \times Y \rightarrow \mathbb{R}_+$. Then the *Monge–Kantorovich problem* consists in minimizing a total *transportation cost*:

$$\mathcal{C}(\gamma) = \mathcal{C}_c(\gamma) := \int_{X \times Y} c(x, y) \, d\gamma(x, y) \rightarrow \min_{\gamma \in \Pi(\mu, \nu)}. \quad (\text{MK})$$

A transport plan γ^* at which the minimum is attained is called *optimal*. The set of all optimal transport plans from μ to ν is denoted by $\Pi_o(\mu, \nu)$. Respectively, the *transportation functional* between μ and ν is the value of the Monge–Kantorovich problem:

$$J(\mu, \nu) = J_c(\mu, \nu) := \inf_{\gamma \in \Pi(\mu, \nu)} \mathcal{C}(\gamma).$$

The Monge–Kantorovich problem can be viewed as a convex relaxation of the *Monge problem*, where one is looking for a push-forward map instead of a transport plan:

$$\int_X c(x, T(x)) \, d\mu(x) \rightarrow \min_T,$$

where the minimization is over the Borel maps T such that $T_{\#}\mu = \nu$. Notice that unlike (MK) this is not an LP problem. As we will see later, the Monge–Kantorovich problem admits a solution under very mild assumptions, which is not the case for the Monge problem. However, sometimes it is possible to show that the values of both problems coincides: e.g. if X and Y are Polish, c is continuous, and μ has no atoms [Pra07].

Let us now recall some properties of the transportation functional J . First of all, since (MK) is an (infinite-dimensional) linear programming problem, one trivially obtains the convexity of its value J (cf. Theorem 4.8 in [Vil09]).

Lemma 2.2.1. *The functional J is convex, i.e. for any measures $\mu_0, \mu_1 \in \mathcal{P}(X)$, $\nu_0, \nu_1 \in \mathcal{P}(Y)$ and $t \in [0, 1]$ it holds that*

$$J(\mu_t, \nu_t) \leq (1-t)J(\mu_0, \nu_0) + tJ(\mu_1, \nu_1),$$

where $\mu_t := (1-t)\mu_0 + t\mu_1$, $\nu_t := (1-t)\nu_0 + t\nu_1$.

Corollary 2.2.2. *Let $Y = X$ and $c(x, x) = 0$ for all $x \in X$. Take $\mu_0, \mu_1 \in \mathcal{P}(X)$. Then for any $0 \leq t < s \leq 1$ it holds that*

$$J(\mu_t, \mu_s) \leq (s-t)J(\mu_0, \mu_1),$$

where $\mu_\tau := (1-\tau)\mu_0 + \tau\mu_1$ for $\tau \in [0, 1]$.

Proof. Since $\mu_s = \frac{1-s}{1-t}\mu_t + \frac{s-t}{1-t}\mu_1$, from the convexity of J it follows that

$$\begin{aligned} J(\mu_t, \mu_s) &\leq \frac{1-s}{1-t}J(\mu_t, \mu_t) + \frac{s-t}{1-t}J(\mu_t, \mu_1) = \frac{s-t}{1-t}J(\mu_t, \mu_1) \\ &\leq \frac{s-t}{1-t}((1-t)J(\mu_0, \mu_1) + tJ(\mu_1, \mu_1)) = (s-t)J(\mu_0, \mu_1). \end{aligned}$$

□

However, in this work we deal with more specific setting. Namely, from now on assume that the cost function is l.s.c. Clearly, in this case \mathcal{C} is also nonnegative and l.s.c. w.r.t. the narrow convergence. Moreover, the problem (MK) enjoys a lot of useful properties under this assumption.

Proposition 2.2.3. *For any $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$ there exists an optimal transport plan. Moreover, if $J(\mu, \nu) < \infty$, then $\Pi_o(\mu, \nu)$ is compact w.r.t. the topology of narrow convergence.*

Proof. Note that $\Pi(\mu, \nu)$ is nonempty, closed in the narrow topology, and tight since μ and ν are tight. Then due to Prokhorov’s theorem any minimizing sequence $\{\gamma_n\}_{n \in \mathbb{N}}$ for (MK) has a narrowly convergent subsequence $\gamma_{n_k} \rightharpoonup \gamma \in \Pi(\mu, \nu)$, and we conclude by the lower semicontinuity of \mathcal{C} . □

Notice, however, that an optimal transport plan from μ to ν may not be unique.

Lemma 2.2.4. *The functional J is lower semicontinuous w.r.t. the narrow convergence.*

Proof. Let $\mu_n \rightharpoonup \mu$, $\nu_n \rightharpoonup \nu$ and $\gamma_n \in \Pi_o(\mu_n, \nu_n)$ be an optimal transport plan from μ_n to ν_n . Since $\{\mu_n\}_{n \in \mathbb{N}}$ and $\{\nu_n\}_{n \in \mathbb{N}}$ are tight, $\{\gamma_n\}_{n \in \mathbb{N}}$ is too. W.l.o.g. assume that there exists $\lim J(\mu_n, \nu_n) \in [0, \infty]$. Using Prokhorov’s theorem extract a weakly convergent subsequence $\gamma_{n_k} \rightharpoonup \gamma \in \Pi(\mu, \nu)$. Then due to the lower semicontinuity of \mathcal{C} one obtains

$$J(\mu, \nu) \leq \mathcal{C}(\gamma) \leq \liminf \mathcal{C}(\gamma_{n_k}) = \lim J(\mu_n, \nu_n).$$

□

Corollary 2.2.5. *J is measurable w.r.t. the product of Borel σ -algebras $\mathcal{B}_w(\mathcal{P}(X)) \otimes \mathcal{B}_w(\mathcal{P}(Y))$ induced by the topologies of narrow convergence.*

Kantorovich duality. One of the central points of the optimal transportation theory is a duality. As (MK) is an infinite-dimensional linear programming problem, one can consider a dual problem associated with it, e.g. the following one:

$$\int_X u \, d\mu + \int_Y v \, d\nu \rightarrow \max_{u,v}, \quad (\text{D})$$

where the maximization is over all $u \in L^1(\mu)$ and $v \in L^1(\nu)$ such that $u(x) + v(y) \leq c(x, y)$ for all $x \in X$, $y \in Y$ (we allow u (v) to take infinite values on a μ - (ν -)negligible set). Any solution (u, v) of this problem is called *Kantorovich (dual) potentials* for the transport from μ to ν . Clearly, the value of the dual problem (D) is always not larger than the value of the primal problem (MK) (this is so called weak duality). The question when these values coincide (strong duality) and when there exists a solution of the dual problem is important for the OT theory and is the subject of many research, see e.g. the bibliographical notes after Chapter 5 in [Vil09].

Definition 2.5. Let $u: X \rightarrow \bar{\mathbb{R}}$. Then its c -transform is defined as

$$u^c(y) := \inf_{x \in X} [c(x, y) - u(x)], \quad y \in Y.$$

In the same way, for $v: Y \rightarrow \bar{\mathbb{R}}$

$$v^c(x) := \inf_{y \in Y} [c(x, y) - v(y)], \quad x \in X.$$

If $u = v^c$ for some function $v: Y \rightarrow \bar{\mathbb{R}}$, then we say u is c -concave.

Note that $u^{cc} \geq u$ and $u^{ccc} = u^c$, and the same holds for the c -transform of v . In the dual problem we can hope to choose $v = u^c$ and $u = v^c$, but u^c and v^c can be non-measurable, unless c is continuous (in which case they are upper-semicontinuous).

Another important concept for duality is c -cyclical monotonicity.

Definition 2.6. A set $\Gamma \subset X \times Y$ is c -cyclically monotone if for any pairs $(x_i, y_i) \in \Gamma$, $1 \leq i \leq n \in \mathbb{N}$, it holds that

$$\sum_{i=1}^n c(x_i, y_i) \leq \sum_{i=1}^n c(x_i, y_{i+1}),$$

where $y_{n+1} := y_1$.

Theorem 2.2.6 (Kantorovich duality). *Take $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$. Then the values of problem (MK) and (D) coincide. Moreover, $L^1(\mu)$ and $L^1(\nu)$ in (D) can be replaced with $C_b^0(X)$ and $C_b^0(Y)$. If $J(\mu, \nu) < \infty$, then for any $\gamma \in \Pi(\mu, \nu)$ the following conditions are equivalent:*

- γ is optimal;
- γ is concentrated on some c -cyclically monotone Borel set (which can be chosen dependent only on μ and ν);
- there is a Borel c -concave function $u: X \rightarrow \mathbb{R} \cup -\infty$ such that $u(x) + u^c(y) = c(x, y)$ for γ -a.e. (x, y) . Moreover, u^c coincides with a Borel function ν -a.e.

If, in addition, $c(x, y) \leq c_X(x) + c_Y(y)$, where $c_X \in L^1(\mu)$, $c_Y \in L^1(\nu)$, then the problem (D) admits a solution.

Remark 2.2.7. If c is continuous, then the fact that γ is concentrated on a c -cyclically monotone Borel set is equivalent to c -cyclical monotonicity of $\text{supp } \gamma$. Moreover, as was mentioned above, in this case (Borel) dual potentials u and v can be chosen such that $u = v^c$ and $v = u^c$.

Proof. Inspecting the proof of Theorem 5.10 in [Vil09], we conclude that this works as well for Radon spaces X and Y : indeed, we need only Prokhorov's theorem, inner regularity of any probability measure on $X \times Y$, and an approximation of μ and ν by discrete measures in the topologies of narrow convergence. \square

An important corollary of the above theorem is the stability of optimal transport plans w.r.t. the narrow convergence once c is continuous (this is a trivial counterpart of Theorem 5.20 in [Vil09] for the case of Radon spaces).

Proposition 2.2.8 (Weak stability of optimal transport plans). *Let the cost function be continuous, $\mu_n \rightharpoonup \mu \in \mathcal{P}(X)$, and $\nu_n \rightharpoonup \nu \in \mathcal{P}(Y)$. If $\liminf J(\mu_n, \nu_n) < \infty$ and $\gamma_n \in \Pi_o(\mu_n, \nu_n)$, then there is an optimal transport plan $\gamma \in \Pi(\mu, \nu)$ such that, up to a subsequence, $\gamma_n \rightharpoonup \gamma$.*

The stability result, in turn, yields the existence of a measurable selection of OT plans (cf. Corollary 5.22 in [Vil09]).

Corollary 2.2.9. *Let the cost function c be continuous, then there exists a Borel (w.r.t. the topologies of narrow convergence) map $(\mu, \nu) \mapsto \gamma_o(\mu, \nu) \in \Pi_o(\mu, \nu)$.*

Proof. Consider the set-valued map from $\mathcal{P}(X) \times \mathcal{P}(Y)$ to $\mathcal{P}(X \times Y)$:

$$\Psi(\mu, \nu) := \begin{cases} \Pi_o(\mu, \nu), & \text{if } J(\mu, \nu) < \infty, \\ \{\mu \otimes \nu\}, & \text{otherwise.} \end{cases}$$

Note that $\Psi(\mu, \nu)$ is compact and nonempty for any $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$. Recall that due to Lemma 2.2.4 for any $h > 0$ the set $\{(\mu, \nu) \in \mathcal{P}(X) \times \mathcal{P}(Y) : J(\mu, \nu) \leq h\}$ is closed, hence $\{(\mu, \nu) : J(\mu, \nu) = \infty\}$ is Borel. Now fix a closed set $D \subset \mathcal{P}(X \times Y)$ and $h > 0$. Proposition 2.2.8 yields that the set

$$\{(\mu, \nu) \in \mathcal{P}(X) \times \mathcal{P}(Y) : J(\mu, \nu) \leq h, \Pi_o(\mu, \nu) \cap D \neq \emptyset\}$$

also is closed in $\tau_w \otimes \tau_w$. Then

$$\{(\mu, \nu) \in \mathcal{P}(X) \times \mathcal{P}(Y) : \Psi(\mu, \nu) \cap D \neq \emptyset\} \in \mathcal{B}_w(X) \otimes \mathcal{B}_w(Y)$$

and we can apply Theorem 6.9.4 in [Bog07] (clearly, one can replace an open set in the statement with a closed set; see also the remark after it), which ensures the existence of a Borel selection from Ψ and hence Π_o . \square

Quadratic cost. Let us now consider the case $X = Y = \mathbb{R}^d$ and the cost function $c(x, y) := \frac{\|x-y\|^2}{2}$ (which corresponds to the p -Wasserstein distance, see the next section), where $\|\cdot\|$ is the Euclidean norm. By $\mathcal{P}_2(\mathbb{R}^d)$ we will denote the set of Borel probability measures on \mathbb{R}^d with finite second moment $m_2(\mu) := \int \|x\|^2 d\mu$. Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$, then by Theorem 2.2.6 there exists dual potentials $(u, v) \in L^1(\mu) \times L^1(\nu)$ such that $v = u^c$ and $u = v^c$. Consider now

$$\varphi(x) := \frac{\|x\|^2}{2} - u(x), \quad \psi(y) := \frac{\|y\|^2}{2} - v(y), \quad x \in \mathbb{R}^d.$$

Then it is easy to see that

$$\varphi(x) = \psi^*(x) := \sup_{y \in \mathbb{R}^d} (\langle x, y \rangle - \psi(y)) \quad \text{and} \quad \psi(y) = \varphi^*(y) := \sup_{x \in \mathbb{R}^d} (\langle x, y \rangle - \varphi(x)).$$

We will call (φ, ψ) *Brenier potentials* between μ and ν . The following famous result due to Y. Brenier [Bre91] establishes existence and uniqueness of the optimal transport map for the quadratic cost function.

Proposition 2.2.10 (Brenier's theorem; Theorem 1.20 in [San15]). *Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ and μ be absolutely continuous w.r.t. the Lebesgue measure. Then there exists a unique optimal transport plan $\gamma \in \Pi_o(\mu, \nu)$, it has a form $\gamma = (\text{id}, T)_{\#}\mu$, and $T = \nabla\varphi$, where φ is a Brenier potential between μ and ν .*

2.3 Wasserstein space

Let X be a Radon space with a fixed metric ρ . Fix an arbitrary point $x_0 \in X$ and for $p \geq 1$ define the set of probability measures with finite p -th moment:

$$\mathcal{P}_p(X) := \left\{ \mu \in \mathcal{P}(X) : m_p(\mu) := \int \rho^p(x, x_0) d\mu < \infty \right\}.$$

Now let us take the cost function $c(\cdot, \cdot) := \rho^p(\cdot, \cdot)$ (obviously, it is nonnegative and continuous) and define

$$W_p(\mu, \nu) := (J_c(\mu, \nu))^{1/p} := \left(\min_{\gamma \in \Pi(\mu, \nu)} \int \rho^p(x, y) d\gamma \right)^{1/p}, \quad \mu, \nu \in \mathcal{P}_p(X). \quad (2.2)$$

It follows from the gluing Proposition 2.1.6 and the Minkowski inequality that W_p is a metric on $\mathcal{P}_p(X)$ [AGS08, Sec. 7.1].

Definition 2.7. We call W_p the p -Wasserstein metric, and $(\mathcal{P}_p(X), W_p)$ is the p -Wasserstein space over (X, ρ) .

Note that $W_p(\delta_x, \delta_y) = \rho(x, y)$, thus X can be isometrically embedded into the p -Wasserstein space, and one can hope that its geometry in some sense reflects the structure of X . The next proposition shows that $(\mathcal{P}_p(X), W_p)$ inherits at least some topological properties of X .

Proposition 2.3.1 (Proposition 7.1.5 in [AGS08]). *The p -Wasserstein space is separable. If X is complete, then $(\mathcal{P}_p(X), W_p)$ is also complete. If X is compact, then $(\mathcal{P}_p(X), W_p)$ is compact.*

One of important properties of the Wasserstein distance is that it almost metrizes the narrow convergence. Namely, convergence in W_p is equivalent to the narrow convergence and the convergence of p -th moments:

Proposition 2.3.2 (Criterion of convergence in W_p ; Theorem 6.9 in [Vil09]). *Let X be a Polish space, then $W_p(\mu_n, \mu) \rightarrow 0$ iff $\mu_n \rightarrow \mu$ and $m_p(\mu_n) \rightarrow m_p(\mu)$.*

In particular, if ρ is bounded, then the convergence in W_p is indeed equivalent to the narrow convergence.

Absolutely continuous curves. Now consider again the case $X = \mathbb{R}^d$ with the Euclidean distance. Recall that a curve $\{x_t\}_{t \in [0,1]}$ in a complete metric space (X, ρ) is *absolutely continuous of order $p \in [1, \infty]$* if there is a function $m \in L^p([0, 1])$ such that for all $0 \leq t \leq s \leq 1$

$$\rho(x_t, x_s) \leq \int_t^s m(r) dr. \quad (2.3)$$

According to Theorem 1.1.2 in [AGS08] any absolutely continuous curve admits a *metric derivative* $|x'| \in L^1([0, 1])$, i.e. the minimal (up to negligible sets) function satisfying (2.3).

Proposition 2.3.3 (Theorem 8.3.1 in [AGS08]). *Let $1 < p < \infty$ and $\{\mu_t\}_{t \in [0,1]} \subset \mathcal{P}_p(\mathbb{R}^d)$ be an absolutely continuous curve of order p . Then there is a Borel vector field $(x, t) \mapsto v_t(x) \in \mathbb{R}^d$ such that*

$$\|v_t\|_{L^p(\mathbb{R}^d, \mu_t; \mathbb{R}^d)} = |\mu'| (t) \quad \text{for a.e. } t \in [0, 1],$$

and (μ_t, v_t) satisfies the continuity equation

$$\partial_t \mu + \operatorname{div}(v_t \mu) = 0$$

in a weak sense, i.e. for any $\varphi \in C_c^1([0, 1] \times \mathbb{R}^d)$ it holds that

$$\int_{[0,1]} \int_{\mathbb{R}^d} \partial_t \varphi(t, x) d\mu_t(x) dt + \int_{[0,1]} \int_{\mathbb{R}^d} \langle v_t, \nabla_x \varphi(t, x) \rangle d\mu_t(x) dt = 0.$$

Conversely, if $\{\mu_t\}_{t \in [0,1]} \subset \mathcal{P}_p(\mathbb{R}^d)$ is a narrowly continuous curve satisfying the continuity equation with a field v_t such that $\|v_t\|_{L^p(\mathbb{R}^d, \mu_t; \mathbb{R}^d)} \in L^1([0, 1])$, then it is absolutely continuous and

$$|\mu'| (t) \leq \|v_t\|_{L^p(\mathbb{R}^d, \mu_t; \mathbb{R}^d)} \quad \text{for a.e. } t \in [0, 1].$$

Chapter 3

Fréchet barycenters

3.1 Introduction

In this chapter we consider the Monge–Kantorovich problem on an abstract Radon space X and try to impose minimal assumptions on the cost function that allow the transportation functional J to induce a topology on $\mathcal{P}(X)$ in a reasonable way. We then investigate the properties of this topology and define averaging of probability measures on X , using the optimal transport theory to define a suitable concept of a “typical element”, which extends the notions of the *Fréchet mean* [Fré48] and the *Wasserstein barycenter* [AC11].

We fix a Radon space X (see Definition 2.2), e.g. a Polish space, and a continuous cost function $c: X \times X \rightarrow [0, \infty)$. Assume that $c(x, y) = 0$ iff $x = y$, thus $J(\mu, \nu) = 0$ iff $\mu = \nu$ due to Proposition 2.2.3. In this chapter we sometimes call $J(\mu, \nu)$ the *Monge–Kantorovich distance* between μ and ν , meaning that it quantifies a dissimilarity between measures μ and ν in $\mathcal{P}(X)$, although it is in general non-symmetric and may not satisfy the triangle inequality. Despite J is not a metric, we show that under additional assumptions on c it induces a *transportation topology* on $\mathcal{P}(X)$. The space $\mathcal{P}(X)$ endowed with this topology can be divided into equivalence classes, and each of them is a Radon space (in particular, it is separable and metrizable).

Further, by analogy with a Wasserstein barycenter we introduce a notion of a Fréchet typical element of P w.r.t. J , which we propose to call a *Fréchet barycenter* of P . It is defined as a minimizer of the average transportation cost:

$$\int_{\mathcal{P}(X)} J(\mu, \nu) \, dP(\mu) \rightarrow \min_{\nu \in \mathcal{P}(X)}$$

(rigorous definitions are given in Section 3.5). Suppose $\inf_{\nu \in \mathcal{P}(X)} \int_{\mathcal{P}(X)} J(\mu, \nu) \, dP(\mu) < \infty$. Then we show that a Fréchet barycenter of P exists. Moreover, if the distributions P_n converge to P w.r.t. the transportation cost on $\mathcal{P}(\mathcal{P}(X))$ with J as cost function, then the barycenters of P_n also converge (in an appropriate sense) to a barycenter of P . For instance, this result implies a law of large numbers for Fréchet barycenters. A similar setting was also considered by T. Le Gouic and J.-M. Loubes in [LL17], where a stability result and a law of large numbers were proven for barycenters in the p -Wasserstein space, and by J. Bigot and T. Klein in [BK12]. The current work, in particular, covers the case of the Wasserstein barycenters on an infinite-dimensional uniformly convex separable Banach space X (e.g. a separable Hilbert space), which, to the best of our knowledge, is the first result of this type.

The chapter is organized as follows. In Section 3.2 we impose assumptions on the cost function c and study corresponding properties of the Monge–Kantorovich distance. In Section 3.3 we define the transportation topology on $\mathcal{P}(X)$, and consider its properties such as separability, metrizability, and weak local compactness. In Section 3.4 we deal with the particular case of $X = \mathbb{R}^d$ and $c(x, y) = g(x - y)$, where $g \geq 0$ is a convex function. Then we define in Section 3.5 a generalized barycenter of a distribution on $\mathcal{P}(X)$. The central result of this chapter is proven in Subsection 3.5.2: the convergence of barycenters of distributions P_n is established provided that P_n themselves converge to some distribution P .

Notations. Let ρ be some metric on X , $B_r(x)$ be an open ball in X w.r.t. ρ for $x \in X$ and $r > 0$, then we call its closure $\bar{B}_r(x) \subset \{y \in X : \rho(x, y) \leq r\}$ a closed ball (note that there can be no equality, since we do not require ρ to be an inner metric). Let us define for any $x \in X$ and $r > 0$ an open c -ball $B_r^c(x) := \{y \in X : c(x, y) < r\}$. Then a closed c -ball is $\bar{B}_r^c(x) \subset \{y \in X : c(x, y) \leq r\}$ (again, the inclusion can be strict). In the same way we define an open J -ball $B_r^J(\mu) := \{\nu \in \mathcal{P}(X) : J(\mu, \nu) < r\}$ and a closed J -ball $\bar{B}_r^J(\mu) := \{\nu \in \mathcal{P}(X) : J(\mu, \nu) \leq r\}$ — as we will see, it coincides with the closure of $B_r^J(\mu)$ in a transportation topology.

Further, we assume that there is a weaker metric ρ_w on X (e.g. this can be a metric inducing the weak convergence if X is a normed space). We denote the convergence w.r.t. ρ_w by $x_n \rightarrow_w x$, and the narrow convergence of measures w.r.t. the corresponding topology (which we call the ρ_w -narrow convergence) by $\mu_n \rightarrow_w \mu$. $B_r^w(x)$ and $\bar{B}_r^w(x)$ denote an open and a closed ball w.r.t. ρ_w , respectively.

3.2 Properties of Monge–Kantorovich distance

In this subsection we are going to impose some assumptions on the cost function and discuss related properties of the Monge–Kantorovich distance. The first assumption concerns the topological properties of c .

Assumption 3.1. c is *consistent* in a sense that $c(x, x_n) \rightarrow 0$ iff $c(x_n, x) \rightarrow 0$ iff $x_n \rightarrow x$ for any $x \in X$ and a sequence $\{x_n\}_{n \in \mathbb{N}} \subset X$. Moreover, c is l.s.c. w.r.t. the weak topology induced by ρ_w and satisfies the following Radon–Riesz-type property: if $x_n \rightarrow x$, $y_n \rightarrow_w y$, and $c(x_n, y_n) \rightarrow c(x, y)$, then $y_n \rightarrow y$.

Remark 3.2.1. Note that any ball $B_r^c(x) \in \mathcal{B}(X, \rho_w)$ due to the lower semicontinuity of c , thus the separability of X together with the consistency of c give us $\mathcal{B}(X, \rho) \subset \mathcal{B}(X, \rho_w)$, and hence these two σ -algebras actually coincide. In particular, X endowed with ρ_w also is a Radon space.

Proof. Fix an arbitrary open ρ -ball $B \subset X$. It is enough to show that $B \in \mathcal{B}(X, \rho_w)$. Due to the consistency of c for any $x \in B$ there are $r(x), \delta(x) > 0$ such that $B_{\delta(x)}(x) \subset B_{r(x)}^c(x) \subset B$. Define sets

$$A_n := \left\{ x \in B : \delta(x) \geq \frac{1}{n} \right\}, \quad n \in \mathbb{N}$$

and take their dense countable subsets $S_n \subset A_n$. Then

$$A_n \subset \bigcup_{x \in S_n} B_{1/n}(x) \subset \bigcup_{x \in S_n} B_{r(x)}^c(x) \subset B.$$

Since $B = \bigcup_{n \in \mathbb{N}} A_n$, one obtains that

$$\bigcup_{n \in \mathbb{N}} \bigcup_{x \in S_n} B_{r(x)}^c(x) = B.$$

As $B_{r(x)}^c(x) \in \mathcal{B}(X, \rho_w)$, we conclude that $B \in \mathcal{B}(X, \rho_w)$, thus $\mathcal{B}(X, \rho) = \mathcal{B}(X, \rho_w)$. \square

Let us provided a couple of examples illustrating the above assumption, especially its second part. First of all, if ρ_w is equivalent to ρ , then the Radon–Riesz property trivially follows from the consistency of c . Now consider more reasonable cases.

Example 3.2.2. The main example that we can have in mind, of course, is the cost function given by

$$c(x, y) := f(\rho(x, y)), \quad (3.1)$$

where $f: \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is a continuous function. Then c is consistent once $f(t_n) \rightarrow 0$ iff $t_n \rightarrow 0$. Recall that a normed space X is called Radon–Riesz (or Kadets–Klee) if $x_n \rightarrow x$ is equivalent to $x_n \rightharpoonup x$ and $\|x_n\| \rightarrow \|x\|$. In particular, any uniformly convex Banach space (e.g. a Hilbert space, Lebesgue spaces ℓ^p or L^p for $1 < p < \infty$) satisfies this property. Then $c(x, y) := f(\|x - y\|)$

fulfills the assumption once f is strictly increasing and ρ_w metrizes the weak convergence on bounded sets (see, e.g. Section 5.1.2 in [AGS08]). In particular, $f(t) := t^p$, corresponding to the p -Wasserstein space, satisfies the above assumption. Another example is provided by the optimal transportation theory itself: according to Proposition 2.3.2 the p -Wasserstein distance fulfills these conditions, if ρ_w metrizes the narrow convergence.

First, we recall a connection between the transportation functional J and the narrow convergence, following from the continuity of the cost function. It is quite similar to well-known results for the Wasserstein metric, see Proposition 2.3.2.

Lemma 3.2.3. *Let $\{\mu_n\}_{n \in \mathbb{N}} \subset \mathcal{P}(X)$ be such that $J(\mu, \mu_n) \rightarrow 0$ or $J(\mu_n, \mu) \rightarrow 0$ for some $\mu \in \mathcal{P}(X)$. Then $\mu_n \rightarrow \mu$.*

Proof. Assume $\{\mu_n\}_{n \in \mathbb{N}}$ fails to narrowly converge to μ . Then there exists a closed set $F \subset X$ such that $\limsup \mu_n(F) > \mu(F)$. Let $3\varepsilon := \lim \mu_n(F) - \mu(F) > 0$ (without relabelling). Consider the following open neighborhoods of F :

$$F_r := \left\{ x \in X : \inf_{y \in F} c(x, y) < r \right\} \supset F, \quad r > 0.$$

For any $r > 0$ the set F_r is open due to the continuity of c . On the other hand, the consistency of c yields that for any $x \notin F$ there exists an open c -ball $B_r^c(x)$ such that $B_r^c(x) \cap F = \emptyset$. Therefore, $\bigcap_{r>0} F_r = F$ and thus $\mu(F) = \lim_{r \rightarrow 0} \mu(F_r)$. Let $r_0 > 0$ be such that $\mu(F_{r_0}) < \mu(F) + \varepsilon$. Since $\mu_n(F) > \mu(F) + 2\varepsilon$ for n large enough,

$$\gamma_n((X \setminus F_{r_0}) \times F) = \mu_n(F) - \gamma_n(F_{r_0} \times F) \geq \mu_n(F) - \mu(F_{r_0}) > \varepsilon,$$

where $\gamma_n \in \Pi_o(\mu, \mu_n)$ is an optimal transport plan. Consequently,

$$J(\mu, \mu_n) = \mathcal{C}(\gamma_n) \geq \gamma_n((X \setminus F_{r_0}) \times F) \inf\{c(x, y) : x \notin F_{r_0}, y \in F\} \geq \varepsilon r_0 > 0,$$

which contradicts the assumptions of the lemma. \square

As we have seen, the convergence w.r.t. the transportation functional implies the narrow convergence. Actually, the converse also holds under some additional assumptions.

Lemma 3.2.4. *Let $\mu_n \rightarrow \mu$ and $\text{supp } \mu_n \subset F$ for all n , where $F \subset X$ is a closed set such that $\sup_{x, y \in F} c(x, y) < \infty$. Then $\lim J(\mu_n, \mu) = \lim J(\mu, \mu_n) = 0$.*

Proof. Fix $\varepsilon > 0$. Due to the separability of X and the continuity of c one can cover X with a countable union of closed balls $\bar{B}_{r_i}(x_i)$, $i \in \mathbb{N}$, such that $c(x, y) < \varepsilon$ whenever $x, y \in \bar{B}_{2r_i}(x_i)$. Fix $m \in \mathbb{N}$ such that $\mu(X \setminus \bigcup_{i=1}^m \bar{B}_{r_i}(x_i)) < \varepsilon$ and consider a partition of unity by continuous functions $f_i: X \rightarrow [0, 1]$, $0 \leq i \leq m$, satisfying

$$\begin{aligned} f_0(x) &= 0 \quad \forall x \in \bigcup_{i=1}^m \bar{B}_{r_i}(x_i); \\ f_i(x) &= 0 \quad \forall x \notin \bar{B}_{2r_i}(x_i), \quad 1 \leq i \leq m. \end{aligned}$$

Without loss of generality $\mu(B_{r_i}(x_i)) > 0$ and $f_i > 0$ in $B_{r_i}(x_i)$, thus $\int f_i d\mu > 0$, for all $1 \leq i \leq m$. Define measures

$$\begin{aligned} \lambda_n^i &:= \frac{(f_i \mu_n) \otimes (f_i \mu)}{\max\{\int f_i d\mu_n, \int f_i d\mu\}} \in \mathcal{M}_+(X \times X), \quad 1 \leq i \leq m, \quad n \in \mathbb{N}; \\ \hat{\mu}_n &:= \mu_n - \sum_{i=1}^m \pi_{\#}^1 \lambda_n^i = \left(1 - \sum_{i=1}^m \frac{\int f_i d\mu}{\max\{\int f_i d\mu_n, \int f_i d\mu\}} f_i\right) \mu_n \geq f_0 \mu_n \geq 0; \\ \hat{\mu}_n^* &:= \mu - \sum_{i=1}^m \pi_{\#}^2 \lambda_n^i = \left(1 - \sum_{i=1}^m \frac{\int f_i d\mu_n}{\max\{\int f_i d\mu_n, \int f_i d\mu\}} f_i\right) \mu \geq f_0 \mu \geq 0. \end{aligned}$$

Since $\mu_n \rightarrow \mu$ one has $\int f_i d\mu_n \rightarrow \int f_i d\mu$ for all i , thus

$$\begin{aligned} \hat{\mu}_n(X) &= \hat{\mu}_n^*(X) = \int \left(1 - \sum_{i=1}^m \frac{\int f_i d\mu_n}{\max\{\int f_i d\mu_n, \int f_i d\mu\}} f_i \right) d\mu \\ &\rightarrow \int \left(1 - \sum_{i=1}^m f_i \right) d\mu = \int f_0 d\mu \leq \mu \left(X \setminus \bigcup_{i=1}^m B_{r_i}(x_i) \right) < \varepsilon. \end{aligned}$$

Consider the following transport plans:

$$\gamma_n := \frac{\hat{\mu}_n \otimes \hat{\mu}_n^*}{\hat{\mu}_n(X)} + \sum_{i=1}^m \lambda_n^i \in \Pi(\mu_n, \mu), \quad n \in \mathbb{N}.$$

From $\text{supp } \mu_n \subset F$ it follows that $\text{supp } \mu \subset F$ and $\text{supp } \gamma_n \subset F \times F$. Define $M := \sup_{x,y \in F} c(x,y) < \infty$. $\text{supp } \lambda_n^i \subset \bar{B}_{2r_i}(x_i) \times \bar{B}_{2r_i}(x_i)$ by the definition of λ_n^i and the functions f_i . Now one can obtain that

$$\begin{aligned} \limsup J(\mu_n, \mu) &\leq \limsup \mathcal{C}(\gamma_n) \leq \limsup \left(M \frac{\hat{\mu}_n(X) \hat{\mu}_n^*(X)}{\hat{\mu}_n(X)} + \varepsilon \sum_{i=1}^m \lambda_n^i(X \times X) \right) \\ &\leq M \limsup \hat{\mu}_n(X) + \varepsilon \leq (M+1)\varepsilon. \end{aligned}$$

This proves that $J(\mu_n, \mu) \rightarrow 0$ because of the arbitrary choice of $\varepsilon > 0$. In the same way one can show that $J(\mu, \mu_n) \rightarrow 0$. \square

Now let us formulate the main assumption on the cost function c , which we suppose to hold hereafter in the chapter: a weak triangle inequality.

Assumption 3.2. There exist constants $A, B \geq 0$ such that the inequality holds for all $x, y, z \in X$:

$$c(x, y) \leq A + B(\min\{c(x, z), c(z, x)\} + \min\{c(y, z), c(z, y)\}),$$

This is a quite natural assumption which holds for a wide class of cost functions, e.g. for $c(x, y) = \rho^p(x, y)$ with $p > 0$ (the case of p -Wasserstein spaces) or, more generally, the cost function given by (3.1) if f is strictly increasing and $f(t+s) \leq A(f(t) + f(s))$ for all $t, s \geq 0$. Another example is considered in Section 3.4.

Using “gluing” Proposition 2.1.6 one can trivially show that the Monge–Kantorovich distance “inherits” the inequalities on the cost function:

Lemma 3.2.5. For all $\mu, \nu, \lambda \in \mathcal{P}(X)$

$$J(\mu, \nu) \leq A + B(\min\{J(\mu, \lambda), J(\lambda, \mu)\} + \min\{J(\nu, \lambda), J(\lambda, \nu)\}).$$

Moreover, one can locally amplify inequalities from Assumption 3.2, as the next lemma shows.

Lemma 3.2.6. Let $K \subset X$ be a compact set. Then for any $\varepsilon > 0$ there exist an open neighbourhood $U_\varepsilon(K) \supset K$ and a constant B_ε^K such that

$$\begin{aligned} c(x, y) &\leq \varepsilon + c(x, z) + B_\varepsilon^K c(y, z), \\ c(x, y) &\leq \varepsilon + c(z, y) + B_\varepsilon^K c(z, x) \end{aligned}$$

for all $x, y, z \in U_\varepsilon(K)$.

Proof. Fix $\varepsilon > 0$. As c is continuous, it is uniformly continuous on $K \times K$, hence there exists an open set $V \in X \times X$ such that $\{(y, y) : y \in K\} \subset V$ and $c(x, y) \leq c(x, z) + \varepsilon/2$ for all $x \in K, (y, z) \in V$. Define $M := \max_{x,y \in K} c(x, y) < \infty$ and

$$\delta := \min_{(y,z) \in K^2 \setminus V} c(y, z) > 0,$$

which is positive due to the compactness of K . Thus if $(y, z) \in K^2 \setminus V$, then $c(x, y) \leq M \leq \frac{M}{\delta}c(y, z)$ for all $x \in K$. Consequently,

$$c(x, y) \leq \varepsilon/2 + c(x, z) + \frac{M}{\delta}c(y, z) \quad (3.2)$$

for all $x, y, z \in K$. Denote $\frac{M}{\delta}$ by B_ε^K .

Due to continuity of c one can choose an open neighbourhood W of K^3 such that for all $x, y, z \in W$ there exist $x', y', z' \in K$ for which $|c(x, y) - c(x', y')| < \gamma$, $|c(x, z) - c(x', z')| < \gamma$, and $|c(y, z) - c(y', z')| < \gamma$, where $\gamma := \varepsilon/(4 + 2B_\varepsilon^K)$. Since K^3 is compact, $\rho(K^3, X^3 \setminus W) > 0$ and there is a neighbourhood $U_\varepsilon(K)$ such that $(U_\varepsilon(K))^3 \subset W$. Now, applying inequality (3.2) and the definition of W one can obtain that

$$\begin{aligned} c(x, y) &\leq \gamma + c(x', y') \leq \gamma + \varepsilon/2 + c(x', z') + B_\varepsilon^K c(y', z') \\ &\leq (2 + B_\varepsilon^K)\gamma + \varepsilon/2 + c(x, z) + B_\varepsilon^K c(y, z) \leq \varepsilon + c(x, z) + B_\varepsilon^K c(y, z) \end{aligned}$$

for all $x, y, z \in U_\varepsilon(K)$. The second inequality can be treated in the same way. \square

The next lemma states one of the main results of this subsection: J is continuous w.r.t. to itself, what is essential to define a transportation topology later (cf. Theorem 1.48 in [San15]).

Lemma 3.2.7 (Continuity of J). *Take two sequences $\{\mu_n\}_{n \in \mathbb{N}}$, $\{\nu_n\}_{n \in \mathbb{N}}$ such that $J(\mu, \mu_n) \rightarrow 0$ and $J(\nu, \nu_n) \rightarrow 0$ for some measures $\mu, \nu \in \mathcal{P}(X)$. Then $J(\mu_n, \nu_n) \rightarrow J(\mu, \nu)$.*

Proof. Let $\gamma_n^1 \in \Pi_o(\mu, \mu_n)$, $\gamma^2 \in \Pi_o(\mu, \nu)$, $\gamma_n^3 \in \Pi_o(\nu, \nu_n)$ be optimal transport plans. Consider measures $\sigma_n \in \Pi(\mu_n, \mu, \nu, \nu_n)$ such that $\pi_{\#}^{2,1}\sigma_n = \gamma_n^1$, $\pi_{\#}^{2,3}\sigma_n = \gamma^2$ and $\pi_{\#}^{3,4}\sigma_n = \gamma_n^3$. Since the sequences are tight one can fix $0 < \varepsilon < 1$ and a compact set K such that $\mu_n(X \setminus K)$, $\mu(X \setminus K)$, $\nu_n(X \setminus K)$, $\nu(X \setminus K)$ and $\int_{X^2 \setminus K^2} c(x_2, x_3) d\gamma^2$ are less than ε . Obviously,

$$J(\mu_n, \nu_n) \leq \mathcal{C}(\pi_{\#}^{1,4}\sigma_n) = \int c(x_1, x_4) d\sigma_n.$$

Consider the set $Y := U_\varepsilon(K) \times K^2 \times U_\varepsilon(K)$. Now one can obtain due to Lemma 3.2.6 that

$$\begin{aligned} \int_Y c(x_1, x_4) d\sigma_n &\leq \int_Y (\varepsilon + B_\varepsilon^K c(x_2, x_1) + c(x_2, x_4)) d\sigma_n \\ &\leq \int_Y (\varepsilon + B_\varepsilon^K c(x_2, x_1) + \varepsilon + B_\varepsilon^K c(x_3, x_4) + c(x_2, x_3)) d\sigma_n \\ &\leq 2\varepsilon + B_\varepsilon^K \mathcal{C}(\gamma_n^1) + B_\varepsilon^K \mathcal{C}(\gamma_n^3) + \mathcal{C}(\gamma^2) \\ &= 2\varepsilon + B_\varepsilon^K J(\mu, \mu_n) + B_\varepsilon^K J(\nu, \nu_n) + J(\mu, \nu) \\ &\xrightarrow{n \rightarrow \infty} 2\varepsilon + J(\mu, \nu) \rightarrow J(\mu, \nu) \quad \text{as } \varepsilon \rightarrow 0. \end{aligned}$$

The remaining term may be bounded by Assumption 3.2 in the following way:

$$\begin{aligned} \int_{X^4 \setminus Y} c(x_1, x_4) d\sigma_n &\leq \int_{X^4 \setminus Y} (A + Bc(x_2, x_1) + Bc(x_2, x_4)) d\sigma_n \\ &\leq \int_{X^4 \setminus Y} (A + Bc(x_2, x_1) + AB + B^2c(x_2, x_3) + B^2c(x_3, x_4)) d\sigma_n \\ &\leq A(1 + B)\sigma_n(X^4 \setminus Y) + BJ(\mu, \mu_n) + B^2 \int_{X^4 \setminus Y} c(x_2, x_3) d\sigma_n + B^2 J(\nu, \nu_n) \\ &\leq 4A(1 + B)\varepsilon + BJ(\mu, \mu_n) + B^2 J(\nu, \nu_n) + B^2 \int_{X^4 \setminus Y} c(x_2, x_3) d\sigma_n. \end{aligned}$$

Notice that

$$X^4 \setminus Y = \left[X \times (X^2 \setminus K^2) \times X \right] \cup \left[(X \setminus U_\varepsilon(K)) \times K^2 \times X \right] \cup \left[X \times K^2 \times (X \setminus U_\varepsilon(K)) \right]$$

and

$$\int_{X \times (X^2 \setminus K^2) \times X} c(x_2, x_3) d\sigma_n = \int_{X^2 \setminus K^2} c(x_2, x_3) d\gamma^2 < \varepsilon.$$

Moreover, since $J(\mu, \mu_n) \rightarrow 0$ and $J(\nu, \nu_n) \rightarrow 0$, we have $\gamma_n^1 \rightharpoonup (\text{id}, \text{id})_{\#}\mu$ and $\gamma_n^3 \rightharpoonup (\text{id}, \text{id})_{\#}\nu$, thus $\sigma_n \rightharpoonup (\pi^1, \pi^1, \pi^2, \pi^2)_{\#}\gamma^2$. Since $(X \setminus U_\varepsilon(K)) \times K^2 \times X$ is closed and $c(x_2, x_3)$ is continuous and bounded on it we conclude that

$$\limsup \int_{(X \setminus U_\varepsilon(K)) \times K^2 \times X} c(x_2, x_3) d\sigma_n \leq \int_{(K \cap X \setminus U_\varepsilon(K)) \times K} c(x, y) d\gamma^2 = 0,$$

as $K \cap X \setminus U_\varepsilon(K) = \emptyset$. In the same way one can obtain that

$$\limsup \int_{X \times K^2 \times (X \setminus U_\varepsilon(K))} c(x_2, x_3) d\sigma_n = 0.$$

Thus $J(\mu_n, \nu_n) \rightarrow J(\mu, \nu)$. □

Now let us show that the convergence in J is symmetric and associative.

Lemma 3.2.8. *Let $\{\mu_n\}_{n \in \mathbb{N}}$, $\{\nu_n\}_{n \in \mathbb{N}}$, $\{\lambda_n\}_{n \in \mathbb{N}}$ be tight sequences such that $J(\mu_n, \nu_n) \rightarrow 0$ and $J(\nu_n, \lambda_n) \rightarrow 0$; then $J(\nu_n, \mu_n) \rightarrow 0$ and $J(\mu_n, \lambda_n) \rightarrow 0$.*

Proof. Fix $\varepsilon > 0$ and a compact set $K \subset X$ such that $\mu_n(K)$, $\nu_n(K)$ and $\lambda_n(K)$ are greater than $1 - \varepsilon$. Consider measures $\sigma_n \in \Pi(\mu_n, \nu_n, \lambda_n)$ such that $\pi_{\#}^{1,2}\sigma_n = \gamma_n^1$ and $\pi_{\#}^{2,3}\sigma_n = \gamma_n^2$ where γ_n^1 and γ_n^2 are optimal transport plans from μ_n to ν_n and from ν_n to λ_n , respectively. Due to Assumption 3.2 and Lemma 3.2.6 one can obtain that

$$\begin{aligned} J(\mu_n, \lambda_n) &\leq \mathcal{C}(\pi_{\#}^{1,3}\sigma_n) = \int c(x, z) d\sigma_n \\ &\leq \int_{K^3} (\varepsilon + c(x, y) + B_\varepsilon^K c(y, z)) d\sigma_n + \int_{X^3 \setminus K^3} (A + Bc(x, y) + Bc(y, z)) d\sigma_n \\ &\leq \varepsilon + J(\mu_n, \nu_n) + B_\varepsilon^K J(\nu_n, \lambda_n) + 3\varepsilon A + BJ(\mu_n, \nu_n) + BJ(\nu_n, \lambda_n) \\ &\rightarrow \varepsilon + 3\varepsilon A \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0. \end{aligned}$$

Thus $J(\mu_n, \lambda_n) \rightarrow 0$. Similarly,

$$\begin{aligned} J(\nu_n, \mu_n) &\leq \mathcal{C}(\pi_{\#}^{2,1}\gamma_n^1) = \int c(y, x) d\gamma_n^1 \\ &\leq \int_{K^3} (\varepsilon + B_\varepsilon^K c(x, y)) d\gamma_n^1 + \int_{X^3 \setminus K^3} (A + Bc(x, y)) d\gamma_n^1 \\ &\leq \varepsilon + B_\varepsilon^K J(\mu_n, \nu_n) + 2\varepsilon A + BJ(\mu_n, \nu_n) \rightarrow \varepsilon + 2\varepsilon A, \end{aligned}$$

therefore $J(\nu_n, \mu_n) \rightarrow 0$. □

Before we move to the next result, let us consider the following useful construction: fix some point $x_0 \in X$ and for given $R > 0$ take a continuous function $f_R: X \times X \rightarrow [0, 1]$ such that $f_R(x, y) = 1$ for $x, y \in B_R^c(x_0)$ and $f_R(x, y) = 0$ if $x \notin B_{R+1}^c(x_0)$ or $y \notin B_{R+1}^c(x_0)$. Let us take measures $\mu, \nu, \gamma \in \Pi(\mu, \nu)$ and consider $\lambda := f_R \gamma$. Define

$$\tilde{\gamma} = \tilde{\gamma}_R := \gamma - \lambda + (\pi^2, \pi^2)_{\#}\lambda$$

and $\tilde{\nu} = \tilde{\nu}_R := \pi_{\#}^1 \tilde{\gamma}$. So $\tilde{\gamma} \in \Pi(\tilde{\nu}, \nu)$ and $J(\tilde{\nu}, \nu) \leq \mathcal{C}(\tilde{\gamma}) = \mathcal{C}(\gamma) - \mathcal{C}(\lambda) = \mathcal{C}(\gamma) - \mathcal{C}'(\gamma)$ where $\mathcal{C}'(\gamma) = \mathcal{C}'_R(\gamma) := \mathcal{C}(f_R \gamma)$. Note that $\tilde{\nu} \leq \mu + \nu$ for any R .

Consider a weakly convergent sequence of plans $\Pi(\mu, \nu_n) \ni \gamma_n \rightharpoonup \gamma \in \Pi(\mu, \nu)$. One has $\tilde{\gamma}_n \rightharpoonup \tilde{\gamma}$ hence $\tilde{\nu}_n \rightharpoonup \tilde{\nu}$. But on the complement of the ball $B_{R+1}^c(x_0)$ all the measures $\tilde{\nu}_n$ coincide with μ , consequently, $J(\tilde{\nu}_n, \tilde{\nu}) \rightarrow 0$ by Lemma 3.2.4.

Now we are ready to show that a converse result to Lemma 3.2.7 is also true, namely the following counterpart of Assumption 3.1.

Lemma 3.2.9. *Take two sequences $\{\mu_n\}_{n \in \mathbb{N}}$, $\{\nu_n\}_{n \in \mathbb{N}}$ such that $J(\mu_n, \mu) \rightarrow 0$, $\nu_n \rightharpoonup_w \nu$, and $J(\mu_n, \nu_n) \rightarrow J(\mu, \nu) < \infty$ for some measures $\mu, \nu \in \mathcal{P}(X)$. Then $J(\nu_n, \nu) \rightarrow 0$.*

Proof. Step 1. We start from proving $\nu_n \rightharpoonup \nu$. Assume that it is false, then there is an open set $U \subset X$, $r > 0$, and $\varepsilon > 0$ such that, up to a subsequence,

$$\nu(U) > \nu_n(U_r) + 3\varepsilon \quad \forall n \in \mathbb{N},$$

with $U_r := \bigcup_{x \in U} B_r(x)$. Now consider the product topology τ_{sw} on $(X, \rho) \times (X, \rho_w)$ and recall that $\mathcal{B}(X, \rho_w) = \mathcal{B}(X, \rho)$. Let $\gamma_n \in \Pi_o(\mu_n, \nu_n)$ for all $n \in \mathbb{N}$. Since $\mu_n \rightharpoonup \mu$, $\nu_n \rightharpoonup_w \nu$, the sequence $\{\gamma_n\}_{n \in \mathbb{N}}$ is tight w.r.t. τ_{sw} , hence there is a narrowly (w.r.t. τ_{sw}) convergent subsequence $\gamma_n \rightharpoonup_{\text{sw}} \gamma \in \Pi(\mu, \nu)$ (without relabelling).

According to Assumption 3.1 for all $x, y \in X$ there exists $\delta = \delta(x, y) > 0$ such that $c(x', y') < c(x, y) + 4\delta$ implies $\rho(y', y) < r$ for $x' \in B_\delta(x)$, $y' \in B_\delta^w(y)$. Then one can find $\delta > 0$ satisfying

$$\gamma^* (\{(x, y) \in X \times U : \delta(x, y) \geq \delta\}) > \gamma(X \times U) - \varepsilon = \nu(U) - \varepsilon, \quad (3.3)$$

where γ^* is the outer measure induced by γ .

For given $h > 0$ define a (Lipschitz) continuous function

$$c_h(x, y) := \inf_{x', y' \in X} [c(x', y') + h\rho(x', x) + h\rho_w(y', y)] \leq c(x, y).$$

Clearly, $c_h \nearrow c$ as $h \rightarrow \infty$ due to the lower semicontinuity of c . In particular,

$$\int c_h d\gamma \rightarrow \int c d\gamma \leq \liminf \int c d\gamma_n = \lim J(\mu_n, \nu_n) = J(\mu, \nu) < \infty.$$

Fix $h \geq 1$ such that

$$\int c d\gamma < \int c_h d\gamma + \varepsilon\delta$$

and take an open (in τ_{sw}) set

$$V := \bigcup \left\{ B_{\delta/h}(x) \times B_{\delta/h}^w(y) : x \in X, y \in U, \delta(x, y) \geq \delta \right\}.$$

Obviously, (3.3) yields

$$\gamma(V) \geq \gamma^* (\{(x, y) \in X \times U : \delta(x, y) \geq \delta\}) > \nu(U) - \varepsilon.$$

Since $\gamma_n \rightharpoonup_{\text{sw}} \gamma$, for large enough n we have

$$\gamma_n(V) > \gamma(V) - \varepsilon > \nu(U) - 2\varepsilon > \nu_n(U_r) + \varepsilon = \gamma_n(X \times U_r) + \varepsilon.$$

For any $(x, y) \in V \setminus (X \times U_r)$ there is $(x', y') \in X \times U$ such that $x \in B_{\delta/h}(x')$, $y \in B_{\delta/h}^w(y')$, and $\delta(x', y') \geq \delta$. Since $\rho(y', y) \geq r$, we have $c(x, y) \geq c(x', y') + 4\delta$, therefore

$$c_h(x, y) \leq c(x', y') + h(\rho(x', x) + \rho_w(y', y)) \leq c(x', y') + 2\delta \leq c(x, y) - 2\delta$$

and thus

$$\begin{aligned} \int c d\gamma_n &\geq \int (c_h + 2\delta \mathbb{1}_{V \setminus (X \times U_r)}) d\gamma_n = \int c_h d\gamma_n + 2\delta \gamma_n(V \setminus (X \times U_r)) \\ &\geq \int c_h d\gamma_n + 2\delta(\gamma_n(V) - \gamma_n(X \times U_r)) > \int c_h d\gamma_n + 2\varepsilon\delta. \end{aligned}$$

Finally,

$$\int c \, d\gamma < \int c_h \, d\gamma + \varepsilon\delta \leq \liminf \int c_h \, d\gamma_n + \varepsilon\delta \leq \liminf \int c \, d\gamma_n - \varepsilon\delta,$$

which contradicts the fact that

$$\lim \int c \, d\gamma_n = \lim J(\mu_n, \nu_n) = J(\mu, \nu) \leq \int c \, d\gamma.$$

Consequently, $\nu_n \rightharpoonup \nu$.

Step 2. Now we are going to show that $J(\mu, \nu_n) \rightarrow J(\mu, \nu)$. Apply Proposition 2.1.6 to find $\sigma_n \in \Pi(\mu, \mu_n, \nu_n)$ such that $\pi_{\#}^{1,2} \sigma_n \in \Pi_o(\mu, \mu_n)$ and $\pi_{\#}^{2,3} \sigma_n \in \Pi_o(\mu_n, \nu_n)$, and extract a weakly convergent subsequence $\sigma_n \rightharpoonup \sigma \in \Pi(\mu, \mu, \nu)$. Since

$$J(\mu, \nu) \leq \int c(x_2, x_3) \, d\sigma \leq \liminf \int c(x_2, x_3) \, d\sigma_n = \lim J(\mu_n, \nu_n) = J(\mu, \nu),$$

we conclude that

$$(A + Bc(x_2, x_3))_{\#} \sigma_n \rightharpoonup (A + Bc(x_2, x_3))_{\#} \sigma.$$

Fix $\varepsilon > 0$ and take compact $K \subset X$ such that

$$\int_{X^3 \setminus K^3} (A + Bc(x_2, x_3)) \, d\sigma \leq \varepsilon.$$

Let U be a neighborhood of K from Lemma 3.2.6, then

$$\begin{aligned} J(\mu, \nu_n) &\leq \int c(x_1, x_3) \, d\sigma_n \\ &\leq \int_{U^3} (\varepsilon + c(x_2, x_3) + B_{\varepsilon}^K c(x_2, x_1)) \, d\sigma_n + \int_{X^3 \setminus U^3} (A + Bc(x_2, x_3) + Bc(x_2, x_1)) \, d\sigma_n \\ &\leq \varepsilon + J(\mu_n, \nu_n) + \max\{B, B_{\varepsilon}^K\} J(\mu_n, \mu) + \int_{X^3 \setminus U^3} (A + Bc(x_2, x_3)) \, d\sigma_n. \end{aligned}$$

By the weak convergence

$$\limsup \int_{X^3 \setminus U^3} (A + Bc(x_2, x_3)) \, d\sigma_n \leq \int_{X^3 \setminus U^3} (A + Bc(x_2, x_3)) \, d\sigma \leq \varepsilon,$$

and since $J(\mu_n, \nu_n) \rightarrow J(\mu, \nu)$, $J(\mu_n, \mu) \rightarrow 0$, one has $\limsup J(\mu, \nu_n) \leq J(\mu, \nu) + 2\varepsilon$. At the same time, $J(\mu, \nu) \leq \liminf J(\mu, \nu_n)$, hence $J(\mu, \nu_n) \rightarrow J(\mu, \nu)$.

Step 3. Let $\gamma_n \in \Pi_o(\mu, \nu_n)$ for all $n \in \mathbb{N}$. Since the sequence $\{\gamma_n\}_{n \in \mathbb{N}}$ is tight, one can extract a subsequence $\gamma_n \rightharpoonup \gamma \in \Pi(\mu, \nu)$ (without relabelling). Fix $\varepsilon > 0$ and $R > 0$ such that $\mathcal{C}'(\gamma) = \mathcal{C}'_R(\gamma) > \mathcal{C}(\gamma) - \varepsilon$. Using the construction described before the lemma get transport plans $\Pi(\tilde{\nu}_n, \nu_n) \ni \tilde{\gamma}_n \rightharpoonup \tilde{\gamma} \in \Pi(\tilde{\nu}, \nu)$. Therefore $J(\tilde{\nu}_n, \nu) \rightarrow 0$, $J(\tilde{\nu}, \nu) \leq \mathcal{C}(\tilde{\gamma}) = \mathcal{C}(\gamma) - \mathcal{C}'(\gamma) < \varepsilon$ and

$$\begin{aligned} J(\tilde{\nu}_n, \nu_n) &\leq \mathcal{C}(\tilde{\gamma}_n) = \mathcal{C}(\gamma_n) - \mathcal{C}'(\gamma_n) = J(\mu, \nu_n) - \mathcal{C}'(\gamma_n) \\ &\rightarrow J(\mu, \nu) - \mathcal{C}'(\gamma) \leq \mathcal{C}(\gamma) - \mathcal{C}'(\gamma) < \varepsilon. \end{aligned}$$

So, one can choose $R_n \rightarrow \infty$ such that

$$\lim J((\tilde{\nu}_n)_{R_n}, \nu_n) = \lim J((\tilde{\nu}_n)_{R_n}, \tilde{\nu}_{R_n}) = \lim J(\tilde{\nu}_{R_n}, \nu) = 0.$$

Since $(\tilde{\nu}_n)_{R_n} \leq \mu + \nu_n$ and $\tilde{\nu}_{R_n} \leq \mu + \nu$, all the sequences are tight and thus $J(\nu_n, \nu) \rightarrow 0$ by Lemma 3.2.8. \square

3.3 Transportation topology

Lemma 3.2.7 immediately implies one of the main results of this chapter: there is a topology on $\mathcal{P}(X)$ with the basis of “balls” w.r.t. J , and J is continuous w.r.t. this topology.

Definition 3.1 (Transportation topology). The set of all open J -balls $B_r^J(\mu)$ forms a basis of the *transportation topology* τ_J on $\mathcal{P}(X)$. We denote the convergence of a sequence $\{\nu_n\}_{n \in \mathbb{N}}$ to ν in τ_J (the *transportation convergence*) by $\nu_n \xrightarrow{J} \nu$.

Note that $\nu_n \xrightarrow{J} \nu$ is equivalent to $J(\nu_n, \nu) \rightarrow 0$ and $J(\nu, \nu_n) \rightarrow 0$. If X is a compact space, it follows from Lemmata 3.2.3 and 3.2.4 that the narrow convergence is equivalent to the transportation convergence. In particular, in this case $(\mathcal{P}(X), \tau_J)$ itself is compact. Notice however that if X is not compact, then $(\mathcal{P}(X), \tau_J)$ is neither compact nor locally compact.

Let the relation $\mu \sim \nu$ be defined as $J(\mu, \nu) < \infty$. Then it is an equivalence on $\mathcal{P}(X)$ and splits the space into equivalence classes $E(\mu) := \{\nu \in \mathcal{P}(X) : J(\mu, \nu) < \infty\}$. Notice that every equivalence class is path-connected, even if X is disconnected, since the curve $[0, 1] \ni t \mapsto (1-t)\mu + t\nu$ is continuous by Corollary 2.2.2, whenever $J(\mu, \nu) < \infty$. Let us denote by E_0 the class containing delta-measures, i.e. $E_0 := E(\delta_{x_0}) = \{\nu \in \mathcal{P}(X) : \int c(x_0, x) d\nu(x) < \infty\}$ for an arbitrary $x_0 \in X$ (obviously, it does not depend on the choice of x_0).

Lemmata 3.2.3, 3.2.7, and 3.2.9 immediately give the following necessary and sufficient condition of convergence in τ_J , which relates the transportation and the narrow convergences and is analogous to the one in Proposition 2.3.2.

Theorem 3.3.1 (Criterion of convergence in τ_J). *Take measures ν and $\{\nu_n\}_{n \in \mathbb{N}} \subset \mathcal{P}(X)$. The following conditions are equivalent:*

1. $\nu_n \xrightarrow{J} \nu$;
2. $\nu_n \rightarrow \nu$ and $J(\mu, \nu_n) \rightarrow J(\mu, \nu)$ for all $\mu \in \mathcal{P}(X)$;
3. $\nu_n \rightarrow_w \nu$ and $J(\mu, \nu_n) \rightarrow J(\mu, \nu) < \infty$ for some $\mu \in E(\nu)$.

3.3.1 Class E_0

Furthermore, for the class E_0 there is also a dual formulation of the transportation convergence through the narrow convergence of weighted measures, like in the case of the Wasserstein spaces [cf. Vil09, Theorem 6.9].

Proposition 3.3.2. *Take measures $\nu \in E_0$ and $\{\nu_n\}_{n \in \mathbb{N}} \subset \mathcal{P}(X)$. Then $\nu_n \xrightarrow{J} \nu$ iff $\int f d\nu_n \rightarrow \int f d\nu$ for any continuous function f such that there is $\alpha > 0$ satisfying $|f(x)| \leq \alpha(1 + c(x_0, x))$ for any $x \in X$.*

Proof. 1. Let $\int f d\nu_n \rightarrow \int f d\nu$ for any continuous function f such that $|f(x)| \leq \alpha + \beta c(x_0, x)$. Then $\nu_n \rightarrow \nu$ and for any $x_0 \in X$

$$J(\delta_{x_0}, \nu_n) = \int c(x_0, x) d\nu_n \rightarrow \int c(x_0, x) d\nu = J(\delta_{x_0}, \nu).$$

By Theorem 3.3.1 that implies $\nu_n \xrightarrow{J} \nu$.

2. Now let $\nu_n \xrightarrow{J} \nu$. Then $\nu_n \rightarrow \nu$ and $\int c(x_0, x) d\nu_n \rightarrow \int c(x_0, x) d\nu$. Obviously, it is enough to consider the case when f is nonnegative and $f(x) \leq 1 + c(x_0, x)$. Consider functions $f_h := \min\{h, f\} \in C_b(X)$, $h \geq 0$. From the weak convergence of ν_n it follows

that $\int f_h d\nu_n \rightarrow \int f_h d\nu$ for any $h \geq 0$. On the other hand,

$$\begin{aligned} 0 &\leq \int (f - f_h) d\nu_n = \int (f - h)_+ d\nu_n \leq \int (1 + c(x_0, x) - h)_+ d\nu_n \\ &= \int (c(x_0, x) - c_{h-1}(x_0, x)) d\nu_n \\ &\xrightarrow{n \rightarrow \infty} \int (c(x_0, x) - c_{h-1}(x_0, x)) d\nu \rightarrow 0 \text{ as } h \rightarrow \infty. \end{aligned}$$

Consequently, $\int f d\nu_n \rightarrow \int f d\nu$. □

Corollary 3.3.3. *Let X be a Polish space. Then the space (E_0, τ_J) is also Polish.*

Proof. Consider the following embedding of E_0 to $\mathcal{M}_+(X)$: $\nu \mapsto F(\nu) := (1 + c(x_0, x))\nu$. From Proposition 3.3.2 it follows that $\nu_n \xrightarrow{J} \nu$ iff $F(\nu_n) \rightharpoonup F(\nu)$. Moreover, the image $F(E_0)$ is weakly closed in $\mathcal{M}_+(X)$: indeed, if $\mu_n := F(\nu_n) \rightharpoonup \mu$, then

$$\int \frac{1}{1 + c(x_0, x)} d\mu = \lim \int \frac{1}{1 + c(x_0, x)} d\mu_n = \int d\nu_n = 1,$$

thus $\nu := \frac{1}{1 + c(x_0, x)}\mu \in E_0$. Recall that the space $\mathcal{M}_+(X)$ endowed with the topology of narrow convergence is Polish (Proposition 2.1.2) and (E_0, τ_J) is isomorphic to a closed subspace of it, consequently, it is also Polish. □

As we have seen, the function $\nu \mapsto \int f d\nu$ for $f \in (1 + c(x_0, \cdot))C_b(X)$ is continuous w.r.t. the topology τ_J . Sometimes it is possible to quantify this continuity. For example, if $c(x, y) = \rho^p(x, y)$ with $p \geq 1$, and f is Lipschitz continuous with a constant L , then $|\int f d\mu - \int f d\nu| \leq LJ^{1/p}(\mu, \nu)$. Recall that $J^{1/p}$ itself is a distance (the p -Wasserstein metric when we are talking about $E_0 = \mathcal{P}_p(X)$), thus the function $\mu \mapsto \int f d\mu$ is also L -Lipschitz for this distance. The next proposition is a simple generalization of the above result which concerns quantifying the modulus of continuity of this function.

Proposition 3.3.4. *Take a function f such that $|f(x) - f(y)| \leq g(c(x, y))$ for all $x, y \in X$ with some concave function g . Then for any $\mu, \nu \in \mathcal{P}(X)$ such that $f \in L^1(\mu) \cap L^1(\nu)$ it holds that*

$$\left| \int f d\mu - \int f d\nu \right| \leq g(J(\mu, \nu)).$$

Proof. Let γ be an optimal transport plan from μ to ν . Then by Jensen's inequality

$$\begin{aligned} \left| \int f d\mu - \int f d\nu \right| &= \left| \int f(x) d\gamma - \int f(y) d\gamma \right| \leq \int |f(x) - f(y)| d\gamma \\ &\leq \int g(c(x, y)) d\gamma \leq g\left(\int c d\gamma\right) = g(J(\mu, \nu)). \end{aligned}$$

□

Finally, Theorem 3.3.1 ensures stability of optimal transport plan w.r.t. the transportation topology (cf. Proposition 2.2.8).

Proposition 3.3.5 (Stability of optimal plans). *Let X, Y be Radon spaces and c_X, c_Y be cost functions satisfying Assumptions 3.1 and 3.2; denote the corresponding Monge–Kantorovich distances by J_X and J_Y . Let $c: X \times Y \rightarrow \mathbb{R}_+$ be a continuous cost function and set*

$$c_{XY}((x, y), (x', y')) := c_X(x, x') + c_Y(y, y') \text{ for } x, x' \in X, y, y' \in Y.$$

Take $\mu_n \xrightarrow{J_X} \mu \in E_0(X)$ and $\nu_n \xrightarrow{J_Y} \nu \in E_0(Y)$ such that $\liminf J_c(\mu_n, \nu_n) < \infty$. If γ_n is an optimal transport plan from μ_n to ν_n w.r.t. c for $n \in \mathbb{N}$, then, up to a subsequence, $\gamma_n \xrightarrow{J_{XY}} \gamma \in \Pi_o(\mu, \nu)$, where $J_{XY} = J_{c_{XY}}$.

Proof. According to Proposition 2.2.8 there is a subsequence $\gamma_n \rightharpoonup \gamma$ (without relabelling), where γ is an optimal transport plan between μ and ν w.r.t. c . Fix arbitrary $x_0 \in X$, $y_0 \in Y$. Then

$$\begin{aligned} J_{XY}(\delta_{(x_0, y_0)}, \gamma_n) &= \int (c_X(x_0, x) + c_Y(y_0, y)) d\gamma_n(x, y) \\ &= \int c_X(x_0, x) d\mu_n + \int c_Y(y_0, y) d\nu_n \\ &\rightarrow \int c_X(x_0, x) d\mu + \int c_Y(y_0, y) d\nu = J_{XY}(\delta_{(x_0, y_0)}, \gamma) < \infty, \end{aligned}$$

hence the claim follows by Theorem 3.3.1. \square

3.3.2 Topological properties

As we saw in the previous section the transportation distance inherits a lot of properties of the cost function. Corollary 3.3.3 shows that the Monge–Kantorovich space sometimes also reflects properties of the underlying space X . Now we are going to prove that under the above assumptions any class $(E(\mu_0), \tau_J)$ is separable and metrizable.

Lemma 3.3.6. *Take an arbitrary measure $\mu_0 \in \mathcal{P}(X)$. The equivalence class $E(\mu_0)$ endowed with the topology τ_J is separable and metrizable.*

Proof. 1. Let d_w be a metric on $\mathcal{P}(X)$ inducing the narrow convergence. Then

$$d_J(\mu, \nu) := d_w(\mu, \nu) + |J(\mu_0, \mu) - J(\mu_0, \nu)|$$

is also a metric and, obviously, $\mu_n \xrightarrow{J} \mu \in E(\mu_0)$ iff $d_J(\mu_n, \mu) \rightarrow 0$ by Theorem 3.3.1.

2. Let \mathcal{S}_{μ_0} be a countable family of measures of type $\nu := \mu_0 \lfloor (X \setminus B_m(x_0)) + \alpha \sum_{i=1}^n \delta_{x_i}$ where $m, n \in \mathbb{N}$, all x_i belong to some countable dense subset of X , and α is a normalizing constant. Fix a measure $\mu \in E(\mu_0)$, $\varepsilon > 0$, and $R > 0$ such that

$$\int_{B_R(x_0) \times B_R(x_0)} c(x, y) d\gamma > \mathcal{C}(\gamma) - \varepsilon,$$

where γ is an optimal transport plan from μ_0 to μ . Thus $\mathcal{C}'(\gamma) := \mathcal{C}(f_R\gamma) > \mathcal{C}(\gamma) - \varepsilon$ and $J(\tilde{\mu}, \mu) \leq \mathcal{C}(\gamma) - \mathcal{C}'(\gamma) < \varepsilon$. But $\tilde{\mu}$ obviously lies in the weak closure of \mathcal{S}_{μ_0} , so there exists a sequence $\mathcal{S}_{\mu_0} \ni \nu_n \xrightarrow{J} \tilde{\mu}$ and $\lim J(\nu_n, \mu) = J(\tilde{\mu}, \mu) < \varepsilon$. Consequently, \mathcal{S}_{μ_0} is a dense set in $E(\mu_0)$. \square

We have shown that the pair $(E(\mu_0), J)$ possesses almost all the properties of (X, c) , except the essential fact that X is a Radon space, i.e. that any Borel probability measure on it is tight. To prove that any class $E(\mu_0)$ endowed with the transportation topology is a Radon space, let us introduce the following additional assumption about a “ c -completeness” of X , which allows us to describe compact sets w.r.t. τ_J .

Assumption 3.3. Let $\{K_n\}_{n \in \mathbb{N}}$ be compact subsets of X and a sequence $\{r_n\}_{n \in \mathbb{N}} \subset \mathbb{R}_+$ converge to 0. Then the set $\bigcap_{n \in \mathbb{N}} \bigcup_{x \in K_n} B_{r_n}^c(x)$ is precompact.

Remark 3.3.7. The above property is an analogue of completeness in terms of c . Actually, one can show that in the case of (3.1) it holds iff (X, ρ) is complete.

Again, this assumption yields a counterpart in the space of measures.

Lemma 3.3.8. *Let $\{K_n\}_{n \in \mathbb{N}}$ be compact in τ_J subsets of $\mathcal{P}(X)$ and a sequence $\{r_n\}_{n \in \mathbb{N}} \subset \mathbb{R}_+$ converge to 0. Then the set*

$$\mathcal{H} := \bigcap_{n \in \mathbb{N}} \bigcup_{\mu \in K_n} \bar{B}_{r_n}^J(\mu)$$

is compact in τ_J .

Proof. Take a sequence $\{\nu^k\}_{k \in \mathbb{N}} \subset H$ and measures $\mu_n^k \in \mathcal{K}_n$ such that $J(\mu_n^k, \nu^k) \leq r_n$ for all $n, k \in \mathbb{N}$. Due to the compactness of \mathcal{K}_n , using the diagonal extraction procedure one can find a subsequence such that (without relabelling) $\mu_n^k \xrightarrow[k \rightarrow \infty]{J} \mu_n \in \mathcal{K}_n$ for all n . W.l.o.g. assume $r_n \leq 4^{-n}$. As $\mu_n^k \xrightarrow[k \rightarrow \infty]{} \mu_n$ by Lemma 3.2.3, there are compact sets $K_n \subset X$ such that $\mu_n^k(X \setminus K_n) \leq 2^{-n}$ for all $k, n \in \mathbb{N}$. Since

$$4^{-n} \geq r_n \geq J(\mu_n^k, \nu^k) \geq 2^{-n} \left(\mu_n^k(K_n) - \nu^k(K_n^{2^{-n}}) \right),$$

where $K_n^{2^{-n}} := \bigcup_{x \in K_n} B_{2^{-n}}^c(x)$, we obtain that

$$\nu^k(K_n^{2^{-n}}) \geq \mu_n^k(K_n) - 2^{-n} \geq 2 \cdot 2^{-n}.$$

Define $H_N := \bigcup_{n > N} K_n^{2^{-n}}$, $N \in \mathbb{N}$. By Assumption 3.3 these sets are precompact. Note that

$$\nu^k(X \setminus H_N) \leq 2 \cdot 2^{-N} \quad \forall k, N \in \mathbb{N},$$

hence $\{\nu^k\}_{k \in \mathbb{N}}$ is tight, and by Prokhorov's theorem there is a subsequence such that $\nu^k \rightharpoonup \nu \in \mathcal{P}(X)$ without relabelling. By the lower semicontinuity of the Monge–Kantorovich distance, $J(\mu_n, \nu) \leq r_n$ for all n , thus $\mu_n \xrightarrow{J} \nu$. In particular, this immediately implies that $\nu \in \mathcal{H}$, hence \mathcal{H} is closed in τ_J . Now take sequences $\{n_i\}_{i \in \mathbb{N}}, \{k_i\}_{i \in \mathbb{N}}$ such that $\mu_{n_i}^{k_i} \xrightarrow{J} \nu$. Since

$$J(\mu_{n_i}^{k_i}, \nu^{k_i}) \leq r_{n_i} \rightarrow 0 = J(\nu, \nu),$$

Lemma 3.2.9 yields that $\nu^{k_i} \xrightarrow{J} \nu$. □

Now we are ready to show that $(E(\mu_0), \tau_J)$ is a Radon space. Actually, we will prove even stronger result: $(E(\mu_0), \tau_J)$ is a Polish space.

Theorem 3.3.9. *For any $\mu_0 \in \mathcal{P}(X)$ the class $E(\mu_0)$ endowed with the transportation topology τ_J is a Polish space.*

Proof. Fix a countable dense set $\mathcal{S} = \{\mu_k\}_{k \in \mathbb{N}} \subset E(\mu_0)$ and for any $n \in \mathbb{N}$ define the map $v_n: E(\mu_0) \rightarrow \ell^1$ by

$$v_n(\nu) := \left\{ 2^{-k} (1 - nJ(\mu_k, \nu))_+ \right\}_{k \in \mathbb{N}}, \quad \nu \in E(\mu_0).$$

Clearly, $0 < \|v_n(\nu)\| \leq 1$. Now we define the following metric (the norms are in ℓ^1):

$$d_J(\mu, \nu) := d_w(\mu, \nu) + \sum_{n \in \mathbb{N}} 2^{-n} \left(\|v_n(\mu) - v_n(\nu)\| + \left\| \frac{v_n(\mu)}{\|v_n(\mu)\|} - \frac{v_n(\nu)}{\|v_n(\nu)\|} \right\| \right), \quad \mu, \nu \in E(\mu_0),$$

where d_w is some metric inducing the narrow convergence. Since J is continuous in τ_J and every v_n is bounded by the sequence $\{2^{-k}\}_{k \in \mathbb{N}}$, we conclude that $v_n(\nu_m) \xrightarrow{m \rightarrow \infty} v_n(\nu) \neq 0$ once $\nu_m \xrightarrow{J} \nu \in E(\mu_0)$, hence $\frac{v_n(\nu_m)}{\|v_n(\nu_m)\|} \rightarrow \frac{v_n(\nu)}{\|v_n(\nu)\|}$ and $d_J(\nu_m, \nu) \rightarrow 0$ (recall also that the narrow convergence is weaker than the transportation one). On the other hand, if $d_J(\nu_m, \nu) \rightarrow 0$, then $\nu_m \rightharpoonup \nu$ and $J(\mu_k, \nu_m) \xrightarrow{m \rightarrow \infty} J(\mu_k, \nu)$ once $J(\mu_k, \nu) < 1$, thus $\nu_m \xrightarrow{J} \nu$ due to the density of \mathcal{S} in $E(\mu_0)$ and Theorem 3.3.1. Therefore, d_J induces the same topology τ_J .

Now consider a Cauchy sequence $\{\nu_m\}_{m \in \mathbb{N}} \subset E(\mu_0)$ w.r.t. d_J . Since ℓ^1 is complete, for any $n \in \mathbb{N}$ there is $u_n \in \ell^1$ such that

$$\frac{v_n(\nu_m)}{\|v_n(\nu_m)\|} \rightarrow u_n \quad \text{as } m \rightarrow \infty.$$

Obviously, $\|u_n\| = 1$, thus there is $k_n \in \mathbb{N}$ such that $u_n(k_n) > 0$, hence for some $m_k \in \mathbb{N}$ it holds that $2^{-k_n} (1 - nJ(\mu_{k_n}, \nu_m))_+ > 0$, i.e. $J(\mu_{k_n}, \nu_m) < \frac{1}{n}$, whenever $m > m_k$. Consequently,

$$\nu_m \in B_{1/n}^J(\mu_{k_n}) \cup \bigcup_{j=1}^{m_k} B_{1/n}^J(\nu_j) \quad \text{for all } m \in \mathbb{N}$$

and Lemma 3.3.8 yields that $\{\nu_m\}_{m \in \mathbb{N}}$ is precompact w.r.t. τ_J (and w.r.t. d_J). This immediately implies the convergence of the sequence. The claim follows. \square

Remark 3.3.10. According to the above theorem, Assumption 3.3 ensures that X is also Polish (and hence, automatically, Radon): indeed, the set of Dirac measures is closed in τ_J , and $\delta_{x_n} \xrightarrow{J} \delta_x$ is equivalent to $x_n \rightarrow x$.

Finally, Lemmata 3.2.5, 3.2.9, 3.3.8, and Theorem 3.3.9 show that for any $\mu \in \mathcal{P}(X)$ the pair $(E(\mu), J)$ satisfies the same assumptions as (X, c) . This allows us to consider the Monge–Kantorovich distance on $\mathcal{P}(E(\mu))$ with J as a cost function and apply the results obtained above, which will be used in the next section to show stability of Fréchet barycenters. Moreover, iterating this process one can construct a so-called “tower of measures” (see [Ver06]).

3.3.3 Locally compact X

Finally, we consider the case of locally compact X . This allows us to obtain a weak local compactness of $\mathcal{P}(X)$, which will be essential in the next section to prove existence and stability of Fréchet barycenters.

Assumption 3.4. Any closed c -ball $\bar{B}_r^c(x)$ is compact w.r.t. ρ_w .

If we consider again Example 3.2.2, then this assumption holds once f is strictly increasing and unbounded, due to the Banach–Alaoglu theorem (in the case of a Banach space X) or Proposition 2.3.2 (in the case of the Wasserstein space X).

Notice that under this assumption from $c(x, y) = 0$ iff $x = y$ it follows that $c(x, x_n) \rightarrow 0$ iff $c(x_n, x) \rightarrow 0$ iff $x_n \rightarrow x$, i.e. the consistency of c . Moreover, it ensures Assumption 3.3.

Lemma 3.3.11. *Assumption 3.4 yields Assumption 3.3.*

Proof. Consider the set

$$H := \bigcap_{n \in \mathbb{N}} \bigcup_{x \in K_n} B_{r_n}^c(x).$$

from Assumption 3.3. Let $\{x_k\}_{k \in \mathbb{N}} \subset H$. Obviously, H is bounded w.r.t. c , thus there is a subsequence $x_k \rightarrow_w x$ (without relabelling). The rest of the proof is similar to the proof of Lemma 3.3.8. Take $y_n^k \in K_n$ such that $c(y_n^k, x_k) < r_n$ for all $n, k \in \mathbb{N}$. Again, up to a subsequence, $y_n^k \rightarrow y_n \in K_n$ as $k \rightarrow \infty$. Then $c(y_n, x) \leq \liminf_{k \rightarrow \infty} c(y_n^k, x_k) \leq r_n$, hence there are sequences $\{n_i\}_{i \in \mathbb{N}}$, $\{k_i\}_{i \in \mathbb{N}}$ such that $y_{n_i}^{k_i} \rightarrow x$ and $c(y_{n_i}^{k_i}, x_{k_i}) \rightarrow 0 = c(x, x)$. Therefore, by Assumption 3.1 $x_{k_i} \rightarrow x$. \square

Lemma 3.3.12. *Under Assumption 3.4 any closed J -ball $\bar{B}_r^J(\mu)$ is compact w.r.t. the ρ_w -narrow convergence.*

Proof. Fix $\varepsilon > 0$ and a ball $\bar{B}_m^c(x_0)$ such that $\mu(\bar{B}_m^c(x_0)) > 1 - \varepsilon$. Consider $M := A + Bm + \frac{Br}{\varepsilon}$ and any $\nu \in \bar{B}_r^J(\mu)$. Then

$$\begin{aligned} r \geq J(\mu, \nu) &\geq \int_{\bar{B}_m^c(x_0) \times (X \setminus \bar{B}_M^c(x_0))} c(x, y) \, d\gamma(x, y) \\ &\geq \int_{\bar{B}_m^c(x_0) \times (X \setminus \bar{B}_M^c(x_0))} \left(\frac{c(x_0, y) - Bc(x_0, x) - A}{B} \right) \, d\gamma(x, y) \\ &\geq \frac{M - Bm - A}{B} \gamma(\bar{B}_m^c(x_0) \times (X \setminus \bar{B}_M^c(x_0))) \geq \frac{r}{\varepsilon} [\mu(\bar{B}_m^c(x_0)) - \nu(\bar{B}_M^c(x_0))], \end{aligned}$$

where $\gamma \in \Pi_o(\mu, \nu)$. Hence, $\nu(\bar{B}_M^c(x_0)) \geq \mu(\bar{B}_m^c(x_0)) - \varepsilon > 1 - 2\varepsilon$. Therefore, $\bar{B}_r^J(\mu)$ is tight w.r.t. ρ_w . The claim follows by Prokhorov’s theorem and Lemma 2.2.4. \square

3.4 Case of \mathbb{R}^d

Now consider the locally compact Polish space $X = \mathbb{R}^d$ with the Euclidean metric $\rho(x, y) = \rho_w(x, y) = \|x - y\|$. Take $c(x, y) := g(x - y)$, where g is a real-valued convex function such that $g(0) = 0$ and $g(x) > 0$ whenever $x \neq 0$ (cf. Section 1.3 in [San15]). Obviously, this cost function is continuous and consistent, i.e. $c(x, x_n) \rightarrow 0$ iff $c(x_n, x) \rightarrow 0$ iff $x_n \rightarrow x$. Moreover, the space and the cost function satisfy Assumption 3.4.

First, we assume that the following inequality holds:

$$B := \sup_{x, y} \frac{g(x + y)}{g(x) + g(y)} < \infty. \quad (3.4)$$

Notice that $B \geq 1$ due to the convexity of g .

Proposition 3.4.1. *Let inequality (3.4) hold. Then there exists $q \geq 1$ such that $g^{1/q}$ satisfies the triangle inequality:*

$$g^{1/q}(x + y) \leq g^{1/q}(x) + g^{1/q}(y) \quad \forall x, y \in \mathbb{R}^d.$$

Proof. Consider points $x, y \in \mathbb{R}^d$ such that $g(y) = \xi g(x)$, $\xi \leq 1$. Due to the convexity of g one can obtain that for any $n \geq 1$ it holds

$$g(x + y) \leq \frac{n-1}{n}g(x) + \frac{1}{n}g(x + ny) \leq g(x) + \frac{B}{n}(g(x) + g(ny)).$$

Consider $n = 2^k$; it follows from inequality 3.4 that $g(2^k y) \leq (2B)^k g(y)$ and therefore

$$g(x + y) \leq g(x) + 2^{-k} B g(x) + B^{k+1} g(y) = g(x)(1 + B(2^{-k} + \xi B^k)).$$

Take $k := \lfloor -\frac{\ln \xi}{\ln 2B} \rfloor$; then

$$2^{-k} + \xi B^k \leq 2^{\frac{\ln \xi}{\ln 2 + \ln B} + 1} + \xi B^{-\frac{\ln \xi}{\ln 2 + \ln B}} = 3\xi^{1/q_0},$$

where $q_0 := \frac{\ln 2B}{\ln 2} \geq 1$. Thus $g(x + y) \leq g(x)(1 + 3B\xi^{1/q_0})$. Since $\xi \leq 1$ one can obtain that for $q := \max\{3B, q_0\}$ it holds

$$\begin{aligned} g^{1/q}(x + y) &\leq g^{1/q}(x)(1 + 3B\xi^{1/q_0})^{1/q} \leq g^{1/q}(x) \left(1 + \frac{3B}{q}\xi^{1/q_0}\right) \\ &\leq g^{1/q}(x)(1 + \xi^{1/q}) = g^{1/q}(x) + g^{1/q}(y) \end{aligned}$$

for all $x, y \in \mathbb{R}^d$. □

Corollary 3.4.2. *For all $\mu, \nu, \lambda \in \mathcal{P}(\mathbb{R}^d)$*

$$J^{1/q}(\mu, \nu) \leq J^{1/q}(\mu, \lambda) + J^{1/q}(\lambda, \nu).$$

Proof. Let us take measures $\mu, \nu, \lambda \in \mathcal{P}(\mathbb{R}^d)$ and optimal transport plans $\gamma_1 \in \Pi(\mu, \lambda)$, $\gamma_2 \in \Pi(\lambda, \nu)$. Similarly to the proof of Lemma 3.2.5 consider a measure $\sigma \in \Pi(\mu, \lambda, \nu)$ such that $\pi_{\#}^{1,2}\sigma = \gamma_1$, $\pi_{\#}^{2,3}\sigma = \gamma_2$. Applying Proposition 3.4.1 and the Minkowski inequality one can obtain that

$$\begin{aligned} J^{1/q}(\mu, \nu) &\leq \mathcal{C}^{1/q}(\pi_{\#}^{1,3}\sigma) = \left(\int (g^{1/q}(x - z))^q d\sigma\right)^{1/q} \\ &\leq \left(\int (g^{1/q}(x - y) + g^{1/q}(y - z))^q d\sigma\right)^{1/q} \\ &\leq \left(\int g(x - y) d\sigma\right)^{1/q} + \left(\int g(y - z) d\sigma\right)^{1/q} \\ &= \mathcal{C}^{1/q}(\gamma_1) + \mathcal{C}^{1/q}(\gamma_2) = J^{1/q}(\mu, \lambda) + J^{1/q}(\lambda, \nu). \end{aligned}$$

□

Corollary 3.4.3. *The function $\rho_J(\mu, \nu) := \max \{J^{1/q}(\mu, \nu), J^{1/q}(\nu, \mu)\} \in [0, \infty]$ is a metric on $\mathcal{P}(\mathbb{R}^d)$ (which may take the value $+\infty$).*

As we have seen, under assumption (3.4) $(\mathcal{P}(X), J)$ is similar to a q -Wasserstein space for some exponent q .

Now consider Assumption 3.2 in the Euclidean case. Obviously, one can rewrite it as

$$g(x + y) \leq A + B(g(\pm x) + g(\pm y)).$$

Theorem 3.4.4. *Under Assumption 3.2 for any $\varepsilon > 0$ there exist $q_\varepsilon \geq 1$, $B_\varepsilon > 0$ such that for all $x, y \in \mathbb{R}^d$ it holds that*

$$\begin{aligned} (g(\pm x \pm y) + \varepsilon)^{1/q_\varepsilon} &\leq (g(x) + \varepsilon)^{1/q_\varepsilon} + (g(y) + \varepsilon)^{1/q_\varepsilon}, \\ g(x \pm y) &\leq \varepsilon + (1 + \varepsilon)g(x) + B_\varepsilon g(y). \end{aligned}$$

Proof. Fix $\varepsilon > 0$. Consider $r > 0$ such that $g(x) \leq \varepsilon$ once $\|x\| \leq r$. Since $g(x) = 0$ iff $x = 0$, one has $a(t) := \min_{\|x\| \geq t} g(x) > 0$ for all $t > 0$. If $\|x + y\| > r$, then $\|x\| > r/2$ or $\|y\| > r/2$, and

$$\begin{aligned} g(x + y) &\leq A + B(g(x) + g(y)) \\ &\leq \frac{A}{a(r/2)}(g(x) + g(y)) + B(g(x) + g(y)) = \left(\frac{A}{a(r/2)} + B\right)(g(x) + g(y)). \end{aligned}$$

Consequently, for $D_r := \frac{A}{a(r/2)} + B \geq 1$ it holds that

$$g(\pm x \pm y) \leq \max \{\varepsilon, D_r(g(x) + g(y))\}$$

for all $x, y \in \mathbb{R}^d$. In particular,

$$g(\pm x \pm y) + \varepsilon \leq D_r(g(x) + \varepsilon + g(y) + \varepsilon)$$

and one can prove the first inequality in the same way as in Proposition 3.4.1.

In order to prove the second inequality, let us choose $k \in \mathbb{N}$, $r > 0$ such that

$$2^{-k}B < \varepsilon, \quad 2^{-k}A < \frac{\varepsilon}{2}, \quad 2^{-k}Bg(x) < \frac{\varepsilon}{2} \quad \text{as } \|x\| \leq 2^k r.$$

Then similarly to the proof of Proposition 3.4.1 one can show that

$$\begin{aligned} g(x + y) &\leq (1 + 2^{-k}B)g(x) + 2^{-k}Bg(2^k y) + 2^{-k}A \\ &\leq (1 + \varepsilon)g(x) + \frac{\varepsilon}{2} + \max \left\{ \frac{\varepsilon}{2}, D_r^k Bg(y) \right\} \leq \varepsilon + (1 + \varepsilon)g(x) + B_\varepsilon g(y), \end{aligned}$$

where $B_\varepsilon := D_r^k B$. □

Corollary 3.4.5. *For any $\varepsilon > 0$ and measures $\mu, \nu, \lambda \in \mathcal{P}(\mathbb{R}^d)$ the following inequalities hold:*

$$\begin{aligned} (J(\mu, \nu) + \varepsilon)^{1/q_\varepsilon} &\leq (J(\mu, \lambda) + \varepsilon)^{1/q_\varepsilon} + (J(\lambda, \nu) + \varepsilon)^{1/q_\varepsilon}, \\ J(\mu, \nu) &\leq \varepsilon + (1 + \varepsilon)J(\mu, \lambda) + B_\varepsilon J(\lambda, \nu), \\ J(\mu, \nu) &\leq \varepsilon + (1 + \varepsilon)J(\lambda, \nu) + B_\varepsilon J(\mu, \lambda). \end{aligned}$$

The proof of Corollary 3.4.5 is completely similar to the proofs of Lemma 3.2.5 and Corollary 3.4.2.

3.5 Fréchet barycenters

As we have obtained in Section 3.3, the space of probability measures endowed with the transportation topology has some nice topological properties. In this section the *barycenter* of measures will be defined, i.e. some kind of averaging w.r.t. the transportation structure of the space. It generalizes the construction from [AC11], where the 2-Wasserstein space is considered. Moreover, we consider a more general setting of penalized barycenters, which will be used later in Chapter 5.

In the section the Fréchet barycenter will be shown to be “upper semicontinuous” in some sense and statistically consistent. Analogous results for measures on \mathbb{R} and a convex cost function were proven in [KS15].

3.5.1 Generalized averaging in $\mathcal{P}(X)$

Hereafter we assume that Assumptions 3.1, 3.2, and 3.4 are fulfilled. Let the space $\mathcal{P}(X)$ be endowed with the Borel σ -algebra $\mathcal{B}(\tau_w)$ induced by the topology of narrow convergence τ_w . Note that it is weaker than $\mathcal{B}(\tau_J)$, induced by the transportation topology, but they are equivalent for defining an averaging in $\mathcal{P}(X)$.

Definition 3.2. Take a functional $G: \mathcal{P}(X) \rightarrow \mathbb{R} \cup \{+\infty\}$ (penalty) and a distribution $P \in \mathcal{P}(\mathcal{P}(X))$. A G -regularized Fréchet barycenter $\text{bar}_G(P)$ (or just a Fréchet barycenter $\text{bar}(P)$ if $G \equiv \text{const}$) w.r.t. the transportation functional J is any solution of the following problem:

$$\mathcal{V}_G(\nu; P) := \int J(\mu, \nu) dP(\mu) + G(\nu) \rightarrow \min_{\nu \in \mathcal{P}(X)}. \quad (3.5)$$

Respectively, $\text{Bar}_G(P)$ is the set of all G -regularized Fréchet barycenters of P .

Clearly, for $\text{bar}_G(P)$ to exist it is necessary (but may be not sufficient) that $P(E(\mu_0)) = 1$ for some measure μ_0 . Notice that $E(\mu_0)$ and every ball $B_r^J(\mu)$ belong to $\mathcal{B}(\tau_w)$ due to the lower semicontinuity of J . Thus, the restriction of $\mathcal{B}(\tau_w)$ to $E(\mu_0)$ coincides with $\mathcal{B}(\tau_J)$ since $(E(\mu_0), \tau_J)$ has a countable basis of J -balls. Therefore, it is enough to consider the space $\mathcal{P}(X)$ endowed with $\mathcal{B}(\tau_w)$ instead of the stronger σ -algebra $\mathcal{B}(\tau_J)$.

Assumptions 3.1–3.4 ensure that a G -regularized Fréchet barycenter exists under suitable assumptions on the penalty G : a bound on the negative part and a lower-semicontinuity.

Proposition 3.5.1. *Let $G: E(\mu_0) \rightarrow \mathbb{R} \cup \{+\infty\}$ be such that $G \geq \alpha$ for some functional $\alpha(\mu) = o(J(\mu_0, \mu))$ as $J(\mu_0, \mu) \rightarrow \infty$; G is lower semicontinuous w.r.t. the ρ_w -narrow convergence on any ball $\bar{B}_r^J(\mu_0)$; and $\inf_{\nu \in \mathcal{P}(X)} G(\nu) < \infty$. Let P be a probability distribution on $E(\mu_0)$ such that $\int J(\mu_0, \mu) dP(\mu) < \infty$. Then there exists a G -regularized Fréchet barycenter of P . Moreover, any minimizing sequence for $\mathcal{V}_G(\cdot; P)$ is precompact in τ_J , and every its partial limit is a G -regularized barycenter of P . In particular, $\text{Bar}_G(P)$ is compact.*

Proof. The weak triangle inequality yields that

$$\begin{aligned} \int J(\mu, \nu) dP(\mu) &\geq \int \frac{J(\mu_0, \nu) - BJ(\mu_0, \mu) - A}{B} dP(\mu) \\ &= \frac{J(\mu_0, \nu) - A}{B} - \frac{1}{B} \int J(\mu_0, \mu) dP(\mu) \rightarrow \infty \text{ as } J(\mu_0, \nu) \rightarrow \infty. \end{aligned}$$

Therefore, $\mathcal{V}_G(\nu; P) \geq \alpha(\nu) + \int J(\mu, \nu) dP(\mu) \rightarrow \infty$ once $J(\mu_0, \nu) \rightarrow \infty$, hence any minimizing sequence $\{\nu_n\}_{n \in \mathbb{N}}$ for $\mathcal{V}_G(\cdot; P)$ is bounded in J . By Lemma 3.3.12 there is a subsequence such that $\nu_n \rightarrow_w \nu$ (without relabelling). By Fatou's lemma and the lower semicontinuity of J and G one has

$$\begin{aligned} \mathcal{V}_G(\nu; P) &:= \int J(\mu, \nu) dP(\mu) + G(\nu) \leq \int \liminf J(\mu, \nu_n) dP(\mu) + \liminf G(\nu_n) \\ &\leq \lim \mathcal{V}_G(\nu_n; P) = \inf_{\nu \in \mathcal{P}(X)} \mathcal{V}_G(\nu; P), \end{aligned}$$

i.e. ν is a barycenter of P . Moreover, $J(\mu, \nu) = \liminf J(\mu, \nu_n)$ for P -a.e. μ , so by Theorem 3.3.1 there is a subsequence $\nu_{n_k} \xrightarrow{J} \nu^*$. \square

As an example of a narrowly lower semicontinuous regularizer one can consider a characteristic function of some ρ_w -weakly closed subset $\mathcal{G} \subset \mathcal{P}(X)$, or an entropy-type functional: $G(\nu) := \int g\left(\frac{d\nu}{d\nu_0}\right) d\nu_0$ once $\nu \ll \nu_0$, where g is a convex function. In the last case G may not be bounded from below by a constant or l.s.c. w.r.t. the ρ_w -narrow convergence on the whole space, but still satisfy the assumptions of the above proposition. See Chapter 5 and [BCP19] for more details on entropic-regularized barycenters in the 2-Wasserstein space over \mathbb{R}^d . Note that in both cases G is convex. Due to the convexity of J by Lemma 2.2.1, $\text{Bar}_G(P)$ is a convex set.

Moreover, if $X = \mathbb{R}^d$ and $c(x, y) = g(x - y)$, where g is *strictly* convex, then $J(\mu, \cdot)$ is also strictly convex, whenever μ is absolutely continuous w.r.t. the Lebesgue measure \mathcal{L} . It follows from the fact that in this case for any $\nu \sim \mu$ there exists a unique optimal transport map, see [San15, Section 1.3]. Therefore, there exists a unique barycenter of P , whenever $P(\{\mu : \mu \ll \mathcal{L}\}) > 0$. However, even without any assumption on measures one can take a strictly convex penalty and ensure the uniqueness of the barycenter — e.g. this is the case for entropic-regularized barycenters which will be considered in Chapter 5.

3.5.2 Stability of barycenters

Fix some $\mu_0 \in \mathcal{P}(X)$ and consider distributions on $E = E(\mu_0)$. Let d_w be a metric on E inducing the ρ_w -narrow convergence. One can define the Monge–Kantorovich distance with J as a cost function:

$$\mathcal{J}(P, Q) := \inf_{\Gamma \in \Pi(P, Q)} \int J(\mu, \nu) d\Gamma(\mu, \nu), \quad P, Q \in \mathcal{P}(E).$$

As E equipped with the topology τ_J is a Polish space by Theorem 3.3.9, and J as a cost function satisfies Assumptions 3.1–3.4, all the results from Section 3.3 hold for $\mathcal{P}(E)$ endowed with \mathcal{J} and the topology of d_w -narrow convergence.

Now let us show that convergence of distributions with respect to \mathcal{J} implies the transportation convergence of its barycenters. This result is similar to Theorem 2 from [LL17] in case of p -Wasserstein spaces. Also, we will obtain the law of large numbers for empirical barycenters proven in [BK12, Theorem 6.1] for the 2-Wasserstein space and measures with compact support.

Theorem 3.5.2. *Let $G, G_n : E \rightarrow \mathbb{R}$, $n \in \mathbb{N}$, satisfy assumptions of Proposition 3.5.1 and be bounded from below by the same functional α . Assume that for any J -bounded sequence $\mu_n \xrightarrow{w} \mu$ it holds that $G(\mu) \leq \liminf G_n(\mu_n)$, and for any $\mu \in E$ there is a sequence $\mu_n \xrightarrow{J} \mu$ such that $G(\mu) = \lim G_n(\mu_n)$. Let a sequence $\{P_n\}_{n \in \mathbb{N}} \subset \mathcal{P}(E)$ be such that $P_n \xrightarrow{J} P$ for some distribution P with $\int J(\mu_0, \mu) dP(\mu) < \infty$. Then any sequence of their barycenters $\nu_n \in \text{Bar}_{G_n}(P_n)$ is precompact in τ_J , and every its partial limit is a G -regularized barycenter of P . In particular, if $\nu^* := \text{bar}_G(P)$ is unique, then $\nu_n \xrightarrow{J} \nu^*$.*

Remark 3.5.3. One can rewrite the statement of the theorem in the case of fixed $G_n = G$ as follows: for any $\varepsilon > 0$ there exists $\delta > 0$ such that

$$\text{Bar}_G(P') \subset U_\varepsilon(\text{Bar}_G(P)) \quad \text{as } \mathcal{J}(P, P') < \delta,$$

where $U_\varepsilon(\text{Bar}_G(P)) := \bigcup_{\mu \in \text{Bar}_G(P)} B_\varepsilon^J(\mu)$ is an open neighbourhood of $\text{Bar}_G(P)$. One can say that the set-valued map $P \mapsto \text{Bar}_G(P)$ is upper-semicontinuous w.r.t. a Hausdorff-like convergence.

Notice also that in general case there does not exist a *continuous* function $P \mapsto \text{bar}_G(P)$, even for $G \equiv \text{const}$. However, if G is strictly convex, then $P \mapsto \text{bar}_G(P)$ is actually continuous w.r.t. τ_J .

Remark 3.5.4. The assumption on G_n and G means that G is the Γ -upper limit of G_n w.r.t. τ_J , and the Γ -lower limit w.r.t. d_w on every ball $B_r^J(\mu)$ (see [San15, p. 169] or [Dal12]).

Proof. Let ν^* be a G -regularized barycenter of P . Take a sequence $\mu_n \xrightarrow{J} \mu$ such that $G(\nu^*) = \lim G_n(\mu_n)$. Then

$$\begin{aligned} \mathcal{V}_G(\nu^*; P) &= G(\nu^*) + \mathcal{J}(P, \delta_{\nu^*}) = \lim G_n(\mu_n) + \lim \mathcal{J}(P, \delta_{\mu_n}) \\ &= \lim \mathcal{V}_{G_n}(\mu_n; P_n) \geq \limsup \mathcal{V}_{G_n}(\nu_n; P_n), \end{aligned}$$

but for any $\nu \in E$

$$\begin{aligned} \mathcal{V}_{G_n}(\nu; P_n) &\geq G_n(\nu) + \frac{J(\mu_0, \nu) - A}{B} - \frac{1}{B} \int J(\mu_0, \mu) dP_n(\mu) \\ &\geq \alpha(\nu) + \frac{J(\mu_0, \nu) - A}{B} - \frac{1}{B} \mathcal{J}(\delta_{\mu_0}, P_n) \rightarrow \infty \quad \text{as } J(\mu_0, \nu) \rightarrow \infty. \end{aligned}$$

Therefore, $J(\mu_0, \nu_n)$ are bounded, hence by Lemma 3.3.12 there is a subsequence such that $\nu_n \xrightarrow{w} \nu$ (without relabelling), which is equivalent to the d_w -narrow convergence $\delta_{\nu_n} \xrightarrow{w} \delta_\nu$. $G(\nu) \leq \liminf G_n(\nu_n)$ and $\mathcal{J}(P, \delta_\nu) \leq \liminf \mathcal{J}(P_n, \delta_{\nu_n})$, thus

$$\mathcal{V}_G(\nu; P) \leq \liminf \mathcal{V}_{G_n}(\nu_n; P_n) \leq \liminf \mathcal{V}_{G_n}(\mu_n; P_n) = \mathcal{V}_G(\nu^*; P),$$

i.e. $\nu \in \text{Bar}_G(P)$. Moreover, this yields $\mathcal{J}(P, \delta_\nu) = \liminf \mathcal{J}(P_n, \delta_{\nu_n})$, thus, up to a subsequence, $\delta_{\nu_n} \xrightarrow{\mathcal{J}} \delta_\nu$ by Theorem 3.3.1. The claim follows. \square

In the same way as Corollary 2.2.9 we can obtain the following result.

Corollary 3.5.5. *Let G satisfy the assumptions of Proposition 3.5.1. Then there exists a Borel map $\nu: E(\delta_{\mu_0}) \rightarrow E(\mu_0)$ such that $\nu(P) \in \text{Bar}_G(P)$ for all P .*

Corollary 3.5.6 (Upper semicontinuity of empirical barycenters). *Take sequences of measures $\{\mu_i^n\}_{n \in \mathbb{N}} \subset E$ and weights $\{\lambda_i^n\}_{n \in \mathbb{N}} \subset [0, +\infty)$ such that $\mu_i^n \xrightarrow{J} \mu_i$, $\lambda_i^n \rightarrow \lambda_i$ for $1 \leq i \leq m$, and $\sum_{i=1}^m \lambda_i^n = 1$ for all $n \in \mathbb{N}$. Let $P_n := \sum_{i=1}^m \lambda_i^n \delta_{\mu_i^n}$ and G satisfy the assumptions of Proposition 3.5.1. Then any sequence of Fréchet barycenters $\{\text{bar}_G(P_n)\}_{n \in \mathbb{N}}$ is precompact and every its partial limit is a G -regularized barycenter of $P := \sum_{i=1}^m \lambda_i \delta_{\mu_i}$.*

Proof. Note that $J(\mu_i^n, \mu_j) \rightarrow J(\mu_i, \mu_j)$ for all $1 \leq i, j \leq m$ and $\max_{i,j} J(\mu_i, \mu_j) < \infty$, hence

$$\mathcal{J}(P_n, P) \leq \sum_{i=1}^m \min\{\lambda_i^n, \lambda_i\} J(\mu_i^n, \mu_i) + \max_{i,j} J(\mu_i^n, \mu_j) \sum_{i=1}^m |\lambda_i^n - \lambda_i| \rightarrow 0.$$

This shows that the conditions of Theorem 3.5.2 hold. \square

Corollary 3.5.7 (Law of large numbers). *Let G and P satisfy the assumptions of Proposition 3.5.1, and $\{\mu_n\}_{n \in \mathbb{N}} \subset E$ be a sequence of i.i.d. random measures drawn from P . Define the empirical measures $P_n := \frac{1}{n} \sum_{i=1}^n \delta_{\mu_i}$ and let $\nu_n \in \text{Bar}_G(P_n)_{1 \leq i \leq n}$ be a measurable choice of (random) empirical barycenters. Then the sequence $\{\nu_n\}_{n \in \mathbb{N}}$ is precompact a.s. and every its partial limit is a barycenter of P .*

Proof. By the strong law of large numbers

$$\mathcal{J}(P_n, \delta_{\mu_0}) = \frac{1}{n} \sum_i J(\mu_i, \mu_0) \rightarrow \mathbb{E} J(\mu, \mu_0) = \mathcal{J}(P, \delta_{\mu_0}) < \infty \text{ a.s.},$$

and $P_n \rightarrow P$ a.s. due to Proposition 2.1.2. Then by Theorem 3.3.1 $P_n \xrightarrow{\mathcal{J}} P$ almost surely, i.e. the conditions of Theorem 3.5.2 hold. \square

Notice that all the statements in this section also hold for the space $\mathcal{P}(X)$ instead of $\mathcal{P}(\mathcal{P}(X))$, because one can identify a point $x \in X$ with the Dirac measure $\delta_x \in \mathcal{P}(X)$ so that $J(\delta_x, \delta_y) = c(x, y)$ for all $x, y \in X$, and the set of Dirac measures is closed w.r.t. to the ρ_w -narrow convergence.

Chapter 4

Bures–Wasserstein barycenters

4.1 Introduction

In this chapter we consider 2-Wasserstein barycenters of measures with a special structure (e.g. the Gaussians), and also its generalization to a complex space. Again, we are interested in the stochastic setting, consistency and other related properties of barycenters. As was shown in the previous chapter, a law of large numbers for empirical Wasserstein barycenters of i.i.d. random measures holds in a quite general setting. Having this LLN in mind, it is natural to look for error estimates and asymptotic normality of the error between population Wasserstein barycenters and their empirical counterpart. But establishing a central limit theorem (CLT) for Wasserstein barycenters and, more generally, for Fréchet means over a nonnegatively curved metric space seems to be a delicate task (see [ALP19] for results on concentration of Fréchet mean).

However, sometimes we can obtain more information on Wasserstein barycenters using a special structure of considered measures. Recall that $\mathcal{P}_2(\mathbb{R}^d)$ is the set of Borel probability measures on \mathbb{R}^d having a finite second moment, and equipped with the 2-Wasserstein metric W_2 given by (2.2) it forms the 2-Wasserstein space over \mathbb{R}^d . In most cases there is no closed formula for $W_2(\mu, \nu)$. Two important exceptions are the case of $d = 1$ and of Gaussian measures. In the first case the Wasserstein barycenter of measures is given by averaging their inverse cumulative functions [AC11]. In the second case, if $\mu = \mathcal{N}(a, Q)$, $\nu = \mathcal{N}(b, S)$, then (see [DL82])

$$W_2^2(\mu, \nu) = \|a - b\|^2 + \operatorname{tr} Q + \operatorname{tr} S - 2 \operatorname{tr} \left(Q^{1/2} S Q^{1/2} \right)^{1/2}. \quad (4.1)$$

Moreover, if $P \in \mathcal{P}(\mathcal{P}_2(\mathbb{R}^d))$ is concentrated on Gaussian measures, then (at least one of) its Wasserstein barycenter is also Gaussian [AC11]: it follows from a simple fact that the map $\mu \mapsto \mathcal{N}(\mathbb{E}_\mu X, \operatorname{Var}_\mu X)$ is non-expanding in W_2 , i.e. once $\mathbb{E}_\mu X = a$, $\operatorname{Var}_\mu X = Q$, and $\mathbb{E}_\nu X = b$, $\operatorname{Var}_\nu X = S$, then

$$W_2(\mu, \nu) \geq W_2(\mathcal{N}(a, Q), \mathcal{N}(b, S)).$$

Now we would like to point out that, actually, similar to (4.1) expressions appear not only in the context of Gaussian measures.

Scale-location families. We first present the concept of a scale-location family of measures on \mathbb{R}^d . Let $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$. The *scale-location family* induced by μ_0 is defined as

$$\mathcal{SL}(\mu_0) \stackrel{\text{def}}{=} \left\{ (p + Px)_{\#} \mu : P \in \operatorname{Sym}_+(d), p \in \mathbb{R}^d \right\},$$

where $\operatorname{Sym}_+(d)$ denotes the set of positive semi-definite symmetric matrices of size $d \times d$. If $\mu, \nu \in \mathcal{SL}(\mu_0)$ with $\mathbb{E}_\mu X = a$, $\operatorname{Var}_\mu X = Q$, and $\mathbb{E}_\nu X = b$, $\operatorname{Var}_\nu X = S$, then $W_2(\mu, \nu)$ is given by the same formula (4.1) [Álv+18; MC18]. For a distribution on a general scale-location family it is not true that there always exists a barycenter from this family. However, it still holds once

the covariance matrix of the template measure μ_0 is nondegenerate, by the same arguments as in the Gaussian case.

Scale-location families play an important role in modern data analysis and appear in many practical applications due to being user-friendly in terms of theoretical analysis and, at the same time, possessing high modeling power. For example, it is widely used in medical imaging [Was+10], modeling of molecular dynamic [Gon+17], clustering procedures [Del+17], climate modeling [MF17], and embedding of complex objects in low dimensional spaces [MC18].

Connection to quantum mechanics. The original Bures metric appears in quantum mechanics in relation to the fidelity measure between two quantum states and is used for the measurement of quantum entanglement [MM08; DLH11]. A density matrix ρ is an Hermitian (i.e. complex self-adjoint: $\bar{\rho} = \rho^\top$) positive semi-definite operator with unit trace: $\rho \in \mathbb{H}_+(d)$, $\text{tr} \rho = 1$. It is used to describe a statistical state of a quantum system. For an introduction to the density operators theory one may look [Fan57]. Let ρ and σ be two density matrices. Fidelity of these states, defined as $\mathcal{F}(\rho, \sigma) = \left[\text{tr} \left(\rho^{1/2} \sigma \rho^{1/2} \right)^{1/2} \right]^2$, quantifies a similarity between ρ and σ , see [Joz94]. It corresponds to the *Bures distance*:

$$d_B^2(\rho, \sigma) := 2 \left(1 - \mathcal{F}^{1/2}(\rho, \sigma) \right) = 2 \text{tr} \rho + 2 \text{tr} \sigma - 2 \text{tr} \left(\rho^{1/2} \sigma \rho^{1/2} \right)^{1/2}.$$

Notice that it has the same form (4.1), but now we are working with complex matrices instead of real ones appearing in the classic OT problem.

Given a random ensemble of density matrices, one can recovery its mean using averaging in the Euclidean sense. However, the Fréchet mean suggests an alternative way to define the barycenter in terms of the Bures distance. Given a probability distribution P on $\mathbb{H}_+(d)$, its population barycenter belonging the class of all $d \times d$ -dimensional density operators is defined as

$$\rho_* = \underset{\rho \in \mathbb{H}_+(d): \text{tr} \rho = 1}{\text{argmin}} \int_{\mathbb{H}_+(d)} d_B^2(\sigma, \rho) \, dP(\sigma).$$

It can be easily shown, that neglecting the condition $\text{tr} \rho = 1$, we end up with the global barycenter, which is a solution of the fixed point equation $\rho = \int_{\mathbb{H}_+(d)} (\rho^{1/2} \sigma \rho^{1/2})^{1/2} \, dP(\sigma)$. However, this is a contraction mapping, thus $\text{tr} \rho_*$ can be smaller than 1, and then ρ_* is not a density operator. In other words, the condition $\text{tr} \sigma = 1$ is needed to ensure that a barycenter also belongs to the class of density operators.

4.1.1 Bures–Wasserstein barycenters

Taking into account the considered above examples, we suggest to endow the space of positive semi-definite Hermitian matrices $\mathbb{H}_+(d)$ with the *Bures–Wasserstein distance* d_{BW} , originally introduced in [BJL18]. For a pair of matrices $Q, S \in \mathbb{H}_+(d)$ it is defined as

$$d_{BW}^2(Q, S) := \text{tr} Q + \text{tr} S - 2 \text{tr} \left(Q^{1/2} S Q^{1/2} \right)^{1/2}. \quad (4.2)$$

In particular, if Q and S are real matrices, then d_{BW} coincides with the 2-Wasserstein metric between centered measures from some scale-location family with covariance matrices Q and S ; and if $\text{tr} Q = \text{tr} S = 1$, then it is the Bures distance between Q and S .

As in the previous chapter, we focus on the following statistical setting. Let P be a probability distribution on $\mathbb{H}_+(d)$. Two important characteristics of P are Fréchet mean and variance. While the former is a “typical” representative of a data set in hand, the latter appears in the analysis of data variability (see, e.g., [DLL15]). First, we define

$$\mathcal{V}(Q) := \int_{\mathbb{H}_+(d)} d_{BW}^2(Q, S) \, dP(S), \quad Q \in \mathbb{H}_+(d).$$

A Fréchet mean of P , called here a *Bures–Wasserstein barycenter*, is a minimizer of $\mathcal{V}(Q)$:

$$Q_* := \operatorname{argmin}_{Q \in \mathbb{H}_+(d)} \mathcal{V}(Q).$$

However, as noted for density matrices, in some cases one might be interested in a minimizer belonging to an affine sub-space $\mathbb{A} \subset \mathbb{H}(d)$:

$$Q_* := \operatorname{argmin}_{Q \in \mathbb{H}_+(d) \cap \mathbb{A}} \mathcal{V}(Q). \quad (4.3)$$

Without loss of generality, we further address this problem. Respectively, the Fréchet variance of P is

$$V_* := \inf_{Q \in \mathbb{H}_+(d) \cap \mathbb{A}} \mathcal{V}(Q) = \mathcal{V}(Q_*).$$

Given an i.i.d. sample of matrices $S_1, \dots, S_n \sim P$, we construct an empirical version of $\mathcal{V}(Q)$:

$$\mathcal{V}_n(Q) := \frac{1}{n} \sum_{i=1}^n d_{BW}^2(Q, S_i), \quad Q \in \mathbb{H}_+(d).$$

Respectively, an empirical Bures–Wasserstein barycenter is

$$Q_n := \operatorname{argmin}_{Q \in \mathbb{H}_+(d) \cap \mathbb{A}} \mathcal{V}_n(Q). \quad (4.4)$$

and the empirical Fréchet variance is

$$V_n := \inf_{Q \in \mathbb{H}_+(d) \cap \mathbb{A}} \mathcal{V}_n(Q) = \mathcal{V}_n(Q_n).$$

In this chapter we study the convergence of Q_n to Q_* and V_n to V_* , in particular, a central limit theorem, and investigate their nonasymptotic concentration properties. Under mild assumptions on the distribution P we show the asymptotic normality of the empirical barycenter:

$$\sqrt{n}(Q_n - Q_*) \xrightarrow{d} \mathcal{N}(0, \Xi),$$

where Ξ is a covariance operator on $\mathbb{H}(d)$; and of the variance V_n :

$$\sqrt{n}(V_n - V_*) \xrightarrow{d} \mathcal{N}(0, \operatorname{Var} d_{BW}^2(Q_*, S)).$$

The technique of the proof of the CLT is based on the delta-method, and is also suitable for study of the concentration properties of Q_n and V_n . Namely, assuming the distribution P to be sub-Gaussian we obtain that with high probability

$$\|Q_*^{-1/2} Q_n Q_*^{-1/2} - I\|_F \lesssim \frac{1}{\sqrt{n}}, \quad d_{BW}(Q_n, Q_*) \lesssim \frac{1}{\sqrt{n}}, \quad \text{and} \quad |V_n - V_*| \lesssim \frac{1}{\sqrt{n}}.$$

CLT and asymptotic normality of M-estimators. One of possible approaches to obtain the central limit theorem is to look at a more general result concerning the asymptotic normality of M-estimators. To make the text self-contained, we briefly recall the subject following Section 5.4 in [Van06]. Under the setting (4.4), $d_{BW}^2(Q, S)$ might be considered as a loss function parametrized by elements of the affine subspace, $Q \in \mathbb{A} \cap \mathbb{H}_+(d)$. Thus, to prove the CLT for an empirical barycenter it is enough to validate the following conditions.

(C1) There exists a function $\psi_Q: \mathbb{H}_+(d) \rightarrow \mathbb{H}(d)$ from $L^2(P)$, such that

$$\lim_{Q \rightarrow Q_*} \frac{|d_{BW}^2(Q, S) - d_{BW}^2(Q_*, S) - \langle \psi_{Q_*}(S), Q - Q_* \rangle|}{\|Q - Q_*\|} = 0.$$

(C2) As $Q \rightarrow Q_*$, it holds that

$$\int (d_{BW}^2(Q, S) - d_{BW}^2(Q_*, S)) \, dP(S) = \frac{1}{2} \langle Q - Q_*, \mathbf{V}(Q - Q_*) \rangle + o(\|Q - Q_*\|),$$

where \mathbf{V} is some positive definite operator.

(C3) Let $Q \neq Q_*$, and define $g_Q(S) \stackrel{\text{def}}{=} \frac{d_{BW}^2(Q, S) - d_{BW}^2(Q_*, S)}{\|Q - Q_*\|}$. Suppose that for some $\varepsilon > 0$, the class $\{g_Q : Q \in \mathbb{H}_+(d), \|Q - Q_*\| \leq \varepsilon\}$ has an envelope from $L^2(P)$ and that it is a Donsker class.

Lemma 4.2.11 presents differentiability of the Bures–Wasserstein distance and provides a quadratic approximation for $d_{BW}^2(Q, S)$, what ensures Conditions (C1) and (C2). However, the validation of Condition (C3) is much more subtle. On the other hand, the direct proof of the CLT introduced in the present chapter is also suitable for the proof of the concentration results.

The chapter is organised as follows. Section 4.2 concerns properties of the Bures–Wasserstein distance d_{BW} , optimal transport maps T_Q^S (which are linear in the considered case), and their differentials. In Section 4.3 we impose assumptions on a distribution P , prove existence and uniqueness of its barycenter, and characterize it in terms of optimal maps. Section 4.4 is devoted to one of the main results of this chapter: central limit theorems for barycenters and Fréchet variance. Further, in Section 4.5 we present non-asymptotic concentration bounds on Q_n and V_n under assumption of sub-exponential distribution P . On contrary, Section 4.6 deals with an example of a slow convergence rate of 2-Wasserstein barycenters when the scale-location family is degenerated. The appendix gathers some auxiliary results on concentration of random vectors and matrices.

4.2 Properties of Bures–Wasserstein distance and OT maps

To make the presentation more transparent, we introduce a list of some used notations.

A, B	Matrices or vectors
\mathbf{A}, \mathbf{B}	Operators
$(\square)_{\mathbb{M}}$	Restriction of a quadratic form to a subspace \mathbb{M}
$A \preceq B$	$B - A$ is nonnegative definite
$A \prec B$	$B - A$ is positive definite
$\lambda_{\max}(\square), \lambda_{\min}(\square)$	Largest and smallest eigenvalue of an operator or a matrix
$\kappa(\square) = \ \square\ \cdot \ \square^{-1}\ $	Condition number of an operator or a matrix
$\ \square\ $	Operator norm
$\ \square\ _F$	Frobenius norm
$\ \square\ _1$	1-Schatten (nuclear) norm
$\ \square\ _{\psi_p}$	ψ_p Orlicz norm
$\langle \square, \square \rangle$	Inner product associated to Frobenius norm
\otimes	Tensor product
$\mathcal{L}(X)$	Distribution of a r.v. X
$o_P(\square)$	little o in probability
$O_P(\square)$	big O in probability

Following [BJL18], we continue to investigate properties of $d_{BW}(Q, S)$. Further we present an alternative analytical expression for the distance. This result is well-known for the case of real-valued symmetric matrices $Q, S \in \text{Sym}_+(d)$, see e.g. [OP82], although in [DL82] it is proven for Hermitian matrices. We provide a short proof here for the sake of completeness.

Proposition 4.2.1. *Let $Q, S \in \mathbb{H}_+(d)$ and $Q \succ 0$. Then (4.2) can be rewritten as*

$$d_{BW}^2(Q, S) = \min \left\{ \text{tr}(T - I) Q (T - I) : T \in \mathbb{C}^{d \times d}, TQT^* = S \right\},$$

and the minimum is attained at the optimal map

$$T_Q^S = S^{1/2}(S^{1/2}QS^{1/2})^{-1/2}S^{1/2} = Q^{-1/2}(Q^{1/2}SQ^{1/2})^{1/2}Q^{-1/2}. \quad (4.5)$$

Here by $(S^{1/2}QS^{1/2})^{-1/2}$ we denote the pseudo-inverse matrix $\left((S^{1/2}QS^{1/2})^{1/2}\right)^+$.

Remark 4.2.2. Note that being restricted to the sub-space $\text{Sym}_{++}(d)$, T_Q^S coincides with the (matrix of the) optimal transport map between two centered normal distributions $\mathcal{N}(0, Q)$ and $\mathcal{N}(0, S)$.

Proof. First, we prove that optimal T is self-adjoint. Indeed, assume the opposite, then

$$Q^{1/2}TQT^*Q^{1/2} = \left(Q^{1/2}TQ^{1/2}\right) \left(Q^{1/2}TQ^{1/2}\right)^* = Q^{1/2}SQ^{1/2}$$

and thus $\text{tr} Q^{1/2}TQ^{1/2} < \text{tr} (Q^{1/2}SQ^{1/2})^{1/2}$. Therefore

$$\begin{aligned} \text{tr}(T - I)Q(T^* - I) &= \text{tr} S + \text{tr} Q - 2 \text{tr} TQ = \text{tr} S + \text{tr} Q - 2 \text{tr} Q^{1/2}TQ^{1/2} \\ &> \text{tr} S + \text{tr} Q - 2 \text{tr} \left(Q^{1/2}SQ^{1/2}\right)^{1/2} = d_{BW}^2(Q, S). \end{aligned}$$

If T is Hermitian but not positive semi-definite, then

$$Q^{1/2}TQ^{1/2} \preceq \left(Q^{1/2}SQ^{1/2}\right)^{1/2}, \quad Q^{1/2}TQ^{1/2} \neq \left(Q^{1/2}SQ^{1/2}\right)^{1/2},$$

hence again $\text{tr} Q^{1/2}TQ^{1/2} < \text{tr} (Q^{1/2}SQ^{1/2})^{1/2}$.

Finally, if $T \in \mathbb{H}_+(d)$, then it is straightforward to check that $T = T_Q^S$ given by (4.5) and

$$\text{tr}(T - I)Q(T^* - I) = \text{tr} S + \text{tr} Q - 2 \text{tr} \left(Q^{1/2}SQ^{1/2}\right)^{1/2} = d_{BW}^2(Q, S).$$

□

4.2.1 Properties of T_Q^S

The proof of the central limit theorem mainly relies on the differentiability of the map (4.5). Lemma 4.2.4 shows that T_Q^S can be linearised in the vicinity of Q :

$$T_{Q+X}^S = T_Q^S + d\mathbf{T}_Q^S(X) + o(\|X\|),$$

where $d\mathbf{T}_Q^S: \mathbb{H}(d) \rightarrow \mathbb{H}(d)$ is a self-adjoint negative-definite operator and $\|X\|$ stands for the operator norm of X . Properties of $d\mathbf{T}_Q^S$ are investigated in Lemma 4.2.5. Let us note that the differentiability of an optimal transport map T_Q^S was established several times in different works, e.g. [AC17] or [Lav19b, Section 7.2]. In particular, in [AC17] it was used to prove the CLT in case of discrete distribution P . However, in this work we provide a refined analysis of $d\mathbf{T}_Q^S$ what allows us to obtain the CLT in a much more general setting.

Let us introduce some notation: if $G(A)$ is a functional on matrices, then we denote its differential as $d_A G$.

Lemma 4.2.3. *Map $Q \mapsto g(Q) = Q^{1/2}$ is differentiable on $\mathbb{H}_{++}(d)$, and its differential is given by*

$$d_Q g(X) = U^* \left(\frac{(UXU^*)_{ij}}{\sqrt{q_i} + \sqrt{q_j}} \right)_{i,j=1}^d U, \quad X \in \mathbb{H}(d),$$

where $Q = U^* \text{diag}(q)U$ is the eigenvalue decomposition.

Proof. First, let us consider the map $P \mapsto f(P) := P^2$. It is smooth and its differential

$$d_P f(X) = PX + XP, \quad X \in \mathbb{H}(d)$$

is nondegenerate:

$$\langle d_P f(X), X \rangle = 2 \operatorname{tr} XPX > 0, \quad X \neq 0,$$

whenever $P \in \mathbb{H}_{++}(d)$. From now on $\langle \cdot, \cdot \rangle$ denotes a scalar product associated to Frobenius norm.

Now applying the inverse function theorem we obtain that the inverse map $g := f^{-1}$ is also smooth and its differential enjoys the following equation

$$X = \left(d_P f|_{P=Q^{1/2}} \right) (d_Q g(X)) = Q^{1/2} d_Q g(X) + d_Q g(X) Q^{1/2},$$

thus

$$\begin{aligned} UXU^* &= (\operatorname{diag}(q))^{1/2} U d_Q g(X) U^* + U d_Q g(X) U^* (\operatorname{diag}(q))^{1/2}, \\ (UXU^*)_{ij} &= (\sqrt{q_i} + \sqrt{q_j}) (U d_Q g(X) U^*)_{ij}, \quad 1 \leq i, j \leq d, \end{aligned}$$

and

$$d_Q g(X) = U^* \left(\frac{(UXU^*)_{ij}}{\sqrt{q_i} + \sqrt{q_j}} \right)_{i,j=1}^d U.$$

□

Lemma 4.2.4 (Fréchet-differentiability of the map T_Q^S). *For any $S \in \mathbb{H}_+(d)$ the map $Q \mapsto T_Q^S$ can be linearised in the vicinity of $Q \in \mathbb{H}_{++}(d)$ as*

$$T_{Q+X}^S = T_Q^S + dT_Q^S(X) + o(\|X\|), \quad \text{as } X \rightarrow 0,$$

where

$$dT_Q^S(X) \stackrel{\text{def}}{=} -S^{1/2} U^* \Lambda^{-1/2} \delta \Lambda^{-1/2} U S^{1/2}, \quad X \in \mathbb{H}(d), \quad (4.6)$$

$U^* \Lambda U$ is an eigenvalue decomposition of $S^{1/2} Q S^{1/2}$

$$\begin{aligned} U^* \Lambda U &= S^{1/2} Q S^{1/2}, \quad U^* U = U U^* = I, \quad \Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_{\operatorname{rank}(S)}, 0, \dots, 0), \\ \Lambda^{-1/2} &= \left(\Lambda^{1/2} \right)^+ = \operatorname{diag}(\lambda_1^{-1/2}, \dots, \lambda_{\operatorname{rank}(S)}^{-1/2}, 0, \dots, 0), \\ \delta &= (\delta_{ij})_{i,j=1}^d, \quad \delta_{ij} = \begin{cases} \frac{\Delta_{ij}}{\sqrt{\lambda_i} + \sqrt{\lambda_j}}, & i, j \leq \operatorname{rank}(S) \\ 0, & \text{otherwise} \end{cases}, \quad \Delta = U S^{1/2} X S^{1/2} U^*. \end{aligned}$$

Proof. The proof mainly relies on the differentiation of the pseudo-inverse term $(S^{1/2} Q S^{1/2})^{-1/2}$, as long as

$$dT_Q^S(X) = S^{1/2} d_Q \left(S^{1/2} Q S^{1/2} \right)^{-1/2} (X) S^{1/2}.$$

Obviously, we can consider only the restriction to $\operatorname{range}(S)$ and therefore assume w.l.o.g. $S \succ 0$. As $(S^{1/2}(Q+X)S^{1/2})^{-1/2} = U^* (\Lambda + \Delta)^{-1/2} U$, by Lemma 4.2.3 and von Neumann series expansion we obtain for infinitesimal $X \in \mathbb{H}(d)$ and corresponding Δ that

$$\begin{aligned} (\Lambda + \Delta)^{-1/2} &= \left(\Lambda^{1/2} + \delta + o(\|\Delta\|) \right)^{-1} \\ &= \left(\Lambda^{1/4} \left(I + \Lambda^{-1/4} \delta \Lambda^{-1/4} + o(\|\Delta\|) \right) \Lambda^{1/4} \right)^{-1} \\ &= \Lambda^{-1/4} \left(I - \Lambda^{-1/4} \delta \Lambda^{-1/4} + o(\|\Delta\|) \right) \Lambda^{-1/4} \\ &= \Lambda^{-1/2} - \Lambda^{-1/2} \delta \Lambda^{-1/2} + o(\|\Delta\|). \end{aligned}$$

Then the differential $\mathbf{d}_Q (S^{1/2}QS^{1/2})^{-1/2} (X)$ is written as

$$\mathbf{d}_Q \left(S^{1/2}QS^{1/2} \right)^{-1/2} (X) = -U^* \Lambda^{-1/2} \delta \Lambda^{-1/2} U.$$

Therefore,

$$T_{Q+X}^S = T_Q^S + \mathbf{dT}_Q^S(X) + o(\|X\|),$$

where $\mathbf{dT}_Q^S(X)$ is defined by (4.6). \square

Lemmas 4.2.5 and 4.2.8 are technical and explore properties of \mathbf{dT}_Q^S .

Lemma 4.2.5. *For any $S \in \mathbb{H}_+(d)$, $Q \in \mathbb{H}_{++}(d)$, the properties of operator \mathbf{dT}_Q^S defined in (4.6) are following:*

- (I) *it is self-adjoint;*
- (II) *it is negative semi-definite;*
- (III) *it enjoys the following bounds:*

$$\begin{aligned} -\langle \mathbf{dT}_Q^S(X), X \rangle &\leq \frac{\lambda_{\max}^{1/2}(S^{1/2}QS^{1/2})}{2} \left\| Q^{-1/2} X Q^{-1/2} \right\|_F^2, \\ -\langle \mathbf{dT}_Q^S(X), X \rangle &\geq \frac{\lambda_{\min}^{1/2}(S^{1/2}QS^{1/2})}{2} \left\| Q^{-1/2} X Q^{-1/2} \right\|_F^2; \end{aligned}$$

- (IV) *it is homogeneous w.r.t. Q with degree $-\frac{3}{2}$ and w.r.t. S with degree $\frac{1}{2}$, i.e. $\mathbf{dT}_{aQ}^S = a^{-3/2} \mathbf{dT}_Q^S$ and $\mathbf{dT}_Q^{aS} = a^{1/2} \mathbf{dT}_Q^S$ for any $a > 0$;*

- (V) *it is monotone w.r.t. $S^{1/2}QS^{1/2}$ (once the range of S is fixed): $\mathbf{dT}_{Q_0}^{S_0} \preceq \mathbf{dT}_{Q_1}^{S_1}$ in the sense of self-adjoint operators on $\mathbb{H}(d)$ whenever $S_0^{1/2}Q_0S_0^{1/2} \preceq S_1^{1/2}Q_1S_1^{1/2}$ and $\text{range}(S_0) = \text{range}(S_1)$; in particular, \mathbf{dT}_Q^S is monotone w.r.t. $Q \in \mathbb{H}_{++}(d)$ for fixed S .*

Proof. Slightly changing notations, we rewrite (4.6) as

$$\mathbf{dT}_Q^S(X) = -S^{1/2}U^* \Lambda^{-1/2} \delta^X \Lambda^{-1/2} U S^{1/2},$$

where matrices U and Λ come from Lemma 4.2.4 and

$$\delta^X = (\delta_{ij}^X)_{i,j=1}^d, \quad \delta_{ij}^X = \frac{\Delta_{ij}^X}{\sqrt{\lambda_i} + \sqrt{\lambda_j}}, \quad \Delta^X = U S^{1/2} X S^{1/2} U^*.$$

(I) Self-adjointness

Consider a scalar product

$$\begin{aligned} \langle \mathbf{dT}_Q^S(X), Y \rangle &= \text{tr}(\mathbf{dT}_Q^S(X)Y) = -\text{tr}(S^{1/2}U^* \Lambda^{-1/2} \delta^X \Lambda^{-1/2} U S^{1/2} Y) \\ &= -\text{tr}(\Lambda^{-1/2} \delta^X \Lambda^{-1/2} U S^{1/2} Y S^{1/2} U^*). \end{aligned}$$

We now introduce a following notation

$$\Delta^Y \stackrel{\text{def}}{=} U S^{1/2} Y S^{1/2} U^*.$$

Then the above equality can be continued as follows:

$$\begin{aligned} -\text{tr}(\Lambda^{-1/2} \delta^X \Lambda^{-1/2} U S^{1/2} Y S^{1/2} U^*) &= -\text{tr}(\Lambda^{-1/2} \delta^X \Lambda^{-1/2} \Delta^Y) \\ &= -\sum_{i,j=1}^r \frac{\delta_{ij}^X}{\sqrt{\lambda_i} \lambda_j} \Delta_{ij}^Y = -\sum_{i,j=1}^r \frac{\Delta_{ij}^X \Delta_{ij}^Y}{\sqrt{\lambda_i} \lambda_j (\sqrt{\lambda_i} + \sqrt{\lambda_j})} \\ &= \text{tr}(\mathbf{dT}_Q^S(Y)X) = \text{tr}(X \mathbf{dT}_Q^S(Y)) = \langle X, \mathbf{dT}_Q^S(Y) \rangle, \end{aligned}$$

where $r := \text{rank}(S)$. Thus the operator is self-adjoint.

(II) Boundedness and (III) eigenvalues

Denoting Δ^X by Δ (i.e. now $\Delta = US^{1/2}XS^{1/2}U^*$) and taking into account the above expansion of an inner product, one obtains

$$-\langle d\mathbf{T}_Q^S(X), X \rangle = \sum_{i,j=1}^r \frac{\Delta_{ij}^2}{\sqrt{\lambda_i \lambda_j}(\sqrt{\lambda_i} + \sqrt{\lambda_j})} = \sum_{i,j=1}^r \left(\frac{\Delta_{ij}}{\sqrt{\lambda_i \lambda_j}} \right)^2 \frac{\sqrt{\lambda_i \lambda_j}}{\sqrt{\lambda_i} + \sqrt{\lambda_j}}. \quad (4.7)$$

Note that the function

$$f(\lambda_i, \lambda_j) \stackrel{\text{def}}{=} \frac{\sqrt{\lambda_i \lambda_j}}{\sqrt{\lambda_i} + \sqrt{\lambda_j}}$$

is monotonously increasing in both arguments λ_i and λ_j , thus

$$\max_{i,j} f(\lambda_i, \lambda_j) = \frac{\lambda_{\max}^{1/2}(\Lambda)}{2}, \quad \min_{i,j} f(\lambda_i, \lambda_j) = \frac{\lambda_{\min}^{1/2}(\Lambda)}{2}. \quad (4.8)$$

For the sake of simplicity we introduce a new variable

$$\zeta \stackrel{\text{def}}{=} Q^{-1/2} X Q^{-1/2},$$

its Frobenius norm is written as

$$\|\zeta\|_F^2 = \text{tr}(XQ^{-1}XQ^{-1}).$$

Moreover, the following inequality for trace holds:

$$\begin{aligned} \text{tr}(XQ^{-1}XQ^{-1}) &\geq \text{tr}(\Pi_S X \Pi_S Q^{-1} \Pi_S X \Pi_S Q^{-1} \Pi_S) \\ &= \text{tr}(\Delta \Lambda^+ \Delta \Lambda^+) = \left\| \Lambda^{-1/2} \Delta \Lambda^{-1/2} \right\|_F^2 = \sum_{i,j=1}^r \frac{\Delta_{ij}^2}{\lambda_i \lambda_j}. \end{aligned}$$

Here Π_S is the orthogonal projector onto the range of S .

Then combining (4.7) with (4.8), the upper and lower bounds can be obtained as follows:

$$\begin{aligned} -\langle d\mathbf{T}_Q^S(X), X \rangle &\leq \max_{i,j} f(\lambda_i, \lambda_j) \sum_{i,j=1}^r \left(\frac{\Delta_{ij}}{\sqrt{\lambda_i \lambda_j}} \right)^2 \leq \frac{\lambda_{\max}^{1/2}(\Lambda)}{2} \|\zeta\|_F^2, \\ -\langle d\mathbf{T}_Q^S(X), X \rangle &\geq \min_{i,j} f(\lambda_i, \lambda_j) \sum_{i,j=1}^r \left(\frac{\Delta_{ij}}{\sqrt{\lambda_i \lambda_j}} \right)^2 = \frac{\lambda_{\min}^{1/2}(\Lambda)}{2} \|\zeta\|_F^2. \end{aligned}$$

Note, that if S is degenerated, the lower bound becomes trivial.

(IV) Homogeneity and (V) monotonicity

Homogeneity follows directly from definition (4.6). Now we prove monotonicity. As the range of $S^{1/2}QS^{1/2}$ is fixed, we may assume $S \succ 0$. Consider

$$\begin{aligned} \langle d\mathbf{T}_Q^S(X), X \rangle &= \text{tr} \left(S^{1/2} U^* \Lambda^{-1/2} \delta \Lambda^{-1/2} U S^{1/2}, X \right) \\ &= \left\langle U^* \Lambda^{-1/2} \delta \Lambda^{-1/2} U, S^{1/2} X S^{1/2} \right\rangle \\ &= \left\langle d_Q \left(S^{1/2} Q S^{1/2} \right)^{-1/2} (X), S^{1/2} X S^{1/2} \right\rangle \\ &= \left\langle d_M M^{-1/2} \left(S^{1/2} X S^{1/2} \right), S^{1/2} X S^{1/2} \right\rangle, \end{aligned}$$

with replacement $M = S^{1/2}QS^{1/2}$ to be change of variables. As long as X is supposed to be fixed, it is enough to show that the differential $d_M M^{-1/2}$ is monotone in M . Notice that the

operator $(\mathbf{d}_M M^{-1/2})^{-1}$ at point M is equal to the differential of the inverse map $P \mapsto P^{-2}$ at point $P = M^{-1/2}$:

$$\mathbf{d}_M M^{-1/2} = (\mathbf{d}_P P^{-2}|_{P=M^{-1/2}})^{-1}.$$

In turn, $\mathbf{d}_P P^{-2}$ can be expressed as

$$\mathbf{d}_P P^{-2}(X) = -P^{-1} (P^{-1}X + XP^{-1}) P^{-1},$$

the right part of the above equation is self-adjoint, negative-definite and

$$\langle -P^{-1} (P^{-1}X + XP^{-1}) P^{-1}, X \rangle = -2 \operatorname{tr} P^{-2} X P^{-1} X.$$

Choose $M_1 \succ M_0 \succ 0$ (thus $M_1^{1/2} \succ M_0^{1/2}$) and let $P_i = M_i^{-1/2}$ for $i = 0, 1$. Then for any fixed $X \in \mathbb{H}(d)$

$$-\operatorname{tr} P_1^{-2} X P_1^{-1} X = -\operatorname{tr} M_1 X M_1^{1/2} X \leq -\operatorname{tr} M_0 X M_0^{1/2} X = -\operatorname{tr} P_0^{-2} X P_0^{-1} X,$$

i.e. $\mathbf{d}_P P^{-2}|_{P_1} \preceq \mathbf{d}_P P^{-2}|_{P_0}$ and hence for the differential of $M \mapsto M^{-1/2}$ the inverse inequality holds: $\mathbf{d}_M M^{-1/2}|_{M_0} \preceq \mathbf{d}_M M^{-1/2}|_{M_1}$. This entails monotonicity of $\mathbf{d}\mathbf{T}_Q^S$. \square

Corollary 4.2.6. *Under conditions of Lemma 4.2.5, it holds*

$$\lambda_{\max}(-\mathbf{d}\mathbf{T}_Q^S) \leq \frac{\lambda_{\max}^{1/2}(S^{1/2}QS^{1/2})}{2\lambda_{\min}^2(Q)}, \quad \lambda_{\min}(-\mathbf{d}\mathbf{T}_Q^S) \geq \frac{\lambda_{\min}^{1/2}(S^{1/2}QS^{1/2})}{2\lambda_{\max}^2(Q)}.$$

Proof. Item (III) from the above lemma ensures that

$$-\langle \mathbf{d}\mathbf{T}_Q^S(X), X \rangle \leq \frac{\lambda_{\max}^{1/2}(S^{1/2}QS^{1/2})}{2} \left\| Q^{-1/2} X Q^{-1/2} \right\|_F^2 \leq \frac{\lambda_{\max}^{1/2}(S^{1/2}QS^{1/2})}{2\lambda_{\min}^2(Q)} \|X\|_F^2.$$

The second bound is proved in a similar way. \square

Corollary 4.2.7. *Define the following rescaled operator*

$$\mathbf{d}\mathbf{T}_Q^S(\zeta) \stackrel{\text{def}}{=} Q^{1/2} \mathbf{d}\mathbf{T}_Q^S(Q^{1/2} \zeta Q^{1/2}) Q^{1/2}, \quad \zeta \in \mathbb{H}(d). \quad (4.9)$$

Then

$$\begin{aligned} \lambda_{\min}(-\mathbf{d}\mathbf{T}_Q^S) &= \frac{1}{2} \lambda_{\min}^{1/2}(S^{1/2}QS^{1/2}), \\ \lambda_{\max}(-\mathbf{d}\mathbf{T}_Q^S) &= \frac{1}{2} \lambda_{\max}^{1/2}(S^{1/2}QS^{1/2}). \end{aligned}$$

Proof. Notice that inequalities

$$\begin{aligned} \lambda_{\min}(-\mathbf{d}\mathbf{T}_Q^S) &\geq \frac{1}{2} \lambda_{\min}^{1/2}(S^{1/2}QS^{1/2}), \\ \lambda_{\max}(-\mathbf{d}\mathbf{T}_Q^S) &\leq \frac{1}{2} \lambda_{\max}^{1/2}(S^{1/2}QS^{1/2}), \end{aligned}$$

are a trivial consequence of Lemma 4.2.5 (III). Now defining for any $1 \leq k \leq \operatorname{rank}(S)$

$$\Delta_{ij}^k = \begin{cases} 1, & i = j = k, \\ 0, & \text{otherwise,} \end{cases}, \quad X^k = S^{-1/2} U \Delta^k U^* S^{-1/2}, \quad \zeta^k = Q^{-1/2} X^k Q^{-1/2}$$

we obtain from (4.7) that

$$-\langle \mathbf{d}\mathbf{T}_Q^S(\zeta^k), \zeta^k \rangle = -\langle \mathbf{d}\mathbf{T}_Q^S(X^k), X^k \rangle = \frac{\lambda_k^{1/2}}{2} \left\| \zeta^k \right\|_F^2.$$

Therefore, the above inequalities are sharp. \square

Lemma 4.2.8. For any $Q_0, Q_1 \in \mathbb{H}_{++}(d)$ and $S \in \mathbb{H}_+(d)$ consider

$$Q_t \stackrel{\text{def}}{=} (1-t)Q_0 + tQ_1, \quad Q' \stackrel{\text{def}}{=} Q_0^{-1/2}Q_1Q_0^{-1/2}. \quad (4.10)$$

Then

$$\begin{aligned} \frac{2}{\lambda_{\min}(Q') + \lambda_{\min}^{1/2}(Q')} d\mathbf{T}_{Q_0}^S &\preceq \int_0^1 d\mathbf{T}_{Q_t}^S dt \\ &\preceq \frac{2}{\lambda_{\max}(Q') + \lambda_{\max}^{1/2}(Q')} d\mathbf{T}_{Q_0}^S \\ &\preceq \frac{1}{1 + 3\|Q' - I\|/4} d\mathbf{T}_{Q_0}^S. \end{aligned}$$

Moreover, if $\|Q' - I\| < 1$, then

$$\int_0^1 d\mathbf{T}_{Q_t}^S dt \succeq \frac{1}{1 - \|Q' - I\|} d\mathbf{T}_{Q_0}^S.$$

Remark 4.2.9. The above inequality might seem confusing due to the fact that $\lambda_{\min}(\cdot) \leq \lambda_{\max}(\cdot)$, however this is explained by the fact that $d\mathbf{T}_Q^S$ is *negative* definite.

Proof. Notice that

$$((1-t) + t\lambda_{\min}(Q')) Q_0 \preceq Q_t = Q_0^{1/2}((1-t)I + tQ')Q_0^{1/2} \preceq ((1-t) + t\lambda_{\max}(Q')) Q_0.$$

Monotonicity and homogeneity with degree $-\frac{3}{2}$ of $d\mathbf{T}_Q^S$ (see Lemma 4.2.5) yield

$$\begin{aligned} d\mathbf{T}_{Q_t}^S &\preceq d\mathbf{T}_{((1-t)+t\lambda_{\max}(Q'))Q_0}^S \\ &= ((1-t) + t\lambda_{\max}(Q'))^{-3/2} d\mathbf{T}_{Q_0}^S \end{aligned}$$

and

$$\begin{aligned} d\mathbf{T}_{Q_t}^S &\succeq d\mathbf{T}_{((1-t)+t\lambda_{\min}(Q'))Q_0}^S \\ &= ((1-t) + t\lambda_{\min}(Q'))^{-3/2} d\mathbf{T}_{Q_0}^S. \end{aligned}$$

Therefore,

$$\begin{aligned} \int_0^1 d\mathbf{T}_{Q_t}^S dt &\preceq d\mathbf{T}_{Q_0}^S \int_0^1 ((1-t) + t\lambda_{\max}(Q'))^{-3/2} dt \\ &= \frac{2}{\lambda_{\max}(Q') + \lambda_{\max}^{1/2}(Q')} d\mathbf{T}_{Q_0}^S \end{aligned}$$

and respectively,

$$\int_0^1 d\mathbf{T}_{Q_t}^S dt \succeq \frac{2}{\lambda_{\min}(Q') + \lambda_{\min}^{1/2}(Q')} d\mathbf{T}_{Q_0}^S.$$

The inequality (II) follows from the fact that

$$\lambda_{\min}(Q') \geq 1 - \|Q' - I\|, \quad \lambda_{\max}(Q') \leq 1 + \|Q' - I\|,$$

and inequalities

$$\begin{aligned} \sqrt{1+x} &\leq 1 + \frac{x}{2} \quad \text{for } x \geq 0, \\ \sqrt{1-x} &\geq 1 - x \quad \text{for } 0 \leq x \leq 1. \end{aligned}$$

□

4.2.2 Properties of $d_{BW}(Q, S)$

The next lemma ensures the strict convexity of $d_{BW}(Q, S)$. In essence, the proof mainly relies on Theorem 7 in [BJL18].

Lemma 4.2.10. *For any $S \in \mathbb{H}_+(d)$ the function $Q \mapsto d_{BW}^2(Q, S)$ is convex on $\mathbb{H}_+(d)$. Moreover, if $S \succ 0$, then it is strictly convex.*

Proof. According to Theorem 7 in [BJL18] the function $h(X) := \text{tr } X^{1/2}$ is strictly concave on $\mathbb{H}_+(d)$, hence the function

$$Q \mapsto d_{BW}^2(Q, S) = \text{tr } S + \text{tr } Q - 2 \text{tr} \left(S^{1/2} Q S^{1/2} \right)^{1/2}$$

is convex on $\mathbb{H}_+(d)$ for any positive semi-definite S . Moreover, if $S \succ 0$, then $Q \mapsto S^{1/2} Q S^{1/2}$ is an injective linear map, and therefore $d_{BW}^2(Q, S)$ is strictly convex. \square

Further we introduce differentiability of $d_{BW}^2(Q, S)$ and provides its quadratic approximation.

Lemma 4.2.11. *For any $Q \in \mathbb{H}_{++}(d)$, $S \in \mathbb{H}_+(d)$ the function $d_{BW}^2(Q, S)$ is twice differentiable in Q with*

$$\begin{aligned} \mathbf{d}_Q d_{BW}^2(Q, S)(X) &= \langle I - T_Q^S, X \rangle, & X \in \mathbb{H}(d), \\ \mathbf{d}_Q^2 d_{BW}^2(Q, S)(X, Y) &= -\langle X, \mathbf{d}T_Q^S(Y) \rangle, & X, Y \in \mathbb{H}(d). \end{aligned}$$

Moreover, the following quadratic approximation holds: for any $Q_0, Q_1 \in \mathbb{H}_{++}(d)$

$$\begin{aligned} & -\frac{2}{(1+\lambda_{\max}^{1/2}(Q'))^2} \langle \mathbf{d}T_{Q_0}^S(Q_1 - Q_0), Q_1 - Q_0 \rangle \\ & \leq d_{BW}^2(Q_1, S) - d_{BW}^2(Q_0, S) + \langle T_{Q_0}^S - I, Q_1 - Q_0 \rangle \\ & \leq -\frac{2}{(1+\lambda_{\min}^{1/2}(Q'))^2} \langle \mathbf{d}T_{Q_0}^S(Q_1 - Q_0), Q_1 - Q_0 \rangle. \end{aligned}$$

with Q' defined in (4.10).

Proof. Derivatives. Note that

$$\mathbf{d}_Q \left(S^{1/2} Q S^{1/2} \right)^{1/2} (X) = U^* \delta U,$$

where δ comes from Lemma 4.2.4. Furthermore, Lemma 4.2.3 implies that

$$\begin{aligned} \mathbf{d}_Q \text{tr} \left(S^{1/2} Q S^{1/2} \right)^{1/2} (X) &= \text{tr } \mathbf{d}_Q \left(S^{1/2} Q S^{1/2} \right)^{1/2} (X) = \text{tr } \delta \\ &= \sum_{i=1}^{\text{rank}(S)} \frac{\Delta_{ii}}{2\sqrt{\lambda_i}} = \frac{1}{2} \text{tr } \Delta \Lambda^{-1/2} \\ &= \frac{1}{2} \text{tr } S^{1/2} X S^{1/2} \left(S^{1/2} Q S^{1/2} \right)^{-1/2} = \frac{1}{2} \langle T_Q^S, X \rangle. \end{aligned}$$

Consequently, $d_{BW}^2(Q, S)$ is differentiable, and

$$\mathbf{d}_Q d_{BW}^2(Q, S)(X) = \text{tr } X - 2 \mathbf{d}_Q \text{tr} \left(S^{1/2} Q S^{1/2} \right)^{1/2} (X) = \langle I - T_Q^S, X \rangle.$$

Applying Lemma 4.2.4 one obtains

$$\mathbf{d}_Q^2 d_{BW}^2(Q, S)(X, Y) = \mathbf{d}_Q \langle I - T_Q^S, X \rangle = -\langle \mathbf{d}T_Q^S(Y), X \rangle (Y).$$

Quadratic approximation. Let $Q_0, Q_1 \in \mathbb{H}_{++}(d)$, $Q_t := (1-t)Q_0 + tQ_1$, $t \in [0, 1]$. The Taylor expansion in the integral form applied to $d_{BW}^2(Q_t, S)$ implies

$$\begin{aligned} d_{BW}^2(Q_1, S) &= d_{BW}^2(Q_0, S) + \langle I - T_{Q_0}^S, Q_1 - Q_0 \rangle \\ &\quad + \int_0^1 (1-t) \langle -dT_{Q_t}^S(Q_1 - Q_0), Q_1 - Q_0 \rangle dt \\ &= d_{BW}^2(Q_0, S) - \langle T_{Q_0}^S - I, Q_1 - Q_0 \rangle \\ &\quad - \left\langle \left[\int_0^1 (1-t) dT_{Q_t}^S dt \right] (Q_1 - Q_0), Q_1 - Q_0 \right\rangle. \end{aligned}$$

Following the same ideas as in the proof of Lemma 4.2.8 one obtains that

$$\begin{aligned} \int_0^1 (1-t) dT_{Q_t}^S dt &\preceq \int_0^1 (1-t) ((1-t) + t\lambda_{\max}(Q'))^{-3/2} dT_{Q_0}^S dt \\ &= \frac{2}{(1+\lambda_{\max}^{1/2}(Q'))^2} dT_{Q_0}^S \end{aligned}$$

and

$$\int_0^1 (1-t) dT_{Q_t}^S dt \succeq \frac{2}{(1+\lambda_{\min}^{1/2}(Q'))^2} dT_{Q_0}^S.$$

Thus

$$\begin{aligned} &-\frac{2}{(1+\lambda_{\max}^{1/2}(Q'))^2} \langle dT_{Q_0}^S(Q_1 - Q_0), Q_1 - Q_0 \rangle \\ &\leq d_{BW}^2(Q_1, S) - d_{BW}^2(Q_0, S) + \langle T_{Q_0}^S - I, Q_1 - Q_0 \rangle \\ &\leq -\frac{2}{(1+\lambda_{\min}^{1/2}(Q'))^2} \langle dT_{Q_0}^S(Q_1 - Q_0), Q_1 - Q_0 \rangle. \end{aligned}$$

□

4.3 Existence and uniqueness of barycenters

Along with knowledge of properties of the Bures–Wasserstein distance in hand, and before moving to more general questions, one should ask her- or himself, whether a Bures–Wasserstein barycenter Q_* exists and, if so, is it unique or not.

Firstly, we assume that \mathbb{A} has a nonempty intersection with the space of positive definite operators.

Assumption 4.1. Given the setting (4.3), we suppose an affine subspace $\mathbb{A} \subset \mathbb{H}(d)$ to be s.t. $\mathbb{H}_{++}(d) \cap \mathbb{A} \neq \emptyset$. By \mathbb{M} we denote the linear subspace of $\mathbb{H}(d)$ associated with \mathbb{A} , i.e. the following representation holds: $\mathbb{A} = \{Q_0\} + \mathbb{M}$ for some $Q_0 \in \mathbb{H}(d)$.

Further, we assume that P assigns positive probability to the space of positive definite Hermitian matrices $\mathbb{H}_{++}(d)$ and that the average of S is finite.

Assumption 4.2. Let the distribution P on $\mathbb{H}_+(d)$ be such that

$$P(\mathbb{H}_{++}(d)) > 0, \quad \mathbb{E} \operatorname{tr} S < +\infty.$$

The next theorem ensures existence and uniqueness of the Fréchet mean introduced in (4.3) under the above assumptions.

Theorem 4.3.1 (Existence and uniqueness of Q_*). *Under Assumptions 4.1 and 4.2, there exists a unique Bures–Wasserstein barycenter Q_* of P . Furthermore, $Q_* \succ 0$ and it is characterised as a unique solution of the equation*

$$\mathbf{\Pi}_{\mathbb{M}} \mathbb{E} T_Q^S = \mathbf{\Pi}_{\mathbb{M}} I, \quad Q \in \mathbb{H}_{++}(d), \quad (4.13)$$

where $\mathbf{\Pi}_{\mathbb{M}}$ is the orthogonal projector onto \mathbb{M} .

Remark 4.3.2. In the case of Gaussian measures, uniqueness and nondegeneracy of Q_* under Assumption 4.2 follows from a general result for 2-Wasserstein barycenters, see e.g. Theorem 3.1 in [KP17]. However, it is not clear if this can be adapted to the considered setting with complex matrices and linear constraints.

Remark 4.3.3. The equation (4.13) generalizes the result for scale-location families in 2-Wasserstein space, presented in [Álv+18, Theorem 3.10], and originally obtained for the Gaussian case in the seminal work [AC11, Theorem 6.1]. Namely, if $\mathbb{A} = \text{Sym}_{++}(d)$, then Q_* exists and is the unique solution of a fixed-point equation:

$$Q = \mathbb{E} \left(Q^{1/2} S Q^{1/2} \right)^{1/2}, \quad Q \in \text{Sym}_{++}(d).$$

Note that it is similar to (4.13), as by multiplying the above equation from both sides by $Q^{-1/2}$ one obtains $\mathbb{E} T_Q^S = I$.

Proof. By Assumption 4.2 $\mathcal{V}(0)$ is finite:

$$\mathcal{V}(0) := \mathbb{E} d_{BW}^2(0, S) = \mathbb{E} \text{tr} S < \infty.$$

Since $d_{BW}(Q, S) \rightarrow \infty$ as $\|Q\| \rightarrow \infty$, one has $\mathcal{V}(Q) \rightarrow \infty$ as $\|Q\| \rightarrow \infty$. Thus, any minimizing sequence for \mathcal{V} is bounded. As \mathcal{V} is continuous, this implies existence of a barycenter Q_* by the compactness argument.

In case $P(\mathbb{H}_{++}(d)) > 0$ applying Lemma 4.2.10 we obtain strict convexity of the integral

$$Q \mapsto \mathbb{E} d_{BW}^2(Q, S) = \mathcal{V}(Q), \quad Q \in \mathbb{H}_+(d),$$

and therefore, uniqueness of the minimizer Q_* .

To prove that $Q_* \succ 0$ consider arbitrary degenerated $Q_0 \in \mathbb{H}_+(d) \cap \mathbb{A}$, $Q_1 \in \mathbb{H}_{++}(d) \cap \mathbb{A}$ (which exists by Assumption 4.1) and $S \in \mathbb{H}_{++}(d)$. Let us define $Q_t = (1-t)Q_0 + tQ_1 \in \mathbb{A}$. We are going to show, that

$$\frac{d}{dt} d_{BW}^2(Q_t, S) = \langle I - T_{Q_t}^S, Q_1 - Q_0 \rangle \rightarrow -\infty \quad \text{as } t \rightarrow 0.$$

To prove this convergence, we consider the following eigen-decomposition

$S^{1/2} Q_0 S^{1/2} = U^* \Lambda U$, $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_r, 0, \dots, 0)$, where $r := \text{rank}(Q_0)$. We denote as $C = U S^{1/2} Q_1 S^{1/2} U^*$, and write it in a block form:

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}, \quad C_{11} \in \mathbb{H}_{++}(r), \quad C_{12} = C_{21}^* \in \mathbb{C}^{r \times (d-r)}, \quad C_{22} \in \mathbb{H}_{++}(d-r).$$

Thus, for all Q_t the following representation holds (see Section A.5.5, paragraph *Inverse of block matrix* in [BV04]):

$$\begin{aligned} U \left(S^{1/2} Q_t S^{1/2} \right)^{-1} U^* &= ((1-t)A + tC)^{-1} \\ &= \begin{pmatrix} E_t^{-1} + t^2 E_t^{-1} C_{12} S_t^{-1} C_{21} E_t^{-1} & -t E_t^{-1} C_{12} S_t^{-1} \\ -t S_t^{-1} C_{21} E_t^{-1} & S_t^{-1} \end{pmatrix}, \end{aligned}$$

where $E_t = (1-t)A_{11} + tC_{11}$, $S_t = tC_{22} - t^2 C_{21} E_t^{-1} C_{12}$, with $A_{11} = \text{diag}(\lambda_1, \dots, \lambda_r)$. When $t \rightarrow 0$, $E_t \rightarrow A_{11} \succ 0$, $\frac{S_t}{t} \rightarrow C_{22} \succ 0$. This yields

$$tU \left(S^{1/2} Q_t S^{1/2} \right)^{-1} U^* \rightarrow \begin{pmatrix} 0 & 0 \\ 0 & C_{22}^{-1} \end{pmatrix},$$

and

$$\sqrt{t}U \left(S^{1/2} Q_t S^{1/2} \right)^{-1/2} U^* \rightarrow \begin{pmatrix} 0 & 0 \\ 0 & C_{22}^{-1/2} \end{pmatrix}.$$

Therefore,

$$\begin{aligned}\sqrt{t}\langle T_{Q_t}^S, Q_0 \rangle &= \sqrt{t} \left\langle \left(S^{1/2} Q_t S^{1/2} \right)^{-1/2}, S^{1/2} Q_0 S^{1/2} \right\rangle \\ &= \left\langle \sqrt{t} U \left(S^{1/2} Q_t S^{1/2} \right)^{-1/2} U^*, U S^{1/2} Q_0 S^{1/2} U^* \right\rangle \\ &\rightarrow \left\langle \begin{pmatrix} 0 & 0 \\ 0 & C_{22}^{-1/2} \end{pmatrix}, \begin{pmatrix} A_{11} & 0 \\ 0 & 0 \end{pmatrix} \right\rangle = 0.\end{aligned}$$

In the same way one can obtain

$$\sqrt{t}\langle T_{Q_t}^S, Q_1 \rangle \rightarrow \left\langle \begin{pmatrix} 0 & 0 \\ 0 & C_{22}^{-1/2} \end{pmatrix}, \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \right\rangle = \operatorname{tr} C_{22}^{1/2} > 0 \text{ as } t \rightarrow 0.$$

Consequently,

$$\frac{d}{dt} d_{BW}^2(Q_t, S) = \langle I - T_{Q_t}^S, Q_1 - Q_0 \rangle = \operatorname{tr} Q_1 - \operatorname{tr} Q_0 - \frac{\operatorname{tr} C_{22}^{1/2} + o(1)}{\sqrt{t}} \rightarrow -\infty.$$

By Assumption 4.1 it holds that $P(\mathbb{H}_{++}(d)) > 0$. Further, since $d_{BW}^2(Q, S)$ is convex, its directional derivatives are bounded by difference quotients, thus one can apply Leibniz integral rule for a Lebesgue-integrable function. This yields the following equality:

$$\frac{d}{dt} \mathcal{V}(Q_t) = \mathbb{E} \frac{d}{dt} d_{BW}^2(Q_t, S) \rightarrow -\infty \text{ as } t \rightarrow 0,$$

thus Q_0 cannot be a barycenter of P . This yields $Q_* \succ 0$.

Since \mathcal{V} is convex and the barycenter of P is positive-definite and unique, it is characterized as a stationary point of the Fréchet variation on subspace \mathbb{A} , i.e. as a solution to equation

$$\mathbf{H}_{\mathbb{M}} \nabla \mathcal{V}(Q) = \mathbf{H}_{\mathbb{M}}(I - \mathbb{E} T_Q^S) = 0, \quad Q \in \mathbb{A} \cap \mathbb{H}_{++}(d),$$

as required. The first equality follows from Lemma 4.2.11. \square

4.4 Central limit theorems

Armed with the knowledge about properties of $d_{BW}(\cdot, \cdot)$, Q_* , and Q_n , we are now equipped enough to introduce the first main result of the current study: the asymptotic normality of empirical barycenters Q_n .

Covariance operators. The proof of the CLT relies on covariance operators on the space of optimal transportation maps and on the space of covariance matrices.

Consider $T_i \stackrel{\text{def}}{=} T_{Q_*}^{S_i}$ and $T_i^n \stackrel{\text{def}}{=} T_{Q_n}^{S_i}$. We define a covariance Σ of T_i , its empirical counterpart Σ_n , and its data-driven estimator $\hat{\Sigma}_n$ as follows:

$$\begin{aligned}\Sigma &\stackrel{\text{def}}{=} \mathbb{E} (T_i - I) \otimes (T_i - I), \quad \Sigma_n \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^n (T_i - I) \otimes (T_i - I), \\ \hat{\Sigma}_n &\stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^n (T_i^n - I) \otimes (T_i^n - I),\end{aligned}$$

where \otimes stands for the tensor product.

The covariance of Q_n and its empirical counterpart are defined as

$$\mathbf{E} \stackrel{\text{def}}{=} \mathbf{F}^{-1}(\Sigma)_{\mathbb{M}} \mathbf{F}^{-1}, \quad \mathbf{E}: \mathbb{M} \rightarrow \mathbb{M}, \quad (4.14)$$

$$\hat{\Xi}_n \stackrel{\text{def}}{=} \hat{F}_n^{-1}(\hat{\Sigma}_n)_{\mathbb{M}} \hat{F}_n^{-1}, \quad \hat{\Xi}_n: \mathbb{M} \rightarrow \mathbb{M}, \quad (4.15)$$

where

$$\begin{aligned} \mathbf{F} &\stackrel{\text{def}}{=} -\mathbb{E} \left(d\mathbf{T}_{Q_*}^S \right)_{\mathbb{M}} & \mathbf{F}_n &\stackrel{\text{def}}{=} -\frac{1}{n} \sum_{i=1}^n \left(d\mathbf{T}_{Q_*}^{S_i} \right)_{\mathbb{M}}, \\ \hat{\mathbf{F}}_n &\stackrel{\text{def}}{=} -\frac{1}{n} \sum_{i=1}^n \left(d\mathbf{T}_{Q_n}^{S_i} \right)_{\mathbb{M}}. \end{aligned} \quad (4.16)$$

Another key object which appears in the proofs quite often is a rescaled empirical barycenter:

$$Q'_n \stackrel{\text{def}}{=} Q_*^{-1/2} Q_n Q_*^{-1/2}. \quad (4.17)$$

Now we are ready to prove the central limit theorem for the empirical barycenter Q_n .

Theorem 4.4.1 (Central limit theorem for empirical barycenter). *Under Assumptions 4.1 and 4.2 the CLT for Bures–Wasserstein barycenter holds:*

$$\sqrt{n}(Q_n - Q_*) \xrightarrow{d} \mathcal{N}(0, \Xi), \quad (\text{A})$$

where Ξ is a self-adjoint linear operator acting on \mathbb{M} defined by (4.14). Moreover, if $(\Sigma)_{\mathbb{M}}$ is nondegenerate, then

$$\sqrt{n} \hat{\Xi}_n^{-1/2} (Q_n - Q_*) \xrightarrow{d} \mathcal{N}(0, (\mathbf{I})_{\mathbb{M}}), \quad (\text{B})$$

where $\hat{\Xi}_n$ is an empirical counterpart of Ξ defined by (4.15).

Proof. Proof of (A). As $0 \leq d_{BW}(Q, S) \leq \text{tr } Q + \text{tr } S$, the random functions \mathcal{V}_n a.s. uniformly converge to the strictly convex function \mathcal{V} on any compact set by the uniform law of large numbers [Jen69, Theorem 2]. Therefore, their minimizers also converge $Q_n \xrightarrow{\text{a.s.}} Q_*$ (see, e.g., Lemma 5.2.2 in [Van06]). In particular, $P(Q_n \succ 0) \rightarrow 1$ as $n \rightarrow \infty$. The expansion from Lemma 4.2.4 at Q_* implies

$$T_i^n = T_i + \int_0^1 d\mathbf{T}_{Q_t}^{S_i}(Q_n - Q_*) dt, \quad (4.18)$$

where $Q_t = (1-t)Q_* + tQ_n$. Note, that the condition for Q_n being a barycenter is $\Pi_{\mathbb{M}} \left(\frac{1}{n} \sum_i T_i^n - I \right) = 0$. This fact together with averaging of (4.18) over i give:

$$\Pi_{\mathbb{M}} I = \Pi_{\mathbb{M}} \bar{T}_n - \mathbf{G}_n(Q_n - Q_*), \quad (4.19)$$

where

$$\bar{T}_n \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^n T_i, \quad \mathbf{G}_n \stackrel{\text{def}}{=} -\frac{1}{n} \sum_i \int_0^1 \left(d\mathbf{T}_{Q_t}^{S_i} \right)_{\mathbb{M}} dt.$$

According to Lemma 4.2.8

$$\frac{2}{\lambda_{\max}(Q'_n) + \lambda_{\max}^{1/2}(Q'_n)} \mathbf{F}_n \preceq \mathbf{G}_n \preceq \frac{2}{\lambda_{\min}(Q'_n) + \lambda_{\min}^{1/2}(Q'_n)} \mathbf{F}_n$$

where \mathbf{F}_n is defined in (4.16), and Q'_n comes from (4.17). Recall that \mathbf{F} introduced in (4.16) is a population counterpart of \mathbf{F}_n . This operator is correctly defined since by Lemma 4.2.5 one can show that it is self-adjoint, positive definite and bounded:

$$\|\mathbf{F}\| \leq \mathbb{E} \|d\mathbf{T}_{Q_*}^S\| \leq \mathbb{E} \frac{\|S^{1/2} Q_* S^{1/2}\|}{2\lambda_{\min}^2(Q_*)} < \infty.$$

This bound follows directly from Corollary 4.2.6.

Since by the law of large numbers $\mathbf{F}_n \xrightarrow{\text{a.s.}} \mathbf{F}$ and $Q'_n \xrightarrow{\text{a.s.}} I$, it holds that $\lambda_{\min}(Q'_n) \xrightarrow{\text{a.s.}} 1$ and $\lambda_{\max}(Q'_n) \xrightarrow{\text{a.s.}} 1$, thus $\mathbf{G}_n \xrightarrow{\text{a.s.}} \mathbf{F}$. Therefore, we obtain from (4.19) that

$$Q_n = Q_* + \mathbf{G}_n^{-1} \mathbf{I}_{\mathbb{M}} (\bar{T}_n - I).$$

Note that $d\mathbf{T}_{Q_*}^S$ is negative definite for any $S \succ 0$ by Lemma 4.2.5, hence \mathbf{F} itself is negative definite and thus can be inverted. In particular, \mathbf{G}_n^{-1} exist asymptotically a.s., and $\mathbf{G}_n^{-1} \xrightarrow{\text{a.s.}} \mathbf{F}^{-1}$. The result (A) follows immediately from the CLT for $\mathbf{I}_{\mathbb{M}} \bar{T}_n$ and Slutsky's theorem.

Proof of (B). Note that result (A) is equivalent to the fact that

$$\sqrt{n} \Xi^{-1/2} (Q_n - Q_*) \xrightarrow{d} \mathcal{N}(0, (\mathbf{I})_{\mathbb{M}}).$$

To ensure convergence of $\hat{\Xi}_n \xrightarrow{\text{a.s.}} \Xi$ we need to show that

- a) $\hat{\Sigma}_n \xrightarrow{\text{a.s.}} \Sigma$ (follows from Lemma 4.A.1, a.s. consistency of Q'_n , and the LLN);
- b) $\hat{\mathbf{F}}_n \xrightarrow{\text{a.s.}} \mathbf{F}$.

Consider

$$\begin{aligned} d\mathbf{T}_{Q_n}^S &\preceq d\mathbf{T}_{\lambda_{\max}(Q'_n)Q_*}^S = (\lambda_{\max}(Q'_n))^{-3/2} d\mathbf{T}_{Q_*}^S, \\ d\mathbf{T}_{Q_n}^S &\succeq d\mathbf{T}_{\lambda_{\min}(Q'_n)Q_*}^S = (\lambda_{\min}(Q'_n))^{-3/2} d\mathbf{T}_{Q_*}^S, \end{aligned}$$

where the inequalities come from monotonicity of $d\mathbf{T}_Q^S$ (see (V) in Lemma 4.2.5) and bounds $\lambda_{\min}(Q'_n)Q_* \preceq Q_n \preceq \lambda_{\max}(Q'_n)Q_*$. The equalities hold due to homogeneity of $d\mathbf{T}_Q^S$ with degree $-\frac{3}{2}$ (see (IV) in Lemma 4.2.5). This naturally leads to the following bounds:

$$\frac{1}{\lambda_{\max}^{3/2}(Q'_n)} \mathbf{F}_n \preceq \hat{\mathbf{F}}_n \preceq \frac{1}{\lambda_{\min}^{3/2}(Q'_n)} \mathbf{F}_n.$$

Since $Q'_n \xrightarrow{\text{a.s.}} I$ and $\mathbf{F}_n \xrightarrow{\text{a.s.}} \mathbf{F}$, this implies $\hat{\mathbf{F}}_n \xrightarrow{\text{a.s.}} \mathbf{F}$ due to the continuity of $\lambda_{\max}(\cdot)$ and $\lambda_{\min}(\cdot)$.

The above results ensure the validity of substitution Ξ by $\hat{\Xi}_n$. This yields (B). \square

The asymptotic convergence result for $d_{BW}(Q_n, Q_*)$ is a straightforward corollary of the above theorem.

Corollary 4.4.2 (Asymptotic distribution of $d_{BW}(Q_n, Q_*)$). *Under conditions of Theorem 4.4.1 it holds that*

$$\sqrt{n} d_{BW}(Q_n, Q_*) \xrightarrow{d} \left\| Q_*^{1/2} d\mathbf{T}_{Q_*}^{Q_*}(Z) \right\|_F,$$

with $Z \sim \mathcal{N}(0, \Xi)$. Moreover, replacing in the limiting distribution Q_* and Z by their empirical counterparts Q_n and $Z_n \sim \mathcal{N}(0, \hat{\Xi}_n)$, respectively, one obtains the following convergence:

$$d_w \left(\mathcal{L}(\sqrt{n} d_{BW}(Q_n, Q_*)), \mathcal{L} \left(\left\| Q_n^{1/2} d\mathbf{T}_{Q_n}^{Q_n}(Z_n) \right\|_F \right) \right) \rightarrow 0,$$

where d_w is any metric inducing the weak convergence.

Proof. Since $Q_n \xrightarrow{\text{a.s.}} Q_*$, Lemma 4.2.11 implies

$$d_{BW}^2(Q_n, Q_*) = -\frac{1 + o_P(1)}{2} \left\langle d\mathbf{T}_{Q_*}^{Q_*}(Q_n - Q_*), Q_n - Q_* \right\rangle.$$

Here o_P denotes little o in probability: recall that $X_n = o_P(1)$ iff $X_n \xrightarrow{P} 0$. Without loss of generality we can consider case $Q_* = \text{diag}(q_1, \dots, q_d)$, thus Lemma 4.2.5 implies (notice that $\Lambda = Q_*^2$ and $\Delta = Q_*^{1/2} X Q_*^{1/2}$)

$$\begin{aligned} -\left\langle d\mathbf{T}_{Q_*}^{Q_*}(X), X \right\rangle &= \sum_{i,j=1}^d \frac{X_{ij}}{q_i + q_j} X_{ij} = \sum_{i,j=1}^d (q_i + q_j) \left(\frac{X_{ij}}{q_i + q_j} \right)^2 \\ &= 2 \sum_{i,j=1}^d \left(\sqrt{q_i} \frac{X_{ij}}{q_i + q_j} \right)^2 = 2 \left\| Q_*^{1/2} d\mathbf{T}_{Q_*}^{Q_*}(X) \right\|_F^2. \end{aligned}$$

By Theorem 4.4.1 $\sqrt{n}(Q_n - Q_*)$ is asymptotically normal and centered, therefore

$$\mathcal{L}(\sqrt{n}d_{BW}(Q_n, Q_*)) \xrightarrow{d} \mathcal{L}\left(\left\| Q_*^{1/2} d\mathbf{T}_{Q_*}^{Q_*}(Z) \right\|_F\right).$$

where $Z \in \mathbb{M} \subset \mathbb{H}(d)$ and $Z \sim \mathcal{N}(0, \Xi)$.

Note, that $Q_n \xrightarrow{\text{a.s.}} Q_*$, $\hat{\Xi}_n \xrightarrow{\text{a.s.}} \Xi$, and $d\mathbf{T}_{Q_n}^{Q_n} \xrightarrow{\text{a.s.}} d\mathbf{T}_{Q_*}^{Q_*}$. The last result follows from Lemma 4.2.5 (IV, V), and can be validated using the same framework as in the proof of (B) in Theorem 4.4.1. Note, that $\lambda_{\min}(Q'_n)Q_* \preceq Q_n \preceq \lambda_{\max}(Q'_n)Q_*$, with Q'_n coming from (4.17). Then

$$\begin{aligned} d\mathbf{T}_{Q_n}^{Q_n} &\preceq d\mathbf{T}_{\lambda_{\max}(Q'_n)Q_*}^{\lambda_{\max}(Q'_n)Q_*} = \frac{1}{\lambda_{\max}(Q'_n)} d\mathbf{T}_{Q_*}^{Q_*} \rightarrow d\mathbf{T}_{Q_*}^{Q_*}, \\ d\mathbf{T}_{Q_n}^{Q_n} &\succeq d\mathbf{T}_{\lambda_{\min}(Q'_n)Q_*}^{\lambda_{\min}(Q'_n)Q_*} = \frac{1}{\lambda_{\min}(Q'_n)} d\mathbf{T}_{Q_*}^{Q_*} \rightarrow d\mathbf{T}_{Q_*}^{Q_*}, \end{aligned}$$

where the inequalities comes from monotonicity (see (V) in Lemma 4.2.5). The equalities hold due to homogeneity (see (IV) in Lemma 4.2.5). Furthermore, the continuity of $\lambda_{\max}(\cdot)$ and $\lambda_{\min}(\cdot)$ yields

$$\mathcal{L}\left(\left\| Q_n^{1/2} d\mathbf{T}_{Q_n}^{Q_n}(Z_n) \right\|_F\right) \xrightarrow{d} \mathcal{L}\left(\left\| Q_*^{1/2} d\mathbf{T}_{Q_*}^{Q_*}(Z) \right\|_F\right),$$

where $Z_n \sim \mathcal{N}(0, \hat{\Xi}_n)$. This, in turn, entails

$$d_w\left(\mathcal{L}(\sqrt{n}d_{BW}(Q_n, Q_*)), \mathcal{L}\left(\left\| Q_n^{1/2} d\mathbf{T}_{Q_n}^{Q_n}(Z_n) \right\|_F\right)\right) \rightarrow 0,$$

where d_w is some metric inducing the weak convergence of the measures. \square

To illustrate the result, we consider the case of a diagonal $Q_* = \text{diag}(q_1, \dots, q_d)$. This setting admits the explicit form of the limiting distribution:

$$\mathcal{L}(\sqrt{n}d_{BW}(Q_n, Q_*)) \xrightarrow{d} \mathcal{L}\left(\sqrt{\sum_{i,j=1}^d \frac{Z_{ij}^2}{2(q_i + q_j)}}\right),$$

where $Z = (Z_{ij})_{i,j=1}^d$. This representation of the limiting distribution is derived in the proof of Corollary 4.4.2 which is based on the fact that

$$d_{BW}^2(Q_n, Q_*) = -\frac{1 + o_P(1)}{2} \left\langle d\mathbf{T}_{Q_*}^{Q_*}(Q_n - Q_*), Q_n - Q_* \right\rangle,$$

and the explicit formula for $d\mathbf{T}_Q^S$ from Lemma 4.2.4.

The last result concerning convergence of empirical barycenter is the central limit theorem for the empirical variance V_n .

Theorem 4.4.3 (Central limit theorem for V_n). *Let Assumptions 4.1 and 4.2 be fulfilled and $\mathbb{E}(\text{tr } S)^2 < \infty$. Then*

$$\sqrt{n}(V_n - V_*) \xrightarrow{d} \mathcal{N}(0, \text{Var } d_{BW}^2(Q_*, S)).$$

Proof. By definition the empirical Fréchet variance is

$$\mathcal{V}_n(Q) = \frac{1}{n} \sum_{i=1}^n d_{BW}^2(Q, S_i).$$

Lemma 4.2.11 ensures the following bound on $\mathcal{V}_n(Q_*) - \mathcal{V}_n(Q_n)$:

$$0 \leq \mathcal{V}_n(Q_*) - \mathcal{V}_n(Q_n) \leq \frac{2}{(1 + \lambda_{\min}^{1/2}(Q'_n))^2} \langle \mathbf{F}_n(Q_n - Q_*), Q_n - Q_* \rangle.$$

The above quadratic bound together with $Q_n \rightarrow Q_*$, $\mathbf{F}_n \rightarrow \mathbf{F}$ and $\sqrt{n}(Q_n - Q_*) \xrightarrow{d} \mathcal{N}(0, \Xi)$ yield:

$$\mathcal{V}_n(Q_n) - \mathcal{V}(Q_*) = \mathcal{V}_n(Q_*) - \mathcal{V}(Q_*) + O_P\left(\frac{1}{n}\right).$$

Recall that $X_n = O_P(a_n)$ means that for any $\varepsilon > 0$ there is $M > 0$ such that $\limsup \mathbb{P}\{|X|_n > M\} \leq \varepsilon$. On the other hand, by the classical central limit theorem we obtain:

$$\begin{aligned} \sqrt{n}(\mathcal{V}_n(Q_*) - \mathcal{V}(Q_*)) &= \sqrt{n} \left(\frac{1}{n} \sum_i d_{BW}^2(Q_*, S_i) - \mathbb{E} d_{BW}^2(Q_*, S) \right) \\ &\xrightarrow{d} \mathcal{N}(0, \text{Var} d_{BW}^2(Q_*, S)). \end{aligned}$$

□

4.5 Concentrations

This section discusses the concentration properties of Q_n and V_n around Q_* and V_* , respectively, under the assumption of sub-Gaussianity of P .

Assumption 4.3 (Sub-Gaussianity of $\sqrt{\text{tr} S}$). Let $\sqrt{\text{tr} S}$ be sub-Gaussian:

$$P \left\{ \sqrt{\text{tr} S} \geq t \right\} \leq B e^{-bt^2} \quad \text{for any } t \geq 0,$$

with some constants $B, b > 0$.

4.5.1 Concentration of Q_n

The next lemma is a key ingredient in the proof of the concentration result for Q_n .

Lemma 4.5.1. *Consider*

$$\eta_n \stackrel{\text{def}}{=} \frac{1}{\lambda_{\min}(\mathbf{F}'_n)} \left\| Q_*^{1/2} \mathbf{I}_{\mathbb{M}} (\bar{T}_n - I) Q_*^{1/2} \right\|_F \quad (4.20)$$

where

$$\mathbf{F}'_n(X) \stackrel{\text{def}}{=} Q_*^{1/2} \mathbf{F}_n \left(Q_*^{1/2} X Q_*^{1/2} \right) Q_*^{1/2}, \quad X \in \left\{ Q_*^{-1/2} Y Q_*^{-1/2} \mid Y \in \mathbb{M} \right\}. \quad (4.21)$$

Then

$$\|Q'_n - I\|_F \leq \frac{\eta_n}{1 - \frac{3}{4}\eta_n}$$

whenever $\eta_n < \frac{4}{3}$ and $Q_n \succ 0$.

Proof. Let us define $Q_t \stackrel{\text{def}}{=} tQ_n + (1-t)Q_*$ for $t \in [0, 1]$. Due to Lemmas 4.2.5 and 4.2.8 we have for any $S \in \mathbb{H}_+(d)$

$$\begin{aligned} \langle \mathbf{I}_{\mathbb{M}} (T_{Q_*}^S - T_{Q_n}^S), Q_n - Q_* \rangle &= \langle T_{Q_*}^S - T_{Q_n}^S, Q_n - Q_* \rangle \\ &= \int_0^1 \langle -d\mathbf{T}_{Q_t}^S(Q_n - Q_*), Q_n - Q_* \rangle dt \\ &\geq \frac{1}{1 + \frac{3}{4}\|Q'_n - I\|} \langle -d\mathbf{T}_{Q_*}^S(Q_n - Q_*), Q_n - Q_* \rangle. \end{aligned}$$

Therefore,

$$\begin{aligned} \langle \mathbf{H}_{\mathbb{M}}(\bar{T}_n - I), Q_n - Q_* \rangle &\geq \frac{1}{1 + \frac{3}{4}\|Q'_n - I\|} \langle \mathbf{F}_n(Q_n - Q_*), Q_n - Q_* \rangle \\ &= \frac{1}{1 + \frac{3}{4}\|Q'_n - I\|} \langle \mathbf{F}'_n(Q'_n - I), Q'_n - I \rangle \\ &\geq \frac{\lambda_{\min}(\mathbf{F}'_n)}{1 + \frac{3}{4}\|Q'_n - I\|} \|Q'_n - I\|_F^2. \end{aligned}$$

At the same time,

$$\begin{aligned} \langle \mathbf{H}_{\mathbb{M}}(\bar{T}_n - I), Q_n - Q_* \rangle &= \left\langle Q_*^{1/2} \mathbf{H}_{\mathbb{M}}(\bar{T}_n - I) Q_*^{1/2}, Q'_n - I \right\rangle \\ &\leq \left\| Q_*^{1/2} \mathbf{H}_{\mathbb{M}}(\bar{T}_n - I) Q_*^{1/2} \right\|_F \|Q'_n - I\|_F. \end{aligned}$$

Hence

$$\|Q'_n - I\|_F \leq \frac{1 + \frac{3}{4}\|Q'_n - I\|}{\lambda_{\min}(\mathbf{F}'_n)} \left\| Q_*^{1/2} \mathbf{H}_{\mathbb{M}}(\bar{T}_n - I) Q_*^{1/2} \right\|_F = (1 + \frac{3}{4}\|Q'_n - I\|) \eta_n.$$

Rewriting the inequality above we obtain

$$\|Q'_n - I\|_F \leq \frac{\eta_n}{1 - \frac{3}{4}\eta_n}$$

provided that $\eta_n < \frac{4}{3}$. □

Before proving concentration results, we define the operator $\mathbf{F}'(X)$ as follows:

$$\mathbf{F}'(X) \stackrel{\text{def}}{=} Q_*^{1/2} \mathbf{F} \left(Q_*^{1/2} X Q_*^{1/2} \right) Q_*^{1/2} \text{ for } X \in \left\{ Q_*^{-1/2} Y Q_*^{-1/2} \mid Y \in \mathbb{M} \right\}. \quad (4.22)$$

The first result concerns the concentration of Q'_n in Frobenius norm. This is a crucial step in the proof of concentration of $d_{BW}(Q_n, Q_*)$.

Theorem 4.5.2 (Concentration of Q'_n). *Let Assumptions 4.1, 4.2, and 4.3 be fulfilled, then*

$$\mathbb{P} \left\{ \|Q'_n - I\|_F \geq \frac{c_Q}{\sqrt{n}} (\sqrt{m} + t) \right\} \leq 2me^{-nt_F} + e^{-t^2/2} + (1-p)^n$$

for any $t \geq 0$ and $n \geq c_Q^2 (\sqrt{m} + t)^2$, with

$$\begin{aligned} m &\stackrel{\text{def}}{=} \dim(\mathbb{M}), \quad p \stackrel{\text{def}}{=} P(\mathbb{H}_{++}(d)), \\ c_Q &\stackrel{\text{def}}{=} \frac{4\|Q_*\|_{\sigma_T}}{\lambda_{\min}(\mathbf{F}')}, \quad t_F \stackrel{\text{def}}{=} \mathbf{C} \min \left(\frac{\lambda_{\min}(\mathbf{F}')}{U \log^{1/2}(U/\sigma_F)}, \frac{\lambda_{\min}^2(\mathbf{F}')}{\sigma_F^2} \right), \end{aligned}$$

where the operator \mathbf{F}' is defined in (4.22), constant σ_T comes from auxiliary Proposition 4.A.4, constants σ_F and U are defined in auxiliary Proposition 4.A.2, and \mathbf{C} denotes a generic constant.

To make the result more transparent, we first discuss it in a less formal way. The proof is based on three steps, and each step yields a bounding term. The first step gives the term $2me^{-nt_F}$. It deals with the concentration of some auxiliary empirical operator \mathbf{F}'_n defined in (4.21) in the vicinity of its population counterpart \mathbf{F}' . These two operators are essentially a price to pay for moving from the space of optimal transportation maps T_Q^S to the space of barycenters. The concentration of \mathbf{F}'_n is derived from a result by [Kol11] which is presented in Proposition 4.A.2. The constants σ_F and U appear due to this concentration. Some prior bounds on σ_F and U are obtained in Lemma 4.A.3. The second step yields the term $e^{-t^2/2}$. It ensures the concentration of $\left\| \frac{1}{n} \sum_i T_{Q_*}^{S_i} - I \right\|_F$, and relies on the result by [HKZ12]. To make the text self-contained, we introduce it in Proposition 4.A.4. The constant σ_T comes from a bound on $\left\| \frac{1}{n} \sum_i T_{Q_*}^{S_i} - I \right\|_F$. The last step yields the term $(1-p)^n$. It comes from the requirement on nondegeneracy of Q_n . In other words, a high degeneracy leads to a smaller p and, thus, to worse bounds.

Proof. Let t_n be s.t. the following upper bound on $\gamma_n(t_n)$ from Proposition 4.A.2 holds:

$$\gamma_n(t_n) := C \max \left(\sigma_F \sqrt{\frac{t_n + \log(2m)}{n}}, U \sqrt{\log \left(\frac{U}{\sigma_F} \right)^{\frac{t_n + \log(2m)}{n}}} \right) \leq \frac{1}{2} \lambda_{\min}(\mathbf{F}').$$

It is easy to see that this condition is fulfilled for $t_n = nt_F - \log(m)$ under a proper choice of generic constant in the definition of t_F . Then with probability at least $1 - 2me^{-nt_F}$ the following bound holds:

$$\lambda_{\min}(\mathbf{F}'_n) \geq \lambda_{\min}(\mathbf{F}') - \|\mathbf{F}'_n - \mathbf{F}'\| \geq \frac{1}{2} \lambda_{\min}(\mathbf{F}'),$$

with \mathbf{F}'_n to be defined in (4.21). The above facts together with definition of η_n (4.20) yield

$$\begin{aligned} \eta_n &\stackrel{\text{def}}{=} \frac{\|Q_*^{1/2} \mathbf{I}_{\mathbb{M}}(\bar{T}_n - I) Q_*^{1/2}\|_F}{\lambda_{\min}(\mathbf{F}'_n)} \\ &\leq \frac{2\|Q_*\|}{\lambda_{\min}(\mathbf{F}')}\|\mathbf{I}_{\mathbb{M}}(\bar{T}_n - I)\|_F = \frac{c_Q}{2\sigma_T}\|\mathbf{I}_{\mathbb{M}}(\bar{T}_n - I)\|_F. \end{aligned}$$

Combining the above bounds with Proposition 4.A.4, we obtain:

$$\mathbb{P} \left\{ \eta_n \geq \frac{c_Q}{2\sqrt{n}}(\sqrt{m} + t) \right\} \leq 2me^{-nt_F} + e^{-t^2/2}.$$

Now it follows from Lemma 4.5.1 that

$$\begin{aligned} \mathbb{P} \left\{ \|Q'_n - I\|_F \geq \frac{c_Q}{\sqrt{n}}(\sqrt{m} + t) \right\} &\leq \mathbb{P} \left\{ 2\eta_n \geq \frac{c_Q}{\sqrt{n}}(\sqrt{m} + t) \right\} + \mathbb{P}\{Q_n \neq 0\} \\ &\leq 2me^{-nt_F} + e^{-t^2/2} + (1-p)^n, \end{aligned}$$

whenever $\frac{c_Q}{2\sqrt{n}}(\sqrt{m} + t) \leq \frac{2}{3}$. Here $Q \neq 0$ means that a matrix Q is not positive definite. We used that $Q_n \succ 0$ if at least one of matrices S_1, \dots, S_n is nondegenerate. \square

The next result deals with the concentration of Q_n in the Bures–Wasserstein distance. It is a corollary of the above theorem.

Corollary 4.5.3 (Concentration of Q_n in d_{BW}). *Under the conditions of Theorem 4.5.2 the following result holds:*

$$\mathbb{P} \left\{ d_{BW}(Q_n, Q_*) \geq \frac{c_Q \|Q_*\|^{1/2}}{\sqrt{n}}(\sqrt{m} + t) \right\} \leq 2me^{-nt_F} + e^{-t^2/2} + (1-p)^n.$$

Proof. To prove this result we use Lemma 4.2.11 and choose $Q_0 = S = Q_*$, $Q_1 = Q_n$. Thus we obtain

$$\begin{aligned} d_{BW}^2(Q_n, Q_*) &\leq \frac{2}{\left(1 + \lambda_{\min}^{1/2}(Q'_n)\right)^2} \left\langle d\mathbf{T}_{Q_*}^{Q_*}(Q_n - Q_*), Q_n - Q_* \right\rangle \\ &\stackrel{\text{Def. 4.9}}{=} \frac{2}{\left(1 + \lambda_{\min}^{1/2}(Q'_n)\right)^2} \left\langle -d\mathbf{T}_{Q_*}^{Q_*}(Q'_n - I), Q'_n - I \right\rangle \\ &\leq 2\lambda_{\max} \left(-d\mathbf{T}_{Q_*}^{Q_*} \right) \|Q'_n - I\|_F^2 \stackrel{C.4.2.7}{=} \lambda_{\max}(Q_*) \|Q'_n - I\|_F^2, \end{aligned}$$

with Q'_n coming from (4.17). Hence by Theorem 4.5.2

$$d_{BW}(Q_n, Q_*) \leq \|Q_*\|^{1/2} \frac{c_Q}{\sqrt{n}}(\sqrt{m} + t)$$

with probability at least $1 - 2me^{-nt_F} - e^{-t^2/2} - (1-p)^n$. \square

4.5.2 Concentration of V_n

The next main result of the current chapter describes the concentration properties of the empirical Fréchet variance V_n .

Theorem 4.5.4 (Concentration of V_n). *Let Assumptions 4.1, 4.2, and 4.3 be fulfilled, then, in the notation of Theorem 4.5.2,*

$$\mathbb{P}\{|V_n - V_*| \geq z(\mu, \nu, d, n, t)\} \leq 2me^{-ntF} + 3e^{-t^2/2} + (1-p)^n$$

with

$$z(b, \nu, d, n, t) \stackrel{\text{def}}{=} \max\left(\frac{\mu t^2}{n}, \frac{\nu t}{\sqrt{n}}\right) + 3\frac{c_Q^2 \|\mathbf{F}'\|}{n}(\sqrt{m} + t)^2.$$

A pair (ν, μ) is the parameters of a sub-exponential r.v. $d_{BW}^2(Q_*, S)$.

Proof. Following the proof of Theorem 4.4.3 we consider $\mathcal{V}_n(Q_*) - \mathcal{V}_n(Q_n)$:

$$\begin{aligned} 0 \leq \mathcal{V}_n(Q_*) - \mathcal{V}_n(Q_n) &\leq \frac{2}{(1+\lambda_{\min}^{1/2}(Q'_n))^2} \langle \mathbf{F}_n(Q_n - Q_*), Q_n - Q_* \rangle \\ &= \frac{2}{(1+\lambda_{\min}^{1/2}(Q'_n))^2} \langle \mathbf{F}'_n(Q'_n - I), Q'_n - I \rangle \\ &\leq 2\|\mathbf{F}'_n\| \cdot \|Q'_n - I\|_F^2, \end{aligned}$$

with \mathbf{F}'_n defined in (4.21), and Q'_n in (4.17).

Following the proof of Theorem 4.5.2, we obtain that with probability at least $1 - 2me^{-tFn} - e^{-t^2/2} - (1-p)^n$ the following upper bounds hold:

$$\|Q'_n - I\|_F \leq \frac{c_Q}{\sqrt{n}}(\sqrt{m} + t), \quad \|\mathbf{F}'_n - \mathbf{F}'\| \leq \frac{1}{2}\lambda_{\min}(\mathbf{F}'),$$

with \mathbf{F}' coming from (4.22). Thus

$$\|\mathbf{F}'_n\| \leq \|\mathbf{F}'\| + \|\mathbf{F}'_n - \mathbf{F}'\| \leq \frac{3}{2}\|\mathbf{F}'\|$$

and consequently

$$0 \leq \mathcal{V}_n(Q_*) - \mathcal{V}_n(Q_n) \leq 3\|\mathbf{F}'\| \frac{c_Q^2}{n}(\sqrt{m} + t)^2.$$

Now we consider the difference $\mathcal{V}_n(Q_*) - \mathcal{V}(Q_*)$. According to Assumption 4.3 S , and therefore $d_{BW}^2(Q_*, S)$, are sub-exponential r.v. with some parameters (ν, μ) . Then Lemma 4.A.5 ensures

$$|\mathcal{V}_n(Q_*) - \mathcal{V}(Q_*)| \leq \max\left(\frac{2\mu t'}{n}, \nu \left(\frac{2t'}{n}\right)^{1/2}\right)$$

with probability at least $1 - 2e^{-t'}$. Combining two above bounds, we obtain:

$$|\mathcal{V}_n(Q_n) - \mathcal{V}(Q_*)| \leq \max\left(\frac{2\mu t'}{n}, \nu \sqrt{\frac{2t'}{n}}\right) + 3\|\mathbf{F}'\| \frac{c_Q^2}{n}(\sqrt{m} + t)^2$$

with probability at least $1 - 2e^{-t'} - 2me^{-ntF} - e^{-t^2/2} - (1-p)^n$. Choosing $t' = t^2/2$, we get

$$\begin{aligned} \mathbb{P}\left\{|\mathcal{V}_n(Q_n) - \mathcal{V}(Q_*)| \geq \max\left(\frac{\mu t^2}{n}, \frac{\nu t}{\sqrt{n}}\right) + 3\|\mathbf{F}'\| \frac{c_Q^2}{n}(\sqrt{m} + t)^2\right\} \\ \leq 2me^{-ntF} + 3e^{-t^2/2} + (1-p)^n. \end{aligned}$$

□

4.6 Slow rate of convergence: example

In this section we demonstrate an example of a distribution on a scale-location family such that the rate of convergence of $W_2(\nu_n, \nu_*)$ is slower than $\frac{1}{\sqrt{n}}$, where ν_* and ν_n are the population and the empirical 2-Wasserstein barycenters, respectively. As was mentioned in the introduction, there is an equivalence between Wasserstein and Bures–Wasserstein barycenters once the scale-location family is induced by a template measure μ_0 with a nondegenerate covariance matrix. Yet, here we will consider a degenerated case.

Theorem 4.6.1. *There exists a scale-location family $\mathcal{SL}(\mu_0) \subset \mathcal{P}_2(\mathbb{R}^2)$ and a distribution P on it such that it has the unique Wasserstein barycenter $\nu_* = \text{bar}(P) \in \mathcal{SL}(\mu_0)$, for any $n \in \mathbb{N}$ there is an empirical barycenter $\nu_n = \text{bar}(P_n) \in \mathcal{SL}(\mu_0)$, and for large enough n with probability at least $\frac{1}{8}$*

$$W_2(\nu_n, \nu_*) \geq \frac{C}{\log n}.$$

Proof. Step 1: construction of P . For any $z \in \mathbb{R}$ define a measure on \mathbb{R}^2

$$\mu_z := \frac{1}{2} (\delta_{a_z} + \delta_{-a_z}),$$

where $a_z := (1 - z, z) \in \mathbb{R}^2$. Let P_Z be a distribution on \mathbb{R} , then $P := (z \mapsto \mu_z)_{\#} P_Z$ is a corresponding distribution on $\mathcal{P}(\mathbb{R}^2)$. Let Z be a random variable drawn from P_Z .

Recall that $\nu_* = \text{bar}(P)$. Set $\tilde{\nu} := \frac{1}{2} (\nu_* + (-\text{id})_{\#} \nu_*)$. Obviously, due to symmetry one has for any $z \in \mathbb{R}$

$$\begin{aligned} W_2^2(\mu_z, \nu_*) &\geq W_2^2(\mu_z, \tilde{\nu}) = \int_{\mathbb{R}^2} \min \{ \|x - a_z\|^2, \|x + a_z\|^2 \} d\tilde{\nu}(x) \\ &= \int_{\mathbb{R}^2} \min \{ \|x - a_z\|^2, \|x + a_z\|^2 \} d\nu_*(x). \end{aligned}$$

Thus, $\tilde{\nu}$ is also a Wasserstein barycenter. Moreover, ν_* -a.e. x is sent by the optimal plan to the closest point among $a_z, -a_z$ a.s., otherwise $\mathbb{E} W_2^2(\mu_z, \nu_*) > \mathbb{E} W_2^2(\mu_z, \tilde{\nu})$ according to the above inequality. In particular,

$$\mathbb{E} W_2^2(\mu_Z, \nu_*) = \mathbb{E} \int_{\mathbb{R}^2} \min \{ \|x - a_Z\|^2, \|x + a_Z\|^2 \} d\nu_*(x) = \int_{\mathbb{R}^2} D(x) d\nu_*(x),$$

where $D(x) := \mathbb{E} \min \{ \|x - a_Z\|^2, \|x + a_Z\|^2 \}$. Due to the symmetry of this function, any symmetric measure concentrated Argmin D is a barycenter of P . Hence

$$\mathbb{E} W_2^2(\mu_Z, \nu_*) = \min_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} \mathbb{E} W_2^2(\mu_Z, \nu) = \min_{x \in \mathbb{R}^d} D(x),$$

and ν_* is concentrated on the set of minimizers of D . Note that D is semi-concave, thus it has directional derivatives at any point $x \in \mathbb{R}^2$.

Let $x = (x_1, x_2)$ and $x_1 < x_2$, then

$$\min \{ \|x - a_z\|^2, \|x + a_z\|^2 \} = \begin{cases} \|x + a_z\|^2, & z \leq z(x), \\ \|x - a_z\|^2, & z \geq z(x), \end{cases}$$

where $z(x) := -\frac{x_1}{x_2 - x_1}$. Therefore, for all $v \in S^1$ one has

$$\begin{aligned} \partial_v D(x) &\leq 2 \mathbb{E} \langle (x + a_Z) \mathbb{1}[Z \leq z(x)] + (x - a_Z) \mathbb{1}[Z > z(x)], v \rangle \\ &= 2 \langle x - \mathbb{E} a_Z + 2 \mathbb{E} a_Z \mathbb{1}[Z \leq z(x)], v \rangle. \end{aligned}$$

If x is a minimum point of $D(x)$, then $\partial_v D(x) \geq 0$ for all v , hence

$$x = \mathbb{E} a_Z - 2 \mathbb{E} a_Z \mathbb{1}[Z \leq z(x)].$$

Set $F(z) := P\{Z \leq z\}$ and $E(z) := \mathbb{E} Z \mathbb{1}[Z \leq z]$ for all $z \in \mathbb{R}$. Then the above equation reads as

$$\begin{cases} x_1 = 1 - \mathbb{E} Z - 2(F(z(x)) - E(z(x))), \\ x_2 = \mathbb{E} Z - 2E(z(x)). \end{cases} \quad (4.23)$$

Substituting it to the formula for $z(x)$, we get the following necessary condition for x to be a minimizer of D :

$$z(x) = \frac{\mathbb{E} Z - 1 + 2F(z(x)) - 2E(z(x))}{2\mathbb{E} Z - 1 + 2F(z(x)) - 4E(z(x))}. \quad (4.24)$$

Respectively, once $x_1 = x_2 \geq 0$, we have

$$\min \{\|x - a_z\|^2, \|x + a_z\|^2\} = \|x - a_z\|^2,$$

and thus

$$\partial_v D(x) \leq 2\langle x - \mathbb{E} a_Z, v \rangle.$$

Then $x = \operatorname{argmin} D(x)$ yields $x = \mathbb{E} a_Z = (1 - \mathbb{E} Z, \mathbb{E} Z)$, which is possible only when $\mathbb{E} Z = \frac{1}{2}$; in this case we set $z(x) := -\infty$, thus x also satisfies (4.23). Similar results for other possible cases follow from the ones considered above by symmetry.

We are going to construct a distribution P_Z such that $Z > 0$ a.s. and $\operatorname{Argmin}_{x \in \mathbb{R}^2} D(x) = \{a_1, -a_1\}$ (thus $\nu_* = \mu_1$). According to (4.23) this implies $\mathbb{E} Z = 1$ since $z(a_1) = 0$ and $F(0) = E(0) = 0$. Obviously, there is no minimum point of D on the diagonal $x_1 = x_2$ because $\mathbb{E} Z \neq \frac{1}{2}$. Further, in this case (4.24) together with (4.23) substituted to $x_1 < x_2$ reads as

$$z(x) = 2 \frac{F(z(x)) - E(z(x))}{1 + 2F(z(x)) - 4E(z(x))} \quad \text{and} \quad 1 + 2F(z(x)) - 4E(z(x)) > 0. \quad (4.25)$$

We want barycenters to be unstable w.r.t. small changes of P , so let us first consider F satisfying (4.25) for all z . It is equivalent to the following equation:

$$\frac{1-z}{1-2z} F(z) = \frac{z}{2(1-2z)} + E(z).$$

If F is absolutely continuous, then $E'(z) = zF'(z)$, and it leads to the ODE

$$\frac{1}{(1-2z)^2} F(z) + \frac{1-z}{1-2z} F'(z) = \frac{1}{2(1-2z)^2} + zF'(z)$$

with a solution F^* given by

$$F^*(z) = \frac{1}{2} \left(1 - \frac{1-2z}{\sqrt{1-2z+2z^2}} \right).$$

It has the density

$$f^*(z) := (F^*)'(z) = \frac{1}{2(1-2z+2z^2)^{3/2}},$$

and the corresponding function $E^*(z) := \mathbb{E}_{Z \sim F^*} Z \mathbb{1}[Z \leq z]$ is

$$E^*(z) = \frac{1}{2} \left(1 - \frac{1-z}{\sqrt{1-2z+2z^2}} \right).$$

We are going to construct F such that it is close to F^* in the vicinity of 0 and ensures the uniqueness of the barycenter $\nu^* = \mu_1$. Consider the density $f := f^* - \delta f$, where $\delta f(z) := \frac{1}{z^2} \exp(-\frac{1}{z})$. Respectively, we denote

$$\delta F(z) := \int_0^z \delta f(s) ds = \exp\left(-\frac{1}{z}\right), \quad \delta E(z) := \int_0^z s \delta f(s) ds.$$

For $0 < z \leq \frac{1}{3}$ we have $\delta f(z) \leq \delta f(\frac{1}{3}) = 9e^{-3} < \frac{1}{2} = f^*(0) \leq f^*(z)$, i.e. $f(z) > 0$. We set $P_Z := f\mathcal{L}|_{[0, z_0]} + (1 - F(z_0))\delta_{z_+}$ with some $0 < z_0 \leq \frac{1}{3}$ and with z_+ still to be fixed. Condition $\mathbb{E}Z = E(z_0) + (1 - F(z_0))z_+ = 1$ yields $z_+ = \frac{1 - E(z_0)}{1 - F(z_0)}$ (clearly, $F(z_0)$ and $E(z_0)$ do not depend on z_+). As was said above, we are interested only in the behavior of F around 0, so the second term is chosen in a simple form (a Dirac measure) that allows us to obtain $\nu_* = \mu_1$.

Since $\delta E(z) < z\delta F(z)$ for all $z > 0$, we have

$$\begin{aligned} z(1 + 2F(z) - 4E(z)) - 2F(z) + 2E(z) &= 2(1 - z)\delta F(z) - 2(1 - 2z)\delta E(z) \\ &\geq 2(1 - z)\delta F(z) - 2(1 - 2z)z\delta F(z) \\ &= 2(1 - 2z + 2z^2)F(z) > 0 \end{aligned}$$

whenever $0 < z \leq z_0$. Consequently, for $z_0 < z < z_+$

$$\begin{aligned} z(1 + 2F(z) - 4E(z)) - 2F(z) + 2E(z) &= z(1 + 2F(z_0) - 4E(z_0)) - 2F(z_0) + 2E(z_0) \\ &\geq z_0(1 + 2F(z_0) - 4E(z_0)) - 2F(z_0) + 2E(z_0) > 0. \end{aligned}$$

Therefore, there is no solution of (4.25) with $0 < z(x) < z_+$. Furthermore, since $F(z_+) = 1$ and $E(z_+) = \mathbb{E}Z = 1$,

$$1 + 2F(z) - 4E(z) = 1 + 2F(z_+) - 4E(z_+) = -1 < 0$$

once $z \geq z_+$, which contradicts to the second inequality in (4.25). Finally, $2\frac{F(z) - E(z)}{1 + 2F(z) - 4E(z)} = 0$ for $z \leq 0$, hence the only solution of (4.25) is $z = 0$, and thus according to (4.23) we obtain that a unique minimum point of D in the upper left half-plane is $a_1 = (0, 1)$. By the symmetry we conclude that $\text{Argmin}_{x \in \mathbb{R}^2} D(x) = \{a_1, -a_1\}$. Therefore, $\nu_* = \frac{1}{2}(\delta_{a_1} + \delta_{-a_1}) = \mu_1$ is the unique Wasserstein barycenter of P .

Step 2: proof of the lower bound. Consider now a random sample $Z_1, \dots, Z_n \sim P_Z$. A corresponding empirical barycenter is

$$\nu_n := \text{bar}(\mu_{Z_1}, \dots, \mu_{Z_n}).$$

According to what was said above, ν_n is concentrated on the set of minimizers of the function

$$D_n(x) := \frac{1}{n} \sum_{i=1}^n \min \{ \|x - a_{Z_i}\|^2, \|x + a_{Z_i}\|^2 \}$$

Moreover, there always exists a barycenter in form $\nu_n = \frac{1}{2}(\delta_x + \delta_{-x})$, thus from the same scale-location family as all μ_z . Indeed, any symmetric measure concentrated on $\text{Argmin}_{x \in \mathbb{R}^2} D_n(x)$ is an empirical barycenter.

Now we consider $x = \text{argmin}_{x \in \mathbb{R}^2} D_n(x)$ with $x_1 \leq x_2$. First note that if $x_1 = x_2$, then $\min \{ \|x - a_1\|, \|x + a_1\| \} \geq \frac{1}{\sqrt{2}}$. Further we assume $x_1 < x_2$. Let us define

$$F_n(z) := \frac{1}{n} \sum_{i=1}^n \mathbb{1}[Z_i \leq z], \quad E_n(z) := \frac{1}{n} \sum_{i=1}^n Z_i \mathbb{1}[Z_i \leq z].$$

Then condition (4.23) with $z = z(x)$ reads as

$$z = \frac{\bar{Z}_n - 1 + 2F_n(z) - 2E_n(z)}{2\bar{Z}_n - 1 + 2F_n(z) - 4E_n(z)}, \quad (4.26)$$

where $\bar{Z}_n := \frac{1}{n} \sum_{i=1}^n Z_i$.

We are going to show that with probability at least $\frac{1}{8}$ it holds that any z satisfying the above equation (4.26) is larger than $\frac{c}{\log n}$. From the standard CLT we obtain that for large enough n with probability at least $\frac{1}{4}$ one has

$$\Delta_n := \bar{Z}_n - \mathbb{E}Z \geq \frac{\sigma}{2\sqrt{n}},$$

where $\sigma^2 := \text{Var } Z$. Using relative concentration inequalities for indicator functions (see Theorem 5.1 and §5.1.2 in [BBL05]), we obtain that with probability at least $\frac{7}{8}$ simultaneously for all $z \geq 0$ one has

$$\begin{aligned} |F_n(z) - F(z)| &\leq 2\sqrt{F(z) \frac{\log(2n+1) + \log 64}{n}} + 4 \frac{\log(2n+1) + \log 64}{n} \\ &\leq 4\sqrt{z \frac{\log 64(2n+1)}{n}} + 4 \frac{\log 64(2n+1)}{n}. \end{aligned}$$

Here we used that $f^*(z) \leq 2^{3/2}$, thus $F(z) \leq 2^{3/2}z \leq 4z$, and that the shatter coefficient $\mathbb{S}_{\mathcal{F}}(Z_1^{2n}) \leq 2n+1$ for the class $\mathcal{F} := \{z \mapsto \mathbb{1}[z \leq a] : a \in \mathbb{R}\}$. Further, note that

$$|E_n(z) - E(z)| \leq z \sup_{s \leq z} |F_n(s) - F(s)|.$$

Moreover,

$$0 \leq \delta F(z) \leq \exp\left(-\frac{1}{z}\right), \quad 0 \leq \delta E(z) \leq z \exp\left(-\frac{1}{z}\right).$$

Now it is easy to see that there are n_0 and $c > 0$ such that for $n \geq n_0$ with probability at least $\frac{1}{8}$ $\Delta_n \geq \frac{\sigma}{2\sqrt{n}}$ and for all $0 \leq z < \min\left\{\frac{c}{\log n}, z_0\right\}$

$$\begin{aligned} |F_n(z) - F(z)| &< \frac{4}{\sqrt{n}} \left(\sqrt{\frac{c \log 64(2n+1)}{\log n}} + \frac{\log 64(2n_0+1)}{\sqrt{n_0}} \right) \leq \frac{\Delta_n}{20}, \\ |E_n(z) - E(z)| &< z_0 \frac{\Delta_n}{20} \leq \frac{\Delta_n}{60}, \end{aligned}$$

and

$$\delta F(z) < n^{-1/c} \leq \frac{\Delta_n}{20}, \quad \delta E(z) < z_0 n^{-1/c} \leq \frac{\Delta_n}{60}.$$

Therefore,

$$\begin{aligned} 2\bar{Z}_n - 1 + 2F_n(z) - 4E_n(z) &= 1 + 2\Delta_n + 2F(z) - 4E(z) + 2(F_n(z) - F(z)) - 4(E_n(z) - E(z)) \\ &\leq 1 + 2F^*(z) - 4E^*(z) + 2\Delta_n + 4\delta E(z) + 2|F_n(z) - F(z)| + 4|E_n(z) - E(z)| \\ &< 1 + 2F^*(z) - 4E^*(z) + \frac{9}{4}\Delta_n, \end{aligned}$$

and

$$\begin{aligned} \bar{Z}_n - 1 + 2F_n(z) - 2E_n(z) &= \Delta_n + 2F(z) - 2E(z) + 2(F_n(z) - F(z)) - 2(E_n(z) - E(z)) \\ &\geq 2(F^*(z) - E^*(z)) + \Delta_n - 2\delta F(z) - 2|F_n(z) - F(z)| - 2|E_n(z) - E(z)| \\ &> 2(F^*(z) - E^*(z)) + \frac{3}{4}\Delta_n. \end{aligned}$$

Since $z(1 + 2F^*(z) - 4E^*(z)) = 2(F^*(z) - E^*(z))$, the above inequalities yield

$$\begin{aligned} z(2\bar{Z}_n - 1 + 2F_n(z) - 4E_n(z)) &\leq 2(F^*(z) - E^*(z)) + \frac{9z}{4}\Delta_n \\ &\leq 2(F^*(z) - E^*(z)) + \frac{3}{4}\Delta_n < \bar{Z}_n - 1 + 2F_n(z) - 2E_n(z), \end{aligned}$$

which contradicts (4.26). Obviously, for $z < 0$

$$\frac{\bar{Z}_n - 1 + 2F_n(z) - 2E_n(z)}{2\bar{Z}_n - 1 + 2F_n(z) - 4E_n(z)} = \frac{\Delta_n}{1 + 2\Delta_n} > 0 > z.$$

Consequently, any solution z of (4.26) must satisfy $z \geq \min\left\{\frac{c}{\log n}, z_0\right\}$. Once $z = z(x)$, this implies that

$$\min\{\|x - a_1\|, \|x + a_1\|\} \geq \frac{c}{\log n}.$$

Hence $d(\text{supp } \nu_n, \text{supp } \nu_*) \geq \frac{c}{\log n}$, and thus the claim follows. \square

Appendix 4.A Auxiliary results

Lemma 4.A.1. *Let $\|Q'_n - I\| \leq \frac{1}{2}$, with Q'_n coming from (4.17); then*

$$\left\| \hat{\Sigma}_n - \Sigma_n \right\|_1 \leq \beta_n \left[2 \left(\frac{1}{n} \sum_i \|T_i - I\|_F^2 \right)^{1/2} + \beta_n \right],$$

where

$$\beta_n \stackrel{\text{def}}{=} \kappa(Q_*) \left(\frac{\frac{1}{n} \sum_i \|S_i\|}{\|Q_*\|} \right)^{1/2} \|Q'_n - I\|_F,$$

$\kappa(Q_*)$ is the condition number of Q_* and $\|\mathbf{A}\|_1$ is the 1-Schatten (nuclear) norm of an operator \mathbf{A} .

Proof. Note, that for any $(T_i^n - I) \otimes (T_i^n - I)$ the following decomposition holds

$$\begin{aligned} (T_i^n - I) \otimes (T_i^n - I) &= (T_i - I) \otimes (T_i - I) + (T_i^n - T_i) \otimes (T_i - I) \\ &\quad + (T_i - I) \otimes (T_i^n - T_i) + (T_i^n - T_i) \otimes (T_i^n - T_i). \end{aligned}$$

Summing over i yields

$$\begin{aligned} \hat{\Sigma}_n - \Sigma_n &= \frac{1}{n} \sum_i (T_i^n - T_i) \otimes (T_i - I) \\ &\quad + \frac{1}{n} \sum_i (T_i - I) \otimes (T_i^n - T_i) + \frac{1}{n} \sum_i (T_i^n - T_i) \otimes (T_i^n - T_i). \end{aligned} \tag{4.27}$$

Note, that each

$$\|(T_i^n - T_i) \otimes (T_i - I)\|_1 \leq \|T_i^n - T_i\|_F \|T_i - I\|_F.$$

Lemmas 4.2.5 (III) and 4.2.8 yield

$$\begin{aligned} \|T_i^n - T_i\|_F &\leq \frac{1}{1 - \|Q'_n - I\|} \left\| d\mathbf{T}_{Q_*}^{S_i}(Q_n - Q_*) \right\|_F \\ &\leq 2 \left\| Q_*^{-1/2} d\mathbf{T}_{Q_*}^{S_i}(Q'_n - I) Q_*^{-1/2} \right\|_F \leq 2 \frac{\lambda_{\max}(d\mathbf{T}_{Q_*}^{S_i})}{\lambda_{\min}(Q_*)} \|Q'_n - I\|_F \\ &\leq \frac{\lambda_{\max}(S_i^{1/2} Q_* S_i^{1/2})}{\lambda_{\min}(Q_*)} \|Q'_n - I\|_F \leq \kappa(Q_*) \left(\frac{\|S_i\|}{\|Q_*\|} \right)^{1/2} \|Q'_n - I\|_F, \end{aligned}$$

where $d\mathbf{T}_Q^S$ is defined in (4.9). Hence $\frac{1}{n} \sum_i \|T_i^n - T_i\|_F^2 \leq \beta_n^2$. The above expression together with (4.27) and Cauchy–Schwarz inequality lead to the upper bound on $\left\| \hat{\Sigma}_n - \Sigma_n \right\|_1$:

$$\begin{aligned} \left\| \hat{\Sigma}_n - \Sigma_n \right\|_1 &\leq \frac{2}{n} \sum_i \|T_i - I\|_F \|T_i^n - T_i\|_F + \frac{1}{n} \sum_i \|T_i^n - T_i\|_F^2 \\ &\leq 2\beta_n \left(\frac{1}{n} \sum_i \|T_i - I\|_F^2 \right)^{1/2} + \beta_n^2. \end{aligned}$$

□

Further we present concentration of \mathbf{F}_n around \mathbf{F} . Denote as $\|X\|_{\psi_2}$ an Orlicz norm with Young function $\psi_2(x) = e^{x^2} - 1$, i.e.

$$\|X\|_{\psi_2} \stackrel{\text{def}}{=} \inf\{c > 0 : \mathbb{E} \psi_2(|X|/c) \leq 1\}.$$

Then sub-Gaussianity of a r.v. X is equivalent to $\|X\|_{\psi_2} < \infty$ and it ensures

$$\text{Var}(X) \leq \sqrt{2} \|X\|_{\psi_2}.$$

Proposition 4.A.2 (Concentration of \mathbf{F}'_n , Proposition 2 in [Kol11]). *Let \mathbf{F}'_n , \mathbf{F}' , and \mathbf{dt}_Q^S be defined as (4.21), (4.22), and (4.9), respectively. There exists a constant $C > 0$ such that for all $t > 0$ it holds with probability at least $1 - e^{-t}$*

$$\|\mathbf{F}'_n - \mathbf{F}'\| \leq \gamma_n(t), \quad \gamma_n(t) \stackrel{\text{def}}{=} C \max \left(\sigma_F \sqrt{\frac{t + \log(2m)}{n}}, U \sqrt{\log \left(\frac{U}{\sigma_F} \right)^{\frac{t + \log(2m)}{n}}} \right),$$

where $\sigma_F^2 \stackrel{\text{def}}{=} \left\| \mathbb{E} \left(\mathbf{dt}_{Q_*}^S - \mathbf{F}' \right)^2 \right\|$, $U \stackrel{\text{def}}{=} \left\| \left\| \mathbf{dt}_{Q_*}^S - \mathbf{F}' \right\| \right\|_{\psi_2}$.

Lemma 4.A.3. *The above constants can be estimated as follows:*

$$\sigma_F \leq \frac{\|Q_*\|^{1/2}}{2} (\mathbb{E}\|S\|)^{1/2}, \quad U \leq \frac{3}{2} \|Q_*\|^{1/2} \|\|S\|\|_{\psi_1}^{1/2},$$

where $\psi_1(x) = e^x - 1$.

Proof. By Corollary 4.2.7 we obtain

$$\sigma_F^2 \stackrel{\text{def}}{=} \left\| \mathbb{E} \left(\mathbf{dt}_{Q_*}^S - \mathbf{F}' \right)^2 \right\| \leq \mathbb{E} \|\mathbf{dt}_{Q_*}^S\|^2 \leq \frac{\|Q_*\|}{4} \mathbb{E}\|S\|$$

and (due to properties of Orlicz norm)

$$\begin{aligned} U &\stackrel{\text{def}}{=} \left\| \left\| \mathbf{dt}_{Q_*}^S - \mathbf{F}' \right\| \right\|_{\psi_2} \leq \frac{\|\mathbf{F}'\|}{\sqrt{\ln 2}} + \left\| \left\| \mathbf{dt}_{Q_*}^S \right\| \right\|_{\psi_2} \\ &\leq \frac{\|Q_*\|^{1/2}}{2} \left[2 \mathbb{E}\|S\|^{1/2} + \|\|S\|^{1/2}\|_{\psi_2} \right] \\ &\leq \frac{\|Q_*\|^{1/2}}{2} \left[2 (\mathbb{E}\|S\|)^{1/2} + \|\|S\|\|_{\psi_1}^{1/2} \right] \\ &\leq \frac{3}{2} \|Q_*\|^{1/2} \|\|S\|\|_{\psi_1}^{1/2}. \end{aligned}$$

□

The next proposition ensures the concentration of \bar{T}_n .

Proposition 4.A.4 (Concentration of \bar{T}_n ; [HKZ12], Theorem 1). *Under Assumption 4.3 it holds*

$$\mathbb{P} \left\{ \left\| \mathbf{I}_M(\bar{T}_n - I) \right\|_F \geq \frac{\sigma_T}{\sqrt{n}} (\sqrt{m} + t) \right\} \leq e^{-t^2/2} \quad \text{for any } t \geq 0.$$

Lemma 4.A.5 (Sub-exponential tail bounds). *Suppose that X is sub-exponential with parameters ν, b . Then*

$$\mathbb{P} \{ X \geq \mathbb{E} X + t \} \leq \begin{cases} \exp(-\frac{t^2}{2\nu^2}), & \text{if } 0 \leq t \leq \frac{\nu^2}{b}, \\ \exp(-\frac{t}{2b}), & \text{if } t \geq \frac{\nu^2}{b}. \end{cases}$$

Chapter 5

Entropic-regularized barycenters

5.1 Introduction

In this chapter we again consider the 2-Wasserstein space over \mathbb{R}^d . As was mentioned in the previous chapter, establishing a central limit theorem (CLT) for Wasserstein barycenters is a nontrivial problem, and such results are known only in very particular cases (dimension one or the case of a scale-location family, see the last chapter). 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 [AC11]). The support of a Wasserstein barycenter is indeed an unknown of the problem and very little is known about its regularity (see [SW16] for counter-examples to convexity). The free-boundary aspect of Wasserstein barycenters actually makes the dependence of the barycenter on the sample possibly nonsmooth and thus prevents one from using a delta method.

Bigot, Cazelles, and Papadakis in [BCP19] observed that when one discretizes continuous measures, the corresponding (discrete) barycenters exhibit strong oscillations and proposed to use an entropic penalization to rule out such discretization artefacts (recall that such penalized barycenters were also considered in a more general setting in Chapter 3). Once one adds an entropic term, the free-boundary aspect of the unregularized Wasserstein problem disappears and one can expect regularity and quite strong estimates by PDE arguments. The objective of this chapter is to investigate the regularizing effect of the entropic penalty term on 2-Wasserstein barycenters. 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 equations). We will then consider again 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 the Wasserstein distance, but also for Sobolev norms) and more importantly, under suitable additional assumptions, we will obtain a CLT.

In Section 5.2, 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 5.3 where we treat the Gaussian case as a simple application. Section 5.4 is devoted to further properties: global moment and Sobolev bounds, strong stability and a maximum principle. Higher regularity is considered in Section 5.5 in the bounded case. Section 5.6 deals with asymptotic results for entropic barycenters of empirical measures with a law of large numbers and a CLT. Finally, the appendix gathers some material related to the linearization of Monge–Ampère equations and to auxiliary probability results which are used in the proof of our CLT.

5.2 Setting, assumptions and preliminaries

Recall that $\mathcal{P}_2(\mathbb{R}^d)$ is the set of Borel probability measures on \mathbb{R}^d having a finite second moment, and equipped with the 2-Wasserstein metric W_2 given by (2.2):

$$W_2^2(\mu, \nu) := \inf_{\gamma \in \Pi(\mu, \nu)} \int \|x - y\|^2 d\gamma(x, y), \quad \mu, \nu \in \mathcal{P}_2(X),$$

it forms the 2-Wasserstein space over \mathbb{R}^d . The Kantorovich duality formula (see Subsection 2.2) enables one to express $\frac{1}{2}W_2^2(\mu, \nu)$ as the maximum of

$$\int_{\mathbb{R}^d} u d\mu + \int_{\mathbb{R}^d} v d\nu$$

among pairs of potentials u and v such that

$$u(x) + v(y) \leq \frac{1}{2}\|x - y\|^2 \quad \forall x, y \in \mathbb{R}^d.$$

Moreover, optimal u and v can be chosen such that Brenier potentials

$$\varphi(x) := \frac{1}{2}\|x\|^2 - u(x), \quad \psi(y) := \frac{1}{2}\|y\|^2 - v(y)$$

are Legendre transforms of each other:

$$\varphi = \psi^*, \quad \psi = \varphi^*.$$

We denote by u_μ^ν any Kantorovich potential from μ to ν and likewise denote by $\varphi_\mu^\nu := \frac{1}{2}\|\cdot\|^2 - u_\mu^\nu$ the corresponding Brenier potential. Moreover, if μ is absolutely continuous w.r.t. the Lebesgue measure, then by Proposition 2.2.10 the optimal transport map $T_\mu^\nu = \nabla \varphi_\mu^\nu$ from μ to ν is unique up to a μ -negligible set. In particular, if μ is absolutely continuous and almost everywhere strictly positive, the Brenier potential φ_μ^ν is uniquely defined on any connected component of $\text{int } \Omega$ up to an additive constant.

Now we give ourselves a Borel (w.r.t. τ_w) probability measure P on $\mathcal{P}_2(\mathbb{R}^d)$ such that

$$\int_{\mathcal{P}_2(\mathbb{R}^d)} m_2(\nu) dP(\nu) < \infty, \quad (5.1)$$

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

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

Given a regularization parameter $\lambda > 0$ and a Borel set $\Omega \subset \mathbb{R}^d$ of positive Lebesgue measure (of particular interest is the case where $\Omega = \mathbb{R}^d$ or Ω is convex), we consider the following problem (which was introduced in [BCP19] as an entropic regularization of the Wasserstein barycenter problem):

$$\mathcal{V}_{\lambda, \Omega}(\rho; P) := \frac{1}{2} \int W_2^2(\rho, \nu) dP(\nu) + \lambda \text{Ent}_\Omega(\rho) \rightarrow \min_{\rho \in \mathcal{P}_2(\mathbb{R}^d)}, \quad (5.2)$$

where Ent_Ω is defined for every $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ by

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

Note that this is nothing but problem (3.5) from Chapter 3 with $G = \lambda \text{Ent}_\Omega$. If $\Omega = \mathbb{R}^d$ we simply denote $\text{Ent}_{\mathbb{R}^d} = \text{Ent}$ and $\mathcal{V}_{\lambda, \mathbb{R}^d} = \mathcal{V}_\lambda$. When considering $\rho \in \mathcal{P}(\mathbb{R}^d)$ absolutely continuous w.r.t. the Lebesgue measure, we shall slightly abuse notations and use the same notation for its density.

Example 5.2.1. If $\Omega = \mathbb{R}^d$ and $P = \sum_{i=1}^I p_i \delta_{x_i}$ is concentrated on Dirac masses, (5.2) 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

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

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

Lemma 5.2.2. *There is a constant $C > 0$ such that for any $\rho \in \mathcal{P}_2(\mathbb{R}^d)$*

$$\text{Ent}(\rho) \geq -\frac{d}{2} \log m_2(\rho) - Cd.$$

Moreover, for any measurable $A \subset \mathbb{R}^d$ with $|A| < 1$ it holds that

$$\rho(A) \leq \left(\text{Ent}(\rho) + \frac{d}{2} (\log m_2(\rho))_+ + Cd \right) \frac{1}{\log(1/|A|)}.$$

Remark 5.2.3. The second claim ensures the uniform integrability of the set $\{\rho \in \mathcal{P}_2(\mathbb{R}^d) : m_2(\rho) \leq C, \text{Ent}(\rho) \leq C\}$ with any $C > 0$. If $|\Omega| < \infty$, then the boundedness of the entropy is enough, but in the general case it becomes trickier since $\rho \log \rho$ can be negative.

Proof. Take the Gaussian density $g := \mathcal{N}(0, \sigma^2 I)$. Then

$$0 \leq KL(\rho, g) := \int \rho \log \frac{\rho}{g} = \text{Ent}(\rho) + \frac{m_2(\rho)}{2\sigma^2} + \frac{d}{2} \log(2\pi\sigma^2).$$

The r.h.s. attains minimum at $\sigma = \sqrt{m_2(\rho)/d}$, which gives us

$$\begin{aligned} \text{Ent}(\rho) &\geq -\frac{d}{2} \left[1 + \log \left(\frac{2\pi m_2(\rho)}{d} \right) \right] \\ &= -\frac{d}{2} \log m_2(\rho) - \frac{d}{2} \log(\pi e) + \frac{d}{2} \log \frac{d}{2} \\ &\geq -\frac{d}{2} \log m_2(\rho) - d \left(\frac{\log(\pi e)}{2} + \frac{1}{e} \right). \end{aligned} \tag{5.3}$$

Here we used that $x \log x \geq -\frac{1}{e} \geq -\frac{d}{e}$ for all $x \geq 0$.

Now consider $A \subset \mathbb{R}^d$ with $|A| < 1$. Define $B := \mathbb{R}^d \setminus A$ and the density $\rho_B := \frac{\rho \mathbb{1}_B}{\rho(B)}$. Using Jensen's inequality we obtain

$$\begin{aligned} \text{Ent}(\rho) &= \rho(B) \int_B \rho_B \log(\rho_B \rho(B)) + \int_A \rho \log \rho \\ &\geq \rho(B) \text{Ent}(\rho_B) + \rho(B) \log \rho(B) + \rho(A) \log \frac{\rho(A)}{|A|} \\ &= \rho(B) \text{Ent}(\rho_B) + \rho(A) \log \frac{1}{|A|} + (\rho(A) \log \rho(A) + \rho(B) \log \rho(B)) \end{aligned}$$

Note that $\rho(B) = 1 - \rho(A)$ and $p \log p + (1-p) \log(1-p) \geq -\log 2$ for any $p \in [0, 1]$. Furthermore, due to (5.3)

$$\begin{aligned} -\rho(B) \text{Ent}(\rho_B) &\leq \frac{d}{2} \rho(B) \log \left(\frac{2\pi e m_2(\rho_B)}{d} \right) \\ &\leq \frac{d}{2} \rho(B) \log \left(\frac{2\pi e m_2(\rho)}{d \rho(B)} \right) \\ &= \frac{d}{2} \rho(B) \log(\pi e m_2(\rho)) - \frac{d}{2} \rho(B) \log \left(\frac{d \rho(B)}{2} \right) \\ &\leq \frac{d}{2} (\log m_2(\rho))_+ + \frac{d}{2} \log(\pi e) + \frac{1}{e}. \end{aligned}$$

Finally, we get

$$\begin{aligned} \rho(A) \log \frac{1}{|A|} &\leq \text{Ent}(\rho) - \rho(B) \text{Ent}(\rho_B) + \log 2 \\ &\leq \text{Ent}(\rho) + \frac{d}{2} (\log m_2(\rho))_+ + d \left(\frac{\log(\pi e)}{2} + \frac{1}{e} + \log 2 \right). \end{aligned}$$

□

Corollary 5.2.4. *For any $R > 0$ the functional Ent_Ω is l.s.c. w.r.t. the narrow convergence on the closed ball $\bar{B}_R^{W_2}(\delta_0) = \{\rho \in \mathcal{P}(\mathbb{R}^d) : m_2(\rho) \leq R^2\}$.*

Remark 5.2.5. Again, if $|\Omega| < \infty$, then the uniform integrability and the Dunford–Pettis theorem [Bel15, Theorem 3] immediately yield that Ent_Ω is l.s.c. w.r.t. the narrow convergence on the whole space $\mathcal{P}(\mathbb{R}^d)$.

Proof. Let $\rho_n \rightharpoonup \rho$, $m_2(\rho_n) \leq R^2$. Then $\text{Ent}(\rho) \leq \liminf \text{Ent}(\rho_n)$, see e.g. the appendix of [Car+17]. W.l.o.g. assume $\text{Ent}(\rho_n) \leq E < \infty$ for all n . It remains to show that $\rho(\Omega) = 1$. By the above lemma there is a constant $C > 0$ such that

$$\rho_n(A) \leq \frac{C}{\log(1/|A|)} \quad \forall n \in \mathbb{N}$$

once $|A| < 1$. For any $0 < \varepsilon < 1$ one can find a closed set $F_\varepsilon \subset \Omega$ such that $|\Omega \setminus F_\varepsilon| \leq \varepsilon$. Then

$$\rho(F_\varepsilon) \geq \limsup \rho_n(F_\varepsilon) = 1 - \liminf \rho_n(\Omega \setminus F_\varepsilon) \geq 1 - \frac{C}{\log(1/\varepsilon)} \rightarrow 1 \quad \text{as } \varepsilon \rightarrow 0.$$

Therefore, $\rho(\Omega) = 1$ and hence

$$\text{Ent}_\Omega(\rho) = \text{Ent}(\rho) \leq \liminf \text{Ent}(\rho_n) = \liminf \text{Ent}_\Omega(\rho_n).$$

□

Now we can conclude that there exists a solution of (5.2), i.e. a corresponding regularized Fréchet barycenter in terms of Chapter 3.

Proposition 5.2.6. *Assume (5.1), then problem (5.2) admits a unique solution.*

Proof. Existence of a solution follows immediately from Proposition 3.5.1: indeed, Lemma 5.2.2 and Corollary 5.2.4 ensure that Ent_Ω satisfies assumptions on a penalty functional. The uniqueness of the minimizer follows from the strict convexity of the entropy and the convexity of the squared 2-Wasserstein distance. □

Entropic-Wasserstein barycenters can therefore be defined as follows.

Definition 5.1. The unique solution $\bar{\rho}$ of (5.2) is called the entropic-Wasserstein barycenter of P w.r.t. λ and Ω and denoted $\text{bar}_{\lambda, \Omega}(P)$ and simply $\text{bar}_\lambda(P)$ if $\Omega = \mathbb{R}^d$.

Remark 5.2.7. If Ω is open and $\lambda_n \rightarrow 0$, then $G_n := \lambda_n \text{Ent}_\Omega$ and

$$G(\mu) := \begin{cases} 0, & \text{if } \mu(\bar{\Omega}) = 1, \\ +\infty, & \text{otherwise} \end{cases}$$

satisfy assumptions of Theorem 3.5.2. Hence, up to extraction of a subsequence,

$$W_2(\text{bar}_{\lambda_n, \Omega}(P), \text{bar}_{0, \bar{\Omega}}(P)) \rightarrow 0,$$

where $\text{bar}_{0, \bar{\Omega}}(P) \in \text{Bar}_G(P)$. Moreover, taking the closure of Ω does not change the entropic-Wasserstein barycenter, thus we have also

$$W_2(\text{bar}_{\lambda_n, \bar{\Omega}}(P), \text{bar}_{0, \bar{\Omega}}(P)) \rightarrow 0.$$

We can immediately state some basic invariance properties of entropic-Wasserstein barycenters in case $\Omega = \mathbb{R}^d$. For instance, if we shift all measures ν 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 Ω is invariant to). The next proposition shows that translations can actually be “factored out” from the barycenter.

Proposition 5.2.8. *Let $\Omega = \mathbb{R}^d$, $\lambda > 0$, P be a measure on $\mathcal{P}_2(\mathbb{R}^d)$ satisfying condition (5.1), and $\bar{\rho} = \text{bar}_\lambda(P)$. Fix a measurable map $\mathbf{s} \in L^2(P; \mathbb{R}^d)$ and define a measure $P_{\mathbf{s}} := (\nu \mapsto \nu + \mathbf{s}(\nu))_{\#}P$, where $\nu \oplus \mathbf{s} := (x \mapsto \mathbf{s}(x) + x)_{\#}\nu$ for all $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ and $\mathbf{s} \in \mathbb{R}^d$. Then $\text{bar}_\lambda(P_{\mathbf{s}}) = \bar{\rho} \oplus \bar{\mathbf{s}}$, with $\bar{\mathbf{s}} := \int \mathbf{s}(\nu) dP(\nu)$.*

Proof. Note that it is enough to consider the case $\mathbb{E}_\nu[X] = 0$ for P -a.e. ν , where $\mathbb{E}_\nu[X] = \int_{\mathbb{R}^d} x d\nu(x)$ 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 $a \in \mathbb{R}^d$

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

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 $\mathcal{V}_\lambda(\rho; P)$ over ρ '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 5.2.9. Note that, when $\Omega = \mathbb{R}^d$, a useful corollary of Proposition 5.2.8 is that the expectation w.r.t. the entropic-Wasserstein barycenter is the average of the expectations:

$$\mathbb{E}_{\bar{\rho}}[X] = \int \mathbb{E}_\nu[X] dP(\nu).$$

5.3 Characterization

From now on we assume that Ω is open, unless explicitly stated otherwise. The entropic term forces the regularized barycenter to be everywhere positive. Indeed, arguing in a similar way as in Lemma 8.6 from [San15], we arrive at:

Lemma 5.3.1. *Let $\bar{\rho} := \text{bar}_{\lambda, \Omega}(P)$ then $\bar{\rho} > 0$ a.e. on Ω and $\log(\bar{\rho}) \in L_{\text{loc}}^1(\Omega)$.*

Proof. Let g be the standard Gaussian density, scaled so as to give mass 1 to Ω . 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

$$\lambda [\text{Ent}_\Omega(\rho_t) - \text{Ent}_\Omega(\bar{\rho})] \geq \frac{t}{2} \int [W_2^2(\bar{\rho}, \nu) - W_2^2(g, \nu)] dP(\nu),$$

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

$$\frac{1}{t} (\text{Ent}_\Omega(\rho_t) - \text{Ent}_\Omega(\bar{\rho})) \geq C. \quad (5.4)$$

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 (5.4) and letting $t \rightarrow 0^+$, we immediately see that $|\{\bar{\rho} = 0\}| = 0$.

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 Ω . Calling μ 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

If Ω is connected, then the fact that the regularized barycenter is everywhere positive guarantees uniqueness (up to a constant) of the Brenier potential between $\bar{\rho}$ and $\nu \in \mathcal{P}_2(\mathbb{R}^d)$, and thus its stability w.r.t. changes of $\bar{\rho}$. However, the case of disconnected Ω seems to be less studied, and for the sake of completeness let us provide in the next lemmas some results based on the analysis of convex potentials φ_ρ^ν .

Lemma 5.3.2. *Let $\mu \in \mathcal{P}(\mathbb{R}^d)$. Then for any compact set $K \subset \Omega$ and any convex function $\varphi: \Omega \rightarrow \mathbb{R}$ one has*

$$\text{osc}_K \varphi := \max_K \varphi - \min_K \varphi \leq \frac{\text{diam}(K) + r}{\inf_{x \in K_{r/2}} \mu(B_{r/2}(x))} \int_\Omega \|\nabla \varphi\| \, d\mu, \quad (5.5)$$

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

$$\text{Lip}(\varphi|_K) \leq \frac{2 \text{diam}(K) + 3r}{r \inf_{x \in K_{3r/4}} \mu(B_{r/4}(x))} \int_\Omega \|\nabla \varphi\| \, d\mu. \quad (5.6)$$

Remark 5.3.3. Notice that Ω is not necessarily convex, thus we say a function φ on Ω is convex if it can be extended to a convex function on \mathbb{R}^d (possibly making value $+\infty$), cf. [Fig17].

Proof. Let $x_1 \in \text{argmax}_K \varphi$, $x_0 \in \text{argmin}_K \varphi$, and $w \in \partial\varphi(x_1)$. Then for any $x \in \Omega$ and $z \in \partial\varphi(x)$ one has

$$\varphi(x_0) + \langle z, x - x_0 \rangle \geq \varphi(x) \geq \varphi(x_1) + \langle w, x - x_1 \rangle,$$

and thus the Cauchy–Schwarz inequality yields

$$\|z\| \geq \frac{\text{osc}_K \varphi + \langle w, x - x_1 \rangle}{\|x - x_0\|}.$$

Therefore,

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

where we have set $W_r(x, w) := \{y \in B_r(x) : \langle w, y - x \rangle \geq 0\}$ and used the fact that $B_{r/2}\left(x + \frac{rw}{2\|w\|}\right) \subset W_r(x, w)$. Finally, the first claim follows from the inclusion $x + \frac{rw}{2\|w\|} \in K_{r/2}$.

To prove (5.6) we apply (5.5) to $K_{r/2}$, which yields

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

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

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

Therefore,

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

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

Corollary 5.3.4. *Let $\rho \in \mathcal{P}_2(\Omega)$ have a positive density, $\rho_n \in \mathcal{P}_2(\mathbb{R}^d)$ be such that $W_2(\rho_n, \rho) \rightarrow 0$, and $\nu_n \in \mathcal{P}_2(\mathbb{R}^d)$ be such that $W_2(\nu_n, \nu) \rightarrow 0$ for some ν . Fix an open connected $U \subset \subset \Omega$ and $x_0 \in U$. If $\varphi_{\rho_n}^{\nu_n}$ is a Brenier potential between ρ_n and ν_n , for all $n \in \mathbb{N}$, then*

$$\varphi_{\rho_n}^{\nu_n} - \varphi_{\rho_n}^{\nu_n}(x_0) \rightrightarrows \varphi_{\rho}^{\nu} \quad \text{on } U,$$

where φ is the uniquely defined on U Brenier potential between ρ and ν , such that $\varphi_{\rho}^{\nu}(x_0) = 0$, and \rightrightarrows stands for the uniform convergence. Moreover, $\nabla \varphi_{\rho_n}^{\nu_n} \rightarrow \nabla \varphi_{\rho}^{\nu}$ a.e. on Ω .

Proof. Let us denote $\varphi_n := \varphi_{\rho_n}^{\nu_n}$ and $\varphi := \varphi_{\rho}^{\nu}$. Since any optimal transport plan from ρ_n to ν_n is concentrated on the graph of φ_n , we have

$$\int_{\Omega} \|\nabla \varphi_n\| \, d\rho_n \leq \int_{\Omega} \|y\| \, d\nu_n = m_1(\nu_n) \rightarrow m_1(\nu).$$

In the same way, since $\nabla \varphi$ is defined a.e. on Ω ,

$$\int_{\Omega} \|\nabla \varphi\| \, d\rho = \int_{\Omega} \|y\| \, d\nu = m_1(\nu).$$

Furthermore, $\inf_{x \in U_{3r/4}} \rho(B_{r/4}(x)) > 0$ since $\rho > 0$, where $0 < r \leq d(U, \partial\Omega) > 0$, thus

$$\liminf \inf_{x \in U_{3r/4}} \rho_n(B_{r/4}(x)) > 0,$$

because $\rho_n \rightarrow \rho$. Then the above lemma and the Arzelà–Ascoli theorem yield that, up to a subsequence,

$$\varphi_n - \varphi_n(x_0) \rightrightarrows \psi \quad \text{on } U$$

for some convex ψ , $\psi(x_0) = 0$. Consequently, $\nabla \varphi_n \rightarrow \nabla \psi$ a.e. on U (recall that ψ and all φ_n are differentiable a.e.) and, moreover, for a.e. $x \in U$

$$d(\nabla \psi(x), \partial\varphi_n(y)) \rightarrow 0 \quad \text{as } y \rightarrow x, n \rightarrow \infty.$$

At the same time, $d(\nabla \varphi(x), \partial\varphi(y)) \rightarrow 0$ as $y \rightarrow x$ for a.e. $x \in U$. Combining this with the stability of optimal transport plans (Proposition 2.2.8) and the uniqueness of Brenier's map we conclude that $\nabla \psi = \nabla \varphi$ a.e. on U , hence $\psi = \varphi$ on U due to the connectedness of U . Extension to the whole Ω is trivial. \square

The uniqueness of the Kantorovich potential between $\bar{\rho}$ and ν in the case of connected Ω is well-known to be very useful in terms of the differentiability of $\mu \mapsto W_2^2(\mu, \nu)$ and $\mu \mapsto \int W_2^2(\mu, \nu) dP(\nu)$ at $\mu = \bar{\rho}$, as expressed in Lemma 5.3.5 below. This is a slight generalization of Proposition 7.14 in [San15], adapted to the case of unbounded domain.

Lemma 5.3.5. *Let Ω be connected, $\bar{\rho} := \text{bar}_{\lambda, \Omega}(P)$, and, given $\nu \in \mathcal{P}_2(\mathbb{R}^d)$, let u_ρ^ν be the (unique on Ω , up to an additive constant) Kantorovich potential between $\bar{\rho}$ and ν . If $\mu \in L^1(\Omega)$ is a probability density such that $\mu - \bar{\rho}$ has compact support in Ω , then defining $\rho_\varepsilon := \bar{\rho} + \varepsilon(\mu - \bar{\rho})$ for $\varepsilon \in (0, \frac{1}{2})$ we have*

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

and

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

Proof. Let us shorten notations by defining

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

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

$$\int_K u_\varepsilon d(\mu - \bar{\rho}) \geq \frac{1}{2\varepsilon} [W_2^2(\rho_\varepsilon, \nu) - W_2^2(\bar{\rho}, \nu)] \geq \int_K u d(\mu - \bar{\rho}). \quad (5.7)$$

Since $W_2^2(\rho_\varepsilon, \bar{\rho}) \leq \varepsilon W_2^2(\mu, \bar{\rho}) \rightarrow 0$ as $\varepsilon \rightarrow 0$, Corollary 5.3.4 yields that $u_\varepsilon \rightrightarrows u$ on K . Passing to the limit in (5.7) gives us the first claim of the lemma.

Now observe that since $(\nabla \varphi_\varepsilon)_{\#} \rho_\varepsilon = \nu$ and $\varepsilon < \frac{1}{2}$, we have

$$\int_{\Omega} \|\nabla \varphi_\varepsilon\| \bar{\rho} \leq 2 \int_{\Omega} \|\nabla \varphi_\varepsilon\| \rho_\varepsilon = 2m_1(\nu). \quad (5.8)$$

Set

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

and note that it follows from (5.7)–(5.8) and Lemma 5.3.2 that $|\theta_\varepsilon(\nu)|$ can be bounded by an affine function of $m_1(\nu)$, the desired result therefore follows from (5.1), Lebesgue's dominated convergence theorem and the first claim. \square

We are now in position to characterize the regularized barycenter.

Theorem 5.3.6. *Let $\bar{\rho} \in \mathcal{P}_2(\Omega)$, then $\bar{\rho} = \text{bar}_{\lambda, \Omega}(P)$ if and only if there is a measurable choice of Brenier potentials φ_ρ^ν such that $\bar{\rho}$ has a continuous density given by*

$$\bar{\rho}(x) = \exp\left(-\frac{1}{2\lambda} \|x\|^2 + \frac{1}{\lambda} \int \varphi_\rho^\nu(x) dP(\nu)\right) \quad (5.9)$$

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

$$x + \lambda \nabla \log(\bar{\rho})(x) = \int \nabla \varphi_\rho^\nu(x) dP(\nu). \quad (5.10)$$

Proof. We start with proving (5.9).

Sufficiency. Assume that $\bar{\rho} \in \mathcal{P}_2(\mathbb{R}^d)$ satisfies (5.9), and let $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ be such that $\text{Ent}_\Omega(\mu) < \infty$. Firstly, using the convexity of the entropy we obtain

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

Secondly, by the Kantorovich duality formula and the fact that $u_\rho^\nu := \frac{1}{2}\|\cdot\|^2 - \varphi_\rho^\nu$ is a Kantorovich potential between $\bar{\rho}$ and ν , we get

$$\frac{1}{2}W_2^2(\mu, \nu) \geq \frac{1}{2}W_2^2(\bar{\rho}, \nu) + \int_{\Omega} u_\rho^\nu d(\mu - \bar{\rho}).$$

Combining the above inequalities, observing that (5.9) means that $\lambda \log \bar{\rho} + \int u_\rho^\nu dP(\nu) = 0$, and using Fubini's theorem, we thus get

$$\mathcal{V}_{\lambda, \Omega}(\mu; P) \geq \mathcal{V}_{\lambda, \Omega}(\bar{\rho}; P),$$

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

Necessity. Step 1: connected Ω . Fix a compact with nonempty interior subset K of Ω and normalize the (unique) dual potential u_ρ^ν such that it has minimum 0 on K . Then, arguing as in the proof of Lemma 5.3.5, there is a constant C_K such that $\|u_\rho^\nu\|_{L^\infty(K)} \leq C_K(1 + m_2(\nu))$ so that the (semi-concave) potential

$$x \mapsto U(x) := \int u_\rho^\nu(x) dP(\nu)$$

is bounded on K . Now we claim that $V := \lambda \log(\bar{\rho}) + U$ (which is integrable on K thanks to Lemma 5.3.1) coincides Lebesgue a.e. with a constant on K (which taking an exhaustive sequence of compact subsets of Ω will enable to find normalizing constants for φ_ρ^ν that do not depend on K and therefore prove (5.9)). 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

$$V \geq \alpha + \delta \text{ a.e. on } K_1, \quad V \leq \alpha - \delta \text{ a.e. on } K_2. \quad (5.11)$$

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

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

With Lemma 5.3.5, the construction of μ , and (5.11), this yields

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

contradicting the optimality of $\bar{\rho}$.

Step 2: general case. Now consider a general open Ω . Take connected open sets $\Omega_n \subset \mathbb{R}^d$ such that $\Omega \subset \Omega_n$ and $|\Omega_n \setminus \Omega| \rightarrow 0$. Let $\bar{\rho}_n := \text{bar}_{\lambda, \Omega_n}(P)$, then Lemma 5.2.2 allows us to apply Theorem 3.5.2, which yields that $W_2(\bar{\rho}_n, \bar{\rho}) \rightarrow 0$. Moreover, according to Step 1 and Lemma 5.3.2 all $\log \bar{\rho}_n$ are locally Lipschitz continuous uniformly in n , hence $\bar{\rho}_n \rightarrow \bar{\rho} > 0$ implies that $\log \bar{\rho}_n$ locally uniformly converge to (the continuous version of) $\log \bar{\rho}$.

Now take a dense countable subset $S = \{x_k\}_{k \in \mathbb{N}}$ of Ω and define functions

$$f_n^k(\nu) := \frac{\varphi_{\bar{\rho}_n}^\nu(x_k)}{m_1(\nu)}, \quad \nu \in \mathcal{P}_2(\mathbb{R}^d).$$

Let $\varphi_{\bar{\rho}_n}^\nu$ be normalized in such way that $\varphi_{\bar{\rho}_n}^\nu(x_0) = c_n = \lambda \log \bar{\rho}_n(x_0) + \frac{\|x_0\|^2}{2}$ for all $\nu \in \mathcal{P}_2(\mathbb{R}^d)$, $n \in \mathbb{N}$, where $x_0 \in \Omega$ is a fixed point. From the stability it follows that every f_n^k is measurable,

and Lemma 5.3.2 ensures that $f_n^k \in L^\infty(P)$. Moreover, since $\bar{\rho}_n(x_0) \rightarrow \bar{\rho}(x_0) > 0$, then c_n are bounded, hence $\{f_n^k\}_{n \in \mathbb{N}}$ is uniformly bounded for every k . By the Banach–Alaoglu theorem and the diagonal extraction argument there is a subsequence such that $f_n^k \rightharpoonup^* f^k \in L^\infty(P)$ for all $k \in \mathbb{N}$ (without relabelling). Define

$$\psi^\nu(x_k) := m_1(\nu) f^k(\nu), \quad \nu \in \mathcal{P}_2(\mathbb{R}^d), \quad k \in \mathbb{N}.$$

Note that if x_k and x_j belong to the same connected component of Ω , then by Corollary 5.3.4

$$f_n^k(\nu) - f_n^j(\nu) \rightarrow \frac{\varphi_{\bar{\rho}}^\nu(x_k) - \varphi_{\bar{\rho}}^\nu(x_j)}{m_1(\nu)} \quad \forall \nu \in \mathcal{P}_2(\mathbb{R}^d).$$

Therefore, for P -a.e. ν on any connected component $\psi^\nu(x_k)$ coincides with $\varphi_{\bar{\rho}}^\nu(x_k)$ for all k , up to an additive constant, hence one can extend ψ^ν to every connected component of Ω by continuity.

Now consider $x_{k_0}, \dots, x_{k_m} \in S$ and $(w_1, \dots, w_m) \in \Delta^{m-1}$ such that $x_{k_0} = \sum_{i=1}^m w_i x_{k_i}$. The convexity of $\varphi_{\bar{\rho}_n}^\nu$ yields that

$$f_n^{k_0} \leq \sum_{i=1}^m w_i f_n^{k_i} \quad \text{for all } n \in \mathbb{N},$$

hence

$$\psi^\nu(x_{k_0}) := m_1(\nu) f_n^{k_0}(\nu) \leq m_1(\nu) \sum_{i=1}^m w_i f_n^{k_i}(\nu) =: \sum_{i=1}^m w_i \psi^\nu(x_{k_i}) \quad \text{for } P\text{-a.e. } \nu.$$

Since there is a countable set of these inequalities and due to the continuity of ψ^ν , this is enough to ensure that it is convex (in the sense of Remark 5.3.3) for P -a.e. ν . Hence $\psi^\nu = \varphi_{\bar{\rho}}^\nu$ for P -a.e. ν . Finally, since $\int m_1(\nu) dP(\nu) < \infty$, we obtain that for all $k \in \mathbb{N}$

$$\begin{aligned} \lambda \log \bar{\rho}_n(x_k) + \frac{\|x_k\|^2}{2} &= \int \varphi_{\bar{\rho}_n}^\nu(x_k) dP(\nu) =: \int m_1(\nu) f_n^k(\nu) dP(\nu) \\ &\rightarrow \int m_1(\nu) f^k(\nu) dP(\nu) =: \int \psi^\nu(x_k) dP(\nu). \end{aligned}$$

As $\log \bar{\rho}_n$ locally uniformly converge to $\log \bar{\rho}$ we conclude that

$$\lambda \log \bar{\rho} + \frac{\|\cdot\|^2}{2} = \int \psi^\nu dP(\nu) \quad \text{in } \Omega.$$

Proof of (5.10). Since

$$\Phi := \int \varphi_{\bar{\rho}}^\nu dP(\nu)$$

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 Φ it also has to be a differentiability point of $\varphi_{\bar{\rho}}^\nu$ for P -almost every ν . Indeed, assume that Φ 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_ν and q_ν in $\partial \varphi_{\bar{\rho}}^\nu(x)$ 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 $(q_\nu, p_\nu) \in \partial \varphi_{\bar{\rho}}^\nu(x)^2$ 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

$$\varphi_{\bar{\rho}}^\nu(x+h) - \varphi_{\bar{\rho}}^\nu(x) - \frac{1}{2} \langle p_\nu + q_\nu, h \rangle \geq \frac{1}{2} |\langle p_\nu - q_\nu, h \rangle|.$$

By integration $s := \int \frac{p_\nu + q_\nu}{2} dP(\nu) \in \partial \Phi(x) = \{\nabla \Phi(x)\}$ and then

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

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

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

Moreover, the left-hand side above is controlled in absolute value by the Lipschitz constant of $\varphi_{\bar{\rho}}^\nu$ in a compact neighborhood of x which, thanks to Lemma 5.3.2, in turn, is controlled by

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

Thanks to (5.1) and Lebesgue's dominated convergence theorem, we thus get

$$\nabla \Phi(x) = \int \nabla \varphi_{\bar{\rho}}^\nu(x) dP(\nu),$$

which shows (5.10). \square

Remark 5.3.7 (First regularizing effect). One immediately deduces from (5.9) and the convexity of $\varphi_{\bar{\rho}}^\nu$, 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 5.3.8 (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 5.2.8 that P -a.e. $\nu = \mathcal{N}(0, S_\nu)$, where S_ν 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{Q} such that

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

In order to see that, recall that the optimal transport from $\rho = \mathcal{N}(0, Q)$ with $Q \succ 0$ to $\nu = \mathcal{N}(0, S)$ is given by $T_\rho^\nu(x) = T_Q^S x$, where $T_Q^S := Q^{-1/2} (Q^{1/2} S Q^{1/2})^{1/2} Q^{-1/2}$ (see Chapter 4). Thus $\varphi_\rho^\nu = \frac{1}{2} \langle x, T_Q^{S_\nu} x \rangle + C$, and the optimality condition (5.9) can be rewritten as

$$-\frac{\lambda}{2} \langle x, \bar{Q}^{-1} x \rangle = -\frac{\|x\|^2}{2} + \frac{1}{2} \mathbb{E}_P \langle x, T_Q^{S_\nu} x \rangle + C,$$

i.e.

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

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

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

This has a solution by Brouwer's fixed-point theorem. Indeed, denote $\alpha_\nu := \lambda_{\max}(S_\nu)$. 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 $\lambda I \preceq Q \preceq \alpha I$ it holds that

$$\lambda_{\max}(F(Q)) \leq \lambda + \mathbb{E}_P \left[(\alpha_\nu \alpha)^{1/2} \right] \leq \lambda + \frac{\alpha}{2} + \frac{\mathbb{E}_P[\alpha_\nu]}{2} \leq \lambda + \frac{\alpha}{2} + \frac{d\sigma^2}{2} = \alpha.$$

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

Example 5.3.9 (Discrete case). Consider now the case where $\Omega = \mathbb{R}^d$ and P is a discrete measure supported on discrete measures:

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

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 ν_i^j are positive. Then it follows from Theorem 5.3.6 that $\bar{\rho} := \text{bar}_\lambda(P)$ has the form

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

where $\nabla \varphi_i$ is the optimal transport map from $\bar{\rho}$ to ν_i . It is given by

$$\varphi_i(x) = \max_{j \in J_i} \{\langle x, x_i^j \rangle - \psi_i^j\} := \varphi_{\psi_i}(x),$$

where the $\psi_i = (\psi_i^j)_{j \in J_i}$ should match the mass conservation condition:

$$\nu_i^j = \bar{\rho}\left(\partial \varphi_{\psi_i}^*(x_i^j)\right) \quad \forall i \in I, j \in J_i. \quad (5.12)$$

In the semi-discrete optimal terminology, $\partial \varphi_{\psi_i}^*(x_i^j)$ is the so-called Laguerre cell, where φ_{ψ_i} coincides with $x \mapsto \langle x, x_i^j \rangle - \psi_i^j$. Computing $\bar{\rho} := \text{bar}_\lambda(P)$ therefore amounts to finding ψ_i^j , $i \in I, j \in J_i$, such that (5.12) holds for $\bar{\rho}$ depending on the ψ_i^j as well:

$$\bar{\rho}(x) = \exp\left(-\frac{1}{2\lambda}\|x\|^2 + \frac{1}{\lambda} \sum_{i \in I} p_i \max_{j \in J_i} \{\langle x, x_i^j \rangle - \psi_i^j\}\right). \quad (5.13)$$

Using results from [KMT19] concerning the differentiability of the Kantorovich functional in the semi-discrete case, it is easy to see that the nonlinear system (5.12)–(5.13) is the system of Euler–Lagrange equations for the finite-dimensional concave maximization problem

$$-\sum_{i \in I} p_i \sum_{j \in J_i} \psi_i^j \nu_i^j - \lambda \int_{\mathbb{R}^d} \exp\left(-\frac{1}{2\lambda}\|x\|^2 + \frac{1}{\lambda} \sum_{i \in I} p_i \max_{j \in J_i} \{\langle x, x_i^j \rangle - \psi_i^j\}\right) dx \rightarrow \max_{\psi_i^j},$$

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

5.4 Properties of the entropic barycenter

5.4.1 Global bounds

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

Lemma 5.4.1. *The entropic-Wasserstein barycenter $\bar{\rho}$ of P satisfies the following bound on the Fisher information:*

$$\int_{\Omega} \|\nabla \log(\bar{\rho})\|^2 \bar{\rho} \leq \frac{1}{\lambda^2} \int W_2^2(\bar{\rho}, \nu) dP(\nu).$$

In particular, $\sqrt{\bar{\rho}} \in H^1(\Omega)$, hence in the case $\Omega = \mathbb{R}^d$ it holds that $\bar{\rho} \in L^\infty(\mathbb{R}^d) \cap C^{0,1/2}(\mathbb{R}^d)$ 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 Theorem 5.3.6

$$\nabla \log(\bar{\rho}(x)) = \frac{1}{\lambda} \int (\nabla \varphi_{\bar{\rho}}^\nu(x) - x) dP(\nu) = -\frac{1}{\lambda} \int \nabla u_{\bar{\rho}}^\nu(x) dP(\nu),$$

thus

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

and using Fubini's Theorem, we get that

$$\int_{\Omega} \frac{\|\nabla \bar{\rho}\|^2}{\bar{\rho}} \leq \frac{1}{\lambda^2} \int \left[\int_{\Omega} \|\nabla u_{\bar{\rho}}^{\nu}\|^2 \bar{\rho} \right] dP(\nu) = \frac{1}{\lambda^2} \int W_2^2(\bar{\rho}, \nu) dP(\nu).$$

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 5.4.2. *Let Ω be a Borel set such that $|\Omega| > 0$ (not necessarily open) and*

$$\int m_p(\nu) dP(\nu) < +\infty \quad (5.14)$$

for some $p \geq 1$ (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

$$m_p(\bar{\rho}) \leq \frac{6^p}{2} \left(r^p + \int m_p(\nu) dP(\nu) \right) + \frac{|B_1(0)| \Gamma\left(\frac{d+p}{2}\right)}{2|\Omega \cap B_r(0)|} (96\lambda)^{(d+p)/2}. \quad (5.15)$$

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

$$m_p(\bar{\rho}) \leq \frac{6^p}{2} \int m_p(\nu) dP(\nu) + (3456\lambda)^{p/2} \Gamma\left(\frac{d+p}{2}\right). \quad (5.16)$$

Proof. Fix $r > 0$ s.t. $|\Omega \cap B_r(0)| > 0$ and denote $S := \Omega \cap B_r(0)$. Now let us take $R > 0$ and consider the set

$$Q_R := \{x \in B_R(0) \setminus B_{R/2}(0) : \|x\| \geq 3(\mathbb{E}\|T_{\bar{\rho}}^{\nu}(x)\| + r)\}, \quad (5.17)$$

where $T_{\bar{\rho}}^{\nu} := \nabla \varphi_{\bar{\rho}}^{\nu}$ is the optimal transport map (here and after, expectations are taken w.r.t. $\nu \sim P$). Assume $\bar{\rho}(Q_R) > 0$ and define

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

Then

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

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

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

which gives us

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

Then it is easy to see that, due to the convexity of W_2^2 ,

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

Therefore,

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

On the other hand, by optimality this derivative should be nonnegative, thus

$$\bar{\rho}(Q_R) \leq \frac{V_d R^d}{|S|} \exp \left(-\frac{R^2}{24\lambda} \right). \quad (5.18)$$

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 (5.17) of Q_R , if $x \in \Omega \setminus \bigcup_{n \in \mathbb{Z}} Q_{R_n}$, then $\|x\| < 3(\mathbb{E} \|T_{\bar{\rho}}^\nu(x)\| + r)$. Consequently,

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

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

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

Now let us bound the second term: due to (5.18) we get

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

Combining the above bounds together we obtain

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

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 $|S| = V_d r^d$ 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 5.4.3. Note that (5.16) (and thus, in some sense, (5.15)) is an interpolation between two bounds. On the one hand, if $\Omega = \mathbb{R}^d$ and $\lambda = 0$, then $\bar{\rho}$ is a standard Wasserstein barycenter and, due to the convexity of m_p along generalized geodesics, one gets the bound

$$m_p(\bar{\rho}) \leq \int m_p(\nu) dP(\nu).$$

On the other hand, if P is concentrated at the measure δ_0 , then $\bar{\rho} = \mathcal{N}(0, \lambda I)$ by Theorem 5.3.6. 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 (5.16) up to a constant factor to the power p and a factor depending on the dimension.

Remark 5.4.4. Let us indicate now a more elementary approach to obtain moment bounds when Ω is convex. Let $V: \mathbb{R}^d \rightarrow \mathbb{R}_+$ be a convex potential such that

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

On the one hand, thanks to (5.10), the convexity of V and the fact that $\nabla \varphi_{\bar{\rho}\#}^V \bar{\rho} = \nu$, we have:

$$\int_{\Omega} V(\lambda \nabla \log \bar{\rho}(x) + x) \bar{\rho}(x) dx \leq \int m_V(\nu) dP(\nu).$$

On the other hand, again by convexity $V(\lambda \nabla \log \bar{\rho}(x) + x) \bar{\rho}(x) \geq V(x) \bar{\rho}(x) + \lambda \langle \nabla V(x), \nabla \bar{\rho}(x) \rangle$. Integrating by parts (which can be justified if V is $C^{1,1}$ and using Lemma 5.4.1), denoting by n the outward normal to Ω on $\partial\Omega$, we thus get

$$\int_{\Omega} (V - \lambda \Delta V) \bar{\rho} \leq \int m_V(\nu) dP(\nu) - \lambda \int_{\partial\Omega} \partial_n V \bar{\rho}. \quad (5.19)$$

Assuming (5.14) and choosing $V(x) = \|x - x_0\|^p$ (actually, some suitable $C^{1,1}$ approximations of V) with $p \geq 2$ in (5.19) with $x_0 \in \Omega$, observing that $\partial_n V \geq 0$ on $\partial\Omega$ since Ω 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 Ω is convex and contains 0, we have

$$m_2(\bar{\rho}) \leq 2\lambda d + \int m_2(\nu) dP(\nu),$$

and for higher moments

$$m_p(\bar{\rho}) \leq \lambda p(p+d-2) m_{p-2}(\bar{\rho}) + \int m_p(\nu) dP(\nu).$$

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

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

Corollary 5.4.5. *Let Ω be open. Under assumptions of Proposition 5.4.2 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 5.4.1. Indeed, by the same arguments (together with the crude bound $\|\nabla\varphi_\rho^\nu(x) - x\|^p \leq 2^{p-1}(\|\nabla\varphi_\rho^\nu(x)\|^p + \|x\|^p)$) we arrive at

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

□

5.4.2 Stability

Following Subsection 3.5.2, 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 5.4.6 (Stability). *Take $p \geq 2$ and let $\{P_n\}_{n \geq 1} \subset \mathcal{P}_p(\mathbb{R}^d)$, $P \in \mathcal{P}_p(\mathbb{R}^d)$ 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*

$$W_p(\bar{\rho}_n, \bar{\rho}) \rightarrow 0, \quad (5.20)$$

$$\bar{\rho}_n^{1/p} \xrightarrow{W^{1,p}(\Omega)} \bar{\rho}^{1/p}, \quad (5.21)$$

$$\log \bar{\rho}_n \xrightarrow{W_{\text{loc}}^{1,q}(\Omega)} \log \bar{\rho}, \quad \forall 1 \leq q < \infty. \quad (5.22)$$

Proof. Proof of (5.20). Note that since $W_2 \leq W_p$ and $\mathcal{W}_2 \leq \mathcal{W}_p$, one has $\mathcal{W}_2(P_n, P) \rightarrow 0$. According to the proof of Proposition 5.2.6, $\text{Ent}_\Omega(\bar{\rho}_n)$ satisfies the assumptions of Theorem 3.5.2, hence the latter yields $W_2(\bar{\rho}_n, \bar{\rho}) \rightarrow 0$.

Arguing in the same way as in the proof of Proposition 5.4.2, one can show that for any $R > 0$

$$\int_{\{\|x\| \geq R\}} \|x\|^p \bar{\rho}_n \leq C \left[\int_{\mathcal{P}_p(\mathbb{R}^d)} \int_{\{\|x\| \geq R\}} (1 + \|\nabla\varphi_{\bar{\rho}_n}^\nu\|^p) \bar{\rho}_n dP_n(\nu) + \int_R^{+\infty} x^{d+p-1} \exp\left(-\frac{x^2}{96\lambda}\right) dx \right], \quad (5.23)$$

where the constant C depends solely on Ω , λ , p , and d .

To prove that $W_p(\bar{\rho}_n, \bar{\rho}) \rightarrow 0$, we use the stability of optimal transport plans from Proposition 3.3.5: once $W_2(\rho_n, \rho) \rightarrow 0$, $W_p(\nu_n, \nu) \rightarrow 0$, and there exists a unique optimal transport plan γ_ρ^ν from ρ to ν for the quadratic cost function, one has $J_c(\gamma_{\bar{\rho}_n}^{\nu_n}, \gamma_\rho^\nu) \rightarrow 0$, where 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 $\gamma_{\bar{\rho}_n}^{\nu_n}$ is any optimal transport plan from $\bar{\rho}_n$ to ν_n for the quadratic cost function. Further, using Proposition 3.3.2, it is easy to show that for any closed set $G \subset \mathbb{R}^d$ the function

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

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

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

Hence for all $R > 0$ one obtains

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

Using this together with (5.23), we get that

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

Thus the measures $\|\cdot\|^p \bar{\rho}_n$ are uniformly integrable, and using the criterion of convergence in the Wasserstein space (see e.g. [Vil09, Theorem 6.9]) we deduce that $W_p(\bar{\rho}_n, \bar{\rho}) \rightarrow 0$.

Proof of (5.21) and (5.22). Fix an arbitrary open set $U \subset \subset \Omega$. By Lemma 5.3.2

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

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

$$\bar{\varphi}_n = \lambda \log \bar{\rho}_n + \frac{\|\cdot\|^2}{2} = \int \varphi_{\bar{\rho}_n}^\nu dP_n(\nu)$$

are uniformly Lipschitz continuous on U for all n since $\int m_2(\nu) dP_n(\nu)$ are uniformly bounded. Furthermore, as $\bar{\rho}_n \rightarrow \bar{\rho} > 0$, $\bar{\varphi}_n$ are also uniformly bounded on U . Then, by the Arzelà–Ascoli theorem, $\bar{\varphi}_n \xrightarrow{C(U)} \bar{\varphi}$, and we deduce from weak convergence that $\bar{\varphi} = \lambda \log \bar{\rho} + \frac{\|\cdot\|^2}{2}$. Moreover, every $\bar{\varphi}_n$ is convex, thus $\nabla \bar{\varphi}_n \rightarrow \nabla \bar{\varphi}$ a.e. on U . Hence, by Lebesgue’s dominated convergence theorem, we get $\bar{\varphi}_n \xrightarrow{W^{1,q}(U)} \bar{\varphi}$ for any $1 \leq q < \infty$ and thus (5.22).

Further, using (5.10), we get

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

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

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

(e.g. in a sense that $\bar{\rho}(\Omega \setminus U) \rightarrow 0$). Finally, this together with (5.22) 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 5.4.6, in Section 5.6 we will obtain a law of large numbers for entropic-Wasserstein barycenters.

5.4.3 Maximum principle

Proposition 5.4.7. *Assume that Ω is convex and $P(\{\nu(\Omega) = 1\}) = 1$, and let $\bar{\rho} := \text{bar}_{\lambda, \Omega}(P)$ be its entropic barycenter. Then*

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

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 5.4.6 (more precisely, its corollary Proposition 5.6.1).

Step 1: the case of finitely many measures. Fix a compact convex set $K \subset \Omega$ with nonempty interior. Assume that $P = \sum_{i=1}^N p_i \delta_{\nu_i}$, where each ν_i is supported in K and has a $C^{0,\alpha}$, bounded away from 0 density on K . Since K is bounded, all $\varphi_{\bar{\rho}}^{\nu_i}$ 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 Ω and $(\nabla \varphi_{\bar{\rho}}^{\nu_i})_{\#} \bar{\rho} = \nu_i$ for all i , there are subgradients $\nabla \varphi_{\bar{\rho}}^{\nu_i}(x) \in K$. Let $y = \sum_{i=1}^N p_i \nabla \varphi_{\bar{\rho}}^{\nu_i}(x) \in K$, $v = \frac{y-x}{\|y-x\|}$, then thanks to (5.9)

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

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 [CF19] yields that $\varphi_{\bar{\rho}}^{\nu_i}$ is in fact $C_{\text{loc}}^{2,\alpha}$. Then at its maximum point $x \in \Omega$ we should have, on the one hand

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

(recall that $A \preceq B$ means that $B - A$ is positive semi-definite). On the other hand, using the Monge–Ampère equation $\bar{\rho} = \det(D^2 \varphi_{\bar{\rho}}^{\nu_i} \nu_i (\nabla \varphi_{\bar{\rho}}^{\nu_i}))$ (see also (5.27)), we get

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

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

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

what 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 ν_i is bounded away from 0 is just here to justify twice differentiability of $\varphi_{\bar{\rho}}^{\nu_i}$, if we drop this assumption replacing ν_i with $\nu_i^n := (1 - \frac{1}{n})\nu_i + \frac{1}{n|K|}$, using Lemma 5.4.6 we get the same conclusion by letting $n \rightarrow \infty$. In a similar way, Hölder regularity of the ν_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 $\mathcal{W}_2^2(P_n, P) \rightarrow 0$, 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 on $\mathcal{P}_2(\mathbb{R}^d)$ satisfying (5.1) and concentrated on measures giving full mass to Ω . Let ν_1, ν_2, \dots be i.i.d. random measures drawn from P . Then, by Proposition 5.6.1, 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 2-Wasserstein distance. Since

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

by the strong law of large numbers, we conclude using Step 1. \square

Remark 5.4.8. If, under 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 [KP17] for 2-Wasserstein barycenters on Riemannian manifolds.

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

Example 5.4.9. 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 $\bar{\rho}_0 := \text{bar}_{0, \Omega}(P)$ is an ordinary Wasserstein barycenter constrained to be supported on Ω . 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 $\bar{\rho}_\lambda := \text{bar}_{\lambda, \Omega}(P)$ and let $\lambda \rightarrow 0$. By compactness, we readily get that $\bar{\rho}_\lambda \rightarrow \bar{\rho}_0$, so, for λ 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 $\lambda > 0$.

5.5 Higher regularity

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

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 $C > 0$

$$P(\mathcal{Q}) = 1, \quad \mathcal{Q} := \left\{ \varrho \in \mathcal{P}_{\text{ac}}(\bar{\Omega}) : \|\log \varrho\|_{C^{k, \alpha}(\bar{\Omega})} \leq C \right\}. \quad (5.24)$$

Remark 5.5.1. 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 $\text{supp } \nu$ are uniformly bounded for P -a.e. ν .

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

Proposition 5.5.2. *Under assumption (5.24), one has*

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

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

$$\|\varphi_\rho^\nu\|_{C^{k+2,\alpha}(\bar{\Omega})}, \|\varphi_\nu^{\bar{\rho}}\|_{C^{k+2,\alpha}(\bar{\Omega})} \leq K \text{ for } P\text{-a.e. } \nu. \quad (5.25)$$

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

Proof. By (5.24) 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 (5.9) 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 λ .

This implies by Caffarelli's regularity theory for Monge–Ampère equations (see [Caf96] for the original paper and Theorem 3.3 [DF14] for a concise formulation) that for any $\nu \in \mathcal{Q}$, $\varphi_\rho^\nu \in C^{2,\alpha}(\bar{\Omega})$ and $\nabla\varphi_\rho^\nu: \bar{\Omega} \rightarrow \bar{\Omega}$ is a diffeomorphism.

For the uniform estimate again by Caffarelli's regularity theory for Monge–Ampère equations (theorem on page 3 of [Caf92]) there is an $\alpha_1 \in (0, 1)$ and constant C_1 (only depending on α_1 , C and R) such that

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

This implies in particular $\bar{\rho} \in C^{1,\alpha_1}(\bar{\Omega})$ by (5.9) and we can apply Theorem 5.A.5 to see that

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

is continuous (where \mathcal{M} denotes the set of $C^{2,\alpha_1}(\bar{\Omega})$ Brenier potentials φ with zero mean such that $\|\nabla\varphi\| = R$ on $\partial\Omega$). Now note that, by the compact embedding of Hölder spaces, \mathcal{Q} is compact in $C^{0,\alpha_1}(\bar{\Omega})$. This implies that $\Phi^{\bar{\rho}}(\mathcal{Q})$ is compact in $C^{2,\alpha_1}(\bar{\Omega})$. Hence, there is a $K_1 > 0$ such that

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

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

$$D^2\varphi_\nu^{\bar{\rho}} \succcurlyeq cI \text{ for } P\text{-a.e. } \nu, \quad (5.26)$$

so that we obtain

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

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

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

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

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

where $A_\nu = \nu(\nabla \varphi_\rho^\nu) \det(D^2 \varphi_\rho^\nu)(D^2 \varphi_\rho^\nu)^{-1}$. Thanks to Lemma 5.A.2 and (5.26) we can finally deduce by classical Schauder estimates (Theorem 6.30 in [GT15]) that there is constant $K > 0$ uniform in ν such that

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

This concludes the uniform estimate of φ_ρ^ν in $C^{3,\alpha}(\bar{\Omega})$ for P -a.e. ν , and by again employing (5.9) we deduce $\bar{\rho} \in C^{3,\alpha}(\bar{\Omega})$. The same bound follows for $\varphi_\nu^{\bar{\rho}}$ by exchanging the role of $\bar{\rho}$ and ν . Higher regularity follows by standard elliptic theory. \square

Note in particular that φ_ρ^ν satisfies the Monge–Ampère equation, subject to the *second boundary value condition*, which encodes the fact that $\nabla \varphi_\rho^\nu$ maps the ball into itself, in the classical sense

$$\begin{aligned} \det(D^2 \varphi_\rho^\nu) \nu(\nabla \varphi_\rho^\nu) &= \bar{\rho} \quad \text{in } B \\ \nabla \varphi_\rho^\nu(B) &\subset B, \end{aligned} \tag{5.27}$$

and that the second boundary value condition is equivalent (see Lemma 5.A.1) to an eikonal equation on the boundary

$$\|\nabla \varphi_\rho^\nu(x)\|^2 = R^2 \quad \forall x \in \partial B.$$

5.6 Statistical properties

5.6.1 Stochastic setting and law of large numbers

Now we consider again the stochastic setting (see Corollary 3.5.7 and Chapter 4): let P , as above, be a distribution on $\mathcal{P}_2(\Omega)$ with finite second moment, and ν_1, ν_2, \dots be independent random measures drawn from P . We will call the barycenter of the first n measures ν_1, \dots, ν_n an empirical barycenter: $\bar{\rho}_n := \operatorname{bar}_{\lambda, \Omega}(P_n)$, 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 5.4, a LLN follows immediately from Lemma 5.4.6.

Proposition 5.6.1 (Law of large numbers). *Assume $\int m_p(\nu) dP(\nu) < +\infty$ for some $p \geq 2$. Let $\bar{\rho}$ be the entropic–Wasserstein barycenter of P and $\{\bar{\rho}_n\}_{n \in \mathbb{N}}$ be empirical barycenters. Then it a.s. holds that*

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

Moreover, under assumption (5.24) $\bar{\rho}_n \xrightarrow{\text{a.s.}} \bar{\rho}$ in $C^{k+2,\beta}(\bar{\Omega})$ for any $\beta \in (0, \alpha)$.

Proof. Then the first part of the theorem follows from Lemma 5.4.6 since P_n converge to P in \mathcal{W}_p metric (recall 3.5.7).

Further, once (5.24) holds, sequence $\{\bar{\rho}_n\}_{n \in \mathbb{N}}$ is uniformly bounded in $C^{k+2,\alpha}(\bar{\Omega})$ by Proposition 5.5.2. Therefore, due to compact Hölder embedding and weak convergence $\bar{\rho}_n \rightharpoonup \bar{\rho}$, the second claim follows. \square

5.6.2 Central limit theorem

Let H 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

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

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 $A_n u \rightarrow A u$ 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 5.B.

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 5.6.2 (Central limit theorem). *Let the assumption (5.24) be fulfilled with $k = 1$. Then a CLT for empirical barycenters holds in $H_\diamond^2(B)$:*

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

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

$$G: u \mapsto \lambda \frac{u}{\bar{\rho}} - \lambda \int_B \frac{u}{\bar{\rho}} - \mathbb{E}(\Phi^\nu)'(\bar{\rho})$$

and $\Phi^\nu(\bar{\rho})$ is the zero-mean Brenier potential between $\bar{\rho}$ and ν .

Proof. Step 1. Let us introduce the following map F :

$$F: \left\{ \rho \in C^2(\bar{B}) : \int_B \rho = 1, \min_{\bar{B}} \rho > 0 \right\} \rightarrow C_\diamond^2(\bar{B})$$

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

It is continuously differentiable and its derivative is

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

Then equation (5.9) can be rewritten (see Appendix 5.A for properties of the map Φ^ν) 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 the differentiability of F and Φ^ν (Theorem 5.A.5), we obtain

$$G_n(\bar{\rho}_n - \bar{\rho}) = F(\bar{\rho}_n) - F(\bar{\rho}) - \frac{1}{n} \sum_{i=1}^n (\Phi^{\nu_i}(\bar{\rho}_n) - \Phi^{\nu_i}(\bar{\rho})) = \frac{1}{n} \sum_{i=1}^n \varphi_i - \mathbb{E} \varphi, \quad (5.28)$$

where $\varphi_i = \varphi_\rho^{\nu_i}$, $\mathbb{E} \varphi = \mathbb{E} \varphi_\rho^\nu$, 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 the delta-method to prove a CLT and to do this we need a convergence (in an appropriate space)

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

We will consider a CLT in $H_\diamond^2(B)$, but first, let us extend all the linear operators above to $L_\diamond^2(B)$. Denote by $\text{Bar}_{\lambda,B}(\mathcal{Q})$ the set of entropic barycenters of all measures supported on \mathcal{Q} :

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

Clearly, the operators $F'(\rho)$ are Hermitian, bounded and positive definite for all $\rho \in \text{Bar}_{\lambda,B}(\mathcal{Q})$. Using (5.25) and (5.9) we conclude that these ρ are uniformly bounded away from zero, thus $F'(\rho)$ are uniformly positive-definite: indeed, for any $u \in L_\diamond^2(B)$

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

For all $\rho \in \text{Bar}_{\lambda,B}(\mathcal{Q})$ and $\nu \in \mathcal{Q}$ it holds that $-(\Phi^\nu)'(\rho)$ are Hermitian and nonnegative. They are also uniformly bounded since all ν and $D^2\varphi'_\rho$ are uniformly bounded away from zero according to (5.24) and Proposition 5.5.2: namely, Theorem 5.A.5 together with the Poincaré inequality and Theorem 6.27 from [Lie13] yield that there is a constant $C_\Phi > 0$ such that

$$\|(\Phi^\nu)'(\rho)u\|_{H^2(B)} \leq C_\Phi \|u\|_{L^2(B)}. \quad (5.29)$$

In particular, the operators G and all G_n are a.s. well-defined, uniformly positive definite, and thus continuously invertible in $L_\diamond^2(B)$ with

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

Now we consider the space $H_\diamond^2(B)$. It is easy to see that $F'(\rho)$ and $(\Phi^\nu)'(\rho)$ can be continuously extended to it for any $\rho \in \text{Bar}_{\lambda,B}(\mathcal{Q})$, $\nu \in \mathcal{Q}$. We are going to show that there exist G^{-1} and G_n^{-1} for all n , and they are uniformly bounded. 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 (5.29) and the Rellich–Kondrachov theorem $(\Phi^\nu)'(\rho)$ are compact and uniformly bounded in $H_\diamond^2(B)$ for all $\rho \in \text{Bar}_{\lambda,B}(\mathcal{Q})$, $\nu \in \mathcal{Q}$, as well as any of their average. Thus $G := F'(\bar{\rho}) - \mathbb{E}(\Phi^\nu)'(\bar{\rho})$ also 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 to any G_n . Let us prove that G_n^{-1} are uniformly bounded in $H_\diamond^2(B)$. Suppose $G_n u = v \in H_\diamond^2(B)$. Then

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

On the other hand,

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

Therefore,

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

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

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

since $\bar{\rho}_n \xrightarrow{C^2(\bar{B})} \bar{\rho}$ a.s. by Proposition 5.6.1. Second, (5.29), the LLN, and the separability of $H_\diamond^2(B)$ 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

$$\frac{1}{n} \sum_{i=1}^n \int_0^1 (\Phi^{\nu_i})'(\bar{\rho}_n^t) dt - \frac{1}{n} \sum_{i=1}^n (\Phi^{\nu_i})'(\bar{\rho}) \xrightarrow{\text{SOT}} 0 \quad \text{a.s.} \quad (5.30)$$

Let $\nu \in \mathcal{Q}$ and $\rho \xrightarrow{C^2(\bar{B})} \bar{\rho}$. Due to Theorem 5.A.5

$$\|(\Phi^\nu)'(\rho)u - (\Phi^\nu)'(\bar{\rho})u\|_{H^2(B)} \rightarrow 0 \quad \text{for any } u \in C_\diamond^{0,\alpha}(\bar{B}),$$

hence (5.29) and the density of $C_\diamond^{0,\alpha}(\bar{B})$ in $L_\diamond^2(B)$ yield that $(\Phi^\nu)'(\rho) \rightarrow (\Phi^\nu)'(\bar{\rho})$ in SOT on $H_\diamond^2(B)$. Now we fix $u \in H_\diamond^2(B)$, then functions

$$f^{\nu_i}(\rho) := \left\| \int_0^1 (\Phi^{\nu_i})'(\rho^t)u dt - (\Phi^{\nu_i})'(\bar{\rho})u \right\|_{H^2(B)},$$

where $\rho^t := (1-t)\bar{\rho} + t\rho$, are bounded, continuous, and $f^{\nu_i}(\bar{\rho}) = 0$. Since $\bar{\rho}_n \xrightarrow{C^2(\bar{B})} \bar{\rho}$ a.s., Lemma 5.B.1 ensures that

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

Taking a dense countable set $\{u_j\}_{j \in \mathbb{N}}$ in $H_\diamond^2(B)$ and using the boundedness of $(\Phi^\nu)'$ by (5.29), one obtains (5.30). Combining the above results we conclude that $G_n \xrightarrow{\text{SOT}} G$ a.s. Finally, for any $u \in H_\diamond^2(B)$ one has

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

since G_n^{-1} are uniformly bounded. I.e., $G_n^{-1} \xrightarrow{\text{SOT}} G^{-1}$ almost surely.

Step 3. Note that $\|\varphi_\rho^\nu\|_{H^2(B)} \leq C\|\varphi_\rho^\nu\|_{C^2(\bar{B})}$, thus $\mathbb{E}\|\varphi_\rho^\nu\|_{H^2(B)}^2 < \infty$, and by the standard CLT in Hilbert spaces (see e.g. [LT13, Theorem 10.5]) applied to $\{\varphi_i\}_{i \in \mathbb{N}}$ we obtain that

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

According to (5.28),

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

Since G_n^{-1} are uniformly bounded and $G_n^{-1} \xrightarrow{\text{SOT}} G^{-1}$ a.s., Lemma 5.B.2 yields the CLT for $\bar{\rho}_n$:

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

□

Remark 5.6.3 (CLT in the discrete case). Let us finally remark that the above delta-method can easily be adapted to the case where Ω is convex and bounded and P is supported on a set of measures of the form $\sum_{j=1}^N \nu^j \delta_{x^j}$ with a lower bound on the mass of atoms $\nu^j \geq \varepsilon$ and the distance between atoms $\|x^i - x^j\| \geq \varepsilon$ once $i \neq j$, for some $\varepsilon > 0$. Of course, in this case, one cannot use the regularity theory for Monge–Ampère and its linearization, but one can instead take advantage of the fine analysis of the semi-discrete case by Kitagawa, Méridot and Thibert [KMT19]. Indeed, in this case $\Phi^\nu(\rho)$ always take the form $x \mapsto \max\{\langle x, x^j \rangle - \psi^j\}$, but it follows from Theorem 5.1 in [KMT19] and the implicit function theorem that the dual variables ψ^j depend in a C^1 way on $\rho \in C^{0,1}(\bar{\Omega})$ as well as an estimate of the form

$$\|(\Phi^\nu)'(\rho)u\|_{L^2(\Omega)} \leq C \sqrt{\sum_{j=1}^N u(V_j)^2}$$

where the V_j 's are the Laguerre cells associated with ρ and ν . Note that the r.h.s. of this inequality depends on finitely many linear functionals of u , therefore $(\Phi^\nu)'(\rho)$ is compact in $L^2_\diamond(\Omega)$. Moreover, one can show that there is a uniform bound

$$\|(\Phi^\nu)'(\rho)\|_{L^2_\diamond(\Omega)} \leq C$$

in the same way as in the proof of Theorem 5.1 in [KMT19], using the Cheeger inequality for graphs together with the lower bounds on ν^j and $\|x^i - x^j\|$, a relative isoperimetric inequality, and uniform bounds on ρ . Since $-(\Phi^\nu)'(\rho)$ is Hermitian and nonnegative definite, we can argue as in the proof above invoking the Fredholm alternative theorem to invert the operators G and G_n in $L^2_\diamond(\Omega)$. This easily yields a CLT in $L^2_\diamond(\Omega)$ in this discrete setting.

Appendix 5.A Linearization of Monge–Ampère equations

Here we collect some results on the linearization of Monge–Ampère equations. For proofs we refer to the original paper [CEK20].

Given a closed ball $\bar{B} := \bar{B}_R(0)$ of radius $R > 0$, $\alpha \in (0, 1)$, and $k \in \mathbb{N}_0$, define

$$\mathcal{S}_{k,\alpha} := \left\{ \varrho \in \mathcal{P}_{\text{ac}}(\bar{B}) : \|\log \varrho\|_{C^{k,\alpha}(\bar{B})} < \infty \right\}.$$

Consider $\mu \in \mathcal{S}_{0,\alpha}$, $\nu \in \mathcal{S}_{1,\alpha}$. Our goal is to linearize the following Monge–Ampère equation with a second boundary value condition:

$$\begin{aligned} \det(D^2\varphi)\nu(\nabla\varphi) &= \mu, \\ \nabla\varphi(\bar{B}) &= \bar{B}. \end{aligned} \tag{5.31}$$

Note that thanks to Brenier's theorem there exists a unique convex solution satisfying (5.31) (a priori in the sense of $\nabla\varphi_{\#}\mu = \nu$), and it is in $C^{2,\alpha}(\bar{B})$ thanks to the regularity theory for Monge–Ampère equations. We will need the following lemmas.

Lemma 5.A.1. *Let $\varphi \in C^1(\bar{B})$ be strictly convex. Then the following are equivalent*

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

Lemma 5.A.2. *For $\varphi \in C^2(\bar{B})$ strongly convex such that $\|\nabla\varphi(x)\|^2 - R^2 = 0$ for $x \in \partial B$, there is $\beta \in C(\partial B)$, $\beta > 0$ such that $(D^2\varphi)^{-1}(x) \cdot x = \beta(x)\nabla\varphi(x)$ for $x \in \partial B$. Furthermore, there exists $\kappa > 0$ such that $|\nabla\varphi(x) \cdot x| \geq \kappa$ for all $x \in \partial B$.*

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

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

Let us also define

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

We now claim that in a neighborhood of a strongly convex function $\varphi_0 \in \mathcal{M}$ this set is the graph of a C^1 -function.

Lemma 5.A.3. *At $\varphi_0 \in \mathcal{M}$ 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 $V \subset F_0 := \{h \in C_{\diamond}^{2,\alpha}(\bar{B}) : \nabla\varphi_0 \cdot \nabla h = 0 \text{ on } \partial B\}$, $U \subset C_{\diamond}^{2,\alpha}(\bar{B})$, with $\varphi_0 \in U$, and a bijective C^1 -function:*

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

Furthermore, for $f_0 := \Pi_{F_0}(\varphi_0)$, where $\Pi_{F_0}(\varphi)$ is defined as a solution of

$$\begin{aligned} -\operatorname{div}(A_0 \nabla f) &= -\operatorname{div}(A_0 \nabla \varphi) + \int_B \operatorname{div}(A_0 \nabla \varphi) && \text{in } B, \\ \nabla\varphi_0 \cdot \nabla f &= 0 && \text{on } \partial B, \end{aligned}$$

it holds that $\chi_0'(f_0) = \operatorname{id}$.

Now for $\varphi_0 \in \mathcal{M}$ take $U \subset C_{\diamond}^{2,\alpha}(\bar{B})$ from Lemma 5.A.3 (and possibly restrict it further such that any $\varphi \in U \cap \mathcal{M}$ is strongly convex) and consider the map

$$\begin{aligned} M_{\nu}: U \cap \mathcal{M} &\rightarrow \left\{ u \in C^{0,\alpha}(\bar{B}) : \int_B u = 1 \right\} \\ \varphi &\mapsto \det(D^2\varphi)\nu(\nabla\varphi) \end{aligned}$$

where ν is a fixed probability density in the set $\mathcal{S}_{1,\alpha}$. Note that this map is well-defined by Lemma 5.A.1 and the fact that the push forward preserves the mass. We want to “take the derivative at $\varphi \in U \cap \mathcal{M}$ ” by pulling back M_{ν} to the linear space F_0 with the map χ_0 from Lemma 5.A.3.

Proposition 5.A.4. *In the setting of Lemma 5.A.3, let $\varphi \in U \cap \mathcal{M}$ be strongly convex. Then $N_{\nu} := M_{\nu} \circ \chi_0$ is continuously differentiable at $f := \Pi_{F_0}\varphi$ and the derivative is given by*

$$\begin{aligned} N'_{\nu}(f): F_0 &\rightarrow C_{\diamond}^{0,\alpha}(\bar{B}) \\ h &\mapsto \operatorname{tr}(A_{\nu} D^2(\chi_0'(f)h)) + \det(D^2\varphi)\nabla\nu(\nabla\varphi) \cdot \nabla(\chi_0'(f)h), \end{aligned}$$

where $F_0 = \{h \in C_{\diamond}^{2,\alpha}(\bar{B}) : \nabla\varphi_0 \cdot \nabla h = 0 \text{ on } \partial B\}$ and $A_{\nu} := \nu(\nabla\varphi) \operatorname{cof}(D^2\varphi)$. In addition, in the weak sense we have

$$N'_{\nu}(f)h = \operatorname{div}(A_{\nu} \nabla(\chi_0'(f)h)).$$

For fixed $\nu \in \mathcal{S}_{1,\alpha}$, consider now the map

$$\begin{aligned} \Phi^{\nu}: \mathcal{S}_{0,\alpha} &\rightarrow \mathcal{M}, \\ \mu &\rightarrow \varphi, \text{ where } \varphi \text{ is strongly convex and } \nabla\varphi_{\#}\mu = \nu. \end{aligned} \tag{5.32}$$

Note that this is well defined thanks to Brenier’s theorem (Theorem 2.12 (ii) [Vil03]) and regularity theory for Monge–Ampère equations (Theorem 3.3 [DF14]). Furthermore, by the considerations before one can show that it is continuously differentiable.

Theorem 5.A.5. *Φ^{ν} as defined in (5.32) is continuously differentiable. More precisely, for every $\mu \in \mathcal{S}_{0,\alpha}$, 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*

$$\begin{aligned} \operatorname{div}(A_{\nu} \nabla h) &= f \text{ in } B, \\ \nabla\varphi_0 \cdot \nabla h &= 0 \text{ on } \partial B, \end{aligned}$$

where $\varphi_0 = \Phi^{\nu}(\mu)$ and $A_{\nu} = \nu(\nabla\varphi_0) \operatorname{cof}(D^2\varphi_0)$.

Appendix 5.B Auxiliary probability results

Lemma 5.B.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^* :

$$\omega_f(\delta, x^*) := \sup_{x \in \bar{B}_\delta(x^*)} |f(x) - f(x^*)|, \quad \delta > 0.$$

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 $\delta > 0$

$$\begin{aligned} \left| \frac{1}{n} \sum_{i=1}^n f_i(X_n) \right| &\leq \frac{1}{n} \sum_{i=1}^n \omega_{f_i}(d(X_n, x^*), x^*) \\ &\leq \frac{1}{n} \sum_{i=1}^n (\omega_{f_i}(\delta, x^*) \mathbb{1}[d(X_n, x^*) \leq \delta] + \sup_{x \in \mathcal{X}} |f_i(X_n)| \mathbb{1}[d(X_n, x^*) > \delta]). \end{aligned}$$

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 5.B.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_ε s.t. $P(\|A_n\| > M_\varepsilon) \leq \varepsilon$ for all n). Let $\{X_n\}$ 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 Π_k be the orthogonal projector onto the first k axes e_1, \dots, e_k . Then

$$A_n X_n = AX_n + (A_n - A)\Pi_k X_n + (A_n - A)(I - \Pi_k) X_n. \quad (5.33)$$

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 (5.33) and $X_n \xrightarrow{d} X$ yields convergence $A_n X_n \xrightarrow{d} AX$. □

Chapter 6

Dirichlet energy and Sobolev spaces of measure-valued maps

6.1 Introduction

In this chapter we study Sobolev spaces of measure-valued maps motivated by a Monge–Kantorovich problem regularized with a “Dirichlet energy” of a transport plan. Let Ω be an open subset of \mathbb{R}^m , and $c: \Omega \times \mathbb{R}^d \rightarrow \mathbb{R}_+$ be a Borel cost function. First, consider the following regularized Monge problem for $\mu \in \mathcal{P}(\Omega)$, $\nu \in \mathcal{P}(\mathbb{R}^d)$:

$$\int_{\Omega} c(x, T(x)) \, d\mu(x) + \int_{\Omega} \|DT(x)\|^p \, dx \rightarrow \min_{T \in W^{1,p}(\Omega; \mathbb{R}^d): T_{\#}\mu = \nu} . \quad (6.1)$$

This was studied by J. Louet in [Lou14], where a PDE characterization of a solution was obtained. In particular, in Section 4.2 he proposed some Kantorovich-like formulation.

However, here we use another approach, based on the theory of Sobolev spaces valued in the Wasserstein space. It was proposed by Y. Brenier in [Bre03] and developed by H. Lavenant in the works [Lav19b; Lav19a] in the context of harmonic mappings valued in the 2-Wasserstein space. Let $\gamma = \gamma(x) \otimes \mu$ be the disintegration of a transport plan γ between μ and ν . Then we consider the following problem:

$$\int c \, d\gamma + \int_{\Omega} \|D\gamma(x)\|^p \, dx \rightarrow \min_{\gamma \in \Pi(\mu, \nu)} ,$$

where $\|D\gamma(x)\|$ to be understood as a “metric gradient” of a Sobolev map from Ω to $\mathcal{P}_p(\mathbb{R}^d)$. Note that a standard p -Sobolev function can be defined up to a set of zero p -capacity, thus we can consider μ which is a.c. w.r.t. the p -capacity, but not necessarily w.r.t. the Lebesgue measure. In this case, of course, we have to extend $\gamma(x)$ to the whole Ω .

We are going to consider some properties of measure-valued Sobolev maps, including fine properties and precise representative, and also define a notion of their convergence which is suitable for studying the regularized Monge–Kantorovich problem.

Notations. Let $\Omega \subset \mathbb{R}^m$ be an open set such that $|\Omega| < \infty$ and D be a closed subset of \mathbb{R}^d . If φ is a function on $\Omega \times D$, then by $\nabla_{\xi}\varphi$ we denote its gradient in Ω , and by $\nabla_x\varphi$ we denote the gradient in D .

Let $1 < p \leq \infty$, then $p' := \frac{p}{p-1}$ is the conjugate index to p , and $p^* := \frac{pm}{m-p}$ is the Sobolev conjugate once $p < m$. Furthermore, for $1 < p < m$, the p -capacity of a set $A \subset \mathbb{R}^m$ is defined as [EG15, Section 4.7]

$$\text{Cap}_p(A) := \inf \left\{ \int_{\mathbb{R}^m} \|\nabla u\|^p \, d\xi : u \in L^{p^*}(\mathbb{R}^m), \nabla u \in L^p(\mathbb{R}^m), u \geq 0, A \subset \text{int}\{u \geq 1\} \right\} .$$

Cap_p is an outer measure on \mathbb{R}^m , but it is not Borel. We say a measure $\mu \ll \text{Cap}_p$ if $\mu^*(A) = 0$ whenever $\text{Cap}_p(A) = 0$, or, equivalently, if for any $A \subset \mathbb{R}^m$ with $\text{Cap}_p(A) = 0$ there is a Borel

set $B \supset A$ such that $\mu(B) = 0$. As mentioned in [EG15, Chapter 4], Cap_p is a suitable measure to study the fine properties of Sobolev functions.

The chapter is organized as follows. In Section 6.2 we define Sobolev maps valued in a metric space and in the space of probability measures and recall some basic properties of them. In Section 6.3 we consider integral mappings of form $\xi \rightarrow \int_D \varphi d\boldsymbol{\mu}[\xi]$ and use them to study the fine properties of Sobolev maps. Section 6.4 is devoted to two notions of convergence in the measure-valued Sobolev space. Finally, in Section 6.5 we define rigorously the regularized Monge–Kantorovich problem, show existence of a solution, and discuss some open questions.

6.2 Sobolev maps valued in metric space

Let (X, ρ) be a metric space and Ω be a domain in \mathbb{R}^m as described above, endowed with the Lebesgue measure $\mathcal{L}|_\Omega$. Then we can naturally define the Lebesgue space $L^p(\Omega; X)$ in the following way.

Definition 6.1. We say that a Borel map $u: \Omega \rightarrow X$ belongs to the Lebesgue space $L^p(\Omega; X)$ for $1 < p < \infty$, if for some (thus any) fixed $x_0 \in X$

$$\int_{\Omega} \rho^p(u(\xi), x_0) d\xi < \infty.$$

A metric on $L^p(\Omega, X)$ is defined as

$$d_p(u, v) = \left(\int_{\Omega} \rho^p(u(\xi), v(\xi)) d\xi \right)^{1/p}, \quad u, v \in L^p(\Omega, X).$$

Of course, d_p is, strictly speaking, a pseudometric between maps, thus we identify maps which coincide a.e. in Ω . An important property of the space $L^p(\Omega; X)$ is that it is complete iff the target space (X, ρ) is complete.

Following Yu. Reshetnyak [Res97], we now give a general definition of the Sobolev space $W^{1,p}(\Omega; X)$. In the case $X = \mathbb{R}^d$ it is equivalent to the standard definition.

Definition 6.2. A map $u \in L^p(\Omega; X)$ belongs to the Sobolev space $W^{1,p}(\Omega; X)$ iff there is $g_u \in L^p(\Omega)$ such that for any L -Lipschitz function $F: X \rightarrow \mathbb{R}$ it holds that $F \circ u \in W^{1,p}(\Omega)$ and $\|\nabla(F \circ u)\| \leq Lg_u$ a.e. in Ω .

Now we pass to a more specific setting, where X is the space $\mathcal{P}_p(D)$ of probability measures on D with finite p -th moment endowed with the p -Wasserstein distance W_p . Then $\boldsymbol{\mu} \in L^p(\Omega, \mathcal{P}_p(D))$ can be equivalently described with a Young measure

$$\boldsymbol{\mu} := \boldsymbol{\mu} \otimes \mathcal{L}|_\Omega \in \mathcal{M}_+(\Omega \times D)$$

such that $\int \|x\|^p d\boldsymbol{\mu}(\xi, x) < \infty$. Indeed, the disintegration of any Young measure $\boldsymbol{\mu} \in \mathcal{M}_+(\Omega \times D)$ (i.e. such that $\pi_{\#}^1 \boldsymbol{\mu} = \mathcal{L}|_\Omega$) satisfying this condition gives us a map $\boldsymbol{\mu} \in L^p(\Omega, \mathcal{P}_p(D))$. Now consider the Sobolev space $W^{1,p}(\Omega; \mathcal{P}_p(D))$ in the sense of the above definition. In Theorem 3.17 in [Lav19b] H. Lavenant shows that there is an equivalent definition based on a multidimensional analogue of the Benamou–Brenier formula (in that work it is proven for $p = 2$ but the proof works for any $p > 1$ as well).

Proposition 6.2.1. *Let $\boldsymbol{\mu} \in L^p(\Omega; \mathcal{P}_p(D))$ for some $1 < p < \infty$. Then $\boldsymbol{\mu} \in W^{1,p}(\Omega; \mathcal{P}(D))$ iff there exists a measurable matrix-valued function $V \in L^p(\Omega \times D, \boldsymbol{\mu}; \mathbb{R}^{m \times d})$ satisfying the following continuity equation in a weak sense:*

$$\nabla_{\xi} \boldsymbol{\mu} + \nabla_x (V \boldsymbol{\mu}) = 0, \tag{6.2}$$

i.e. for any $\varphi \in C_c^1(\Omega \times \mathbb{R}^d)$ it holds that

$$\int \nabla_{\xi} \varphi d\boldsymbol{\mu} + \int V \nabla_x \varphi d\boldsymbol{\mu} = 0.$$

Moreover, there is a constant $C_p > 0$ such that $g_{\boldsymbol{\mu}}^p(\xi) \leq C_p \int \|V\|^p d\boldsymbol{\mu}[\xi]$ for a.e. $\xi \in \Omega$.

Notice that we can replace $\mathcal{P}_p(D)$ with $\mathcal{P}_p(\mathbb{R}^d)$ under the assumption that $\mu[\xi](D) = 1$ for a.e. $\xi \in \Omega$, which immediately follows from Definition 6.2. In this case one can extend V to $\Omega \times \mathbb{R}^d$ with 0.

Again, one can equivalently define the Sobolev space using Young measures. Let $\mu \in W^{1,p}(\Omega; \mathcal{P}(D))$, then we say $\varrho \in \mathcal{M}_+(\Omega \times D \times \mathbb{R}^{m \times d})$ is its *phase measure* if $\pi_{\#}^{1,2} \varrho = \mu$, $\int \|V\|^p d\varrho(\xi, x, V) < \infty$, and for any $\varphi \in C_c^1(\Omega \times \mathbb{R}^d)$

$$\int (\nabla_{\xi} \varphi(\xi, x) + V \nabla_x \varphi(\xi, x)) d\varrho(\xi, x, V) = 0.$$

Given a phase measure ϱ , we can construct an admissible field using the barycentric projection: $\bar{V}(\xi, x) := \int V d\varrho|_{\xi, x}$.

For any $\mu \in W^{1,p}(\Omega; \mathcal{P}(D))$ we define its *Dirichlet energy* as follows:

$$\text{Dir}_p(\mu) := \inf \left\{ \int \|V\|^p d\mu : V \text{ satisfies (6.2)} \right\}.$$

By the direct method in the calculus of variations we obtain the following

Lemma 6.2.2. *Let the norm $\|\cdot\|$ on $\mathbb{R}^{m \times d}$ be strictly convex and $\mu \in W^{1,p}(\Omega; \mathcal{P}(D))$ for some $1 < p < \infty$. Then there exists a unique field V satisfying (6.2) such that $\text{Dir}_p(\mu) = \int \|V\|^p d\mu$.*

We will call the function V from the above lemma the *velocity field* of μ . It is worth to mention that the definition of the Sobolev space does not depend on the choice of a norm on $\mathbb{R}^{m \times d}$, and hence V is for now an auxiliary object. Thus, let us for simplicity use the Frobenius norm, unless explicitly stated otherwise. However, the regularized Monge–Kantorovich problem in Section 6.5 essentially depends on a specific choice of the norm.

6.3 Integral mappings and precise representatives

As shown in [Lav19b, Section 5], if $m > 1$, then a Sobolev map valued in $\mathcal{P}_p(D)$ in general does not satisfy the superposition principle, and moreover, it cannot be represented via a measure on $W^{1,p}(\Omega; D)$. Thus, we cannot rely on this representation to study the properties of Sobolev maps. Instead, we will apply Definition 6.2 and Proposition 6.2.1 to integral mappings of form $\xi \rightarrow \int_D \varphi d\mu[\xi]$.

Lemma 6.3.1. *Let $\varphi \in C^1(\Omega \times \mathbb{R}^d)$ be such that $|\varphi| \leq C(1 + \|x\|^q)$, $\|\nabla_x \varphi\| \leq C(1 + \|x\|^{q-1})$, and $\|\nabla_{\xi} \varphi\| \leq C(1 + \|x\|^q)$ with some constant $C \geq 0$ and exponent $q \geq 1$. Given $\mu \in W^{1,p}(\Omega, \mathcal{P}_p(D))$ for $q \leq p < \infty$, define the function*

$$g(\xi) := \int_D \varphi(\xi, x) d\mu[\xi](x), \quad \xi \in \Omega.$$

Then $g \in W^{1,s}(\Omega)$, where $s := \frac{p}{q}$, and

$$\nabla g(\xi) = \int_D [\nabla_{\xi} \varphi(\xi, x) + V(\xi, x) \nabla_x \varphi(\xi, x)] d\mu[\xi](x).$$

Proof. Step 1: compactly supported φ . Assume that there is a compact set $K \subset D$ such that $\varphi(\xi, \cdot)$ is supported on K for any $\xi \in \Omega$. Clearly, $g \in L^s(\Omega)$. Moreover, (6.2) implies that for any $\eta \in C_c^1(\Omega)$

$$\begin{aligned} \int_{\Omega} g \nabla \eta d\xi &:= \int_{\Omega} \int_D \varphi(\xi, x) \nabla \eta(\xi) d\mu[\xi](x) d\xi \\ &= \int_{\Omega} \int_D [\nabla_{\xi} (\eta(\xi) \varphi(\xi, x)) - \eta(\xi) \nabla_{\xi} \varphi(\xi, x)] d\mu[\xi](x) d\xi \\ &= - \int_{\Omega} \int_D V(\xi, x) \nabla_x (\eta(\xi) \varphi(\xi, x)) d\mu[\xi](x) d\xi - \int_{\Omega} \eta \int_D \nabla_{\xi} \varphi(\xi, x) d\mu[\xi](x) d\xi \\ &= - \int_{\Omega} \eta \int_D [\nabla_{\xi} \varphi(\xi, x) + V(\xi, x) \nabla_x \varphi(\xi, x)] d\mu[\xi](x) d\xi, \end{aligned}$$

where V is the velocity field of $\boldsymbol{\mu}$. Thus

$$\nabla g(\xi) = \int_D [\nabla_\xi \varphi(\xi, x) + V(\xi, x) \nabla_x \varphi(\xi, x)] d\boldsymbol{\mu}[\xi](x)$$

in a weak sense. From the assumptions of the lemma it immediately follows that $\nabla g \in L^p(\Omega; \mathbb{R}^m) \subset L^s(\Omega; \mathbb{R}^m)$.

Step 2: general case. Consider functions $f_n \in C^1(\mathbb{R}^d)$ for $n \in \mathbb{N}$ such that $f_n = 1$ in $B_n(0)$, $f_n = 0$ outside $B_{3n}(0)$, and $\|\nabla f_n\| \leq \frac{1}{n}$. Define $\varphi_n(\xi, x) := f_n(x)\varphi(\xi, x)$ for $\xi \in \Omega$, $x \in \mathbb{R}^d$, and corresponding functions $g_n(\xi) := \int_D \varphi_n(\xi, x) d\boldsymbol{\mu}[\xi](x)$. Since for every $x \in B_{3n}(0)$

$$\begin{aligned} \|\nabla_x \varphi_n\| &= \|f_n \nabla_x \varphi + \varphi \nabla_x f_n\| \leq \|\nabla_x \varphi\| + |\varphi| \cdot \|\nabla_x f_n\| \\ &\leq C(1 + \|x\|^{q-1}) + C \frac{(1 + \|x\|^q)}{n} \leq 4C(1 + \|x\|^{q-1}), \end{aligned}$$

$g_n \in W^{1,s}(\Omega)$ according to Step 1. Furthermore,

$$\begin{aligned} \|g - g_n\|_{L^s(\Omega)}^s &= \int_\Omega \left| \int_D (1 - f_n(x)) \varphi(\xi, x) d\boldsymbol{\mu}[\xi](x) \right|^s d\xi \\ &\leq \int_\Omega \int_{D \setminus B_n(0)} |\varphi(\xi, x)|^s d\boldsymbol{\mu}[\xi](x) d\xi \\ &\leq C^s \int_{\Omega \times (D \setminus B_n(0))} (1 + \|x\|^q)^s d\boldsymbol{\mu}(\xi, x) \\ &\leq (2C)^s \int_{\Omega \times (D \setminus B_n(0))} (1 + \|x\|^p) d\boldsymbol{\mu}(\xi, x) \rightarrow 0 \text{ as } n \rightarrow \infty. \end{aligned}$$

Now define

$$v(\xi) := \int_D [\nabla_\xi \varphi(\xi, x) + V(\xi, x) \nabla_x \varphi(\xi, x)] d\boldsymbol{\mu}[\xi](x).$$

We are going to show that ∇g_n converge to v in $L^s(\Omega; \mathbb{R}^m)$. First of all,

$$\begin{aligned} v(\xi) - \nabla g_n(\xi) &= \int_D \left[(1 - f_n(x)) (\nabla_\xi \varphi(\xi, x) + V(\xi, x) \nabla_x \varphi(\xi, x)) - \varphi(\xi, x) V(\xi, x) \nabla_x f_n(x) \right] d\boldsymbol{\mu}[\xi](x). \end{aligned}$$

From the definition of f_n and the assumptions of the lemma we obtain the following bounds:

$$\begin{aligned} \int_\Omega \left\| \int_D (1 - f_n(x)) \nabla_\xi \varphi(\xi, x) d\boldsymbol{\mu}[\xi](x) \right\|^s d\xi &\leq \int_{\Omega \times (D \setminus B_n(0))} \|\nabla_\xi \varphi\|^s d\boldsymbol{\mu} \\ &\leq C^s \int_{\Omega \times (D \setminus B_n(0))} (1 + \|x\|^q)^s d\boldsymbol{\mu}(\xi, x) \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

Furthermore,

$$\begin{aligned} &\int_\Omega \left\| \int_D (1 - f_n(x)) V(\xi, x) \nabla_x \varphi(\xi, x) d\boldsymbol{\mu}[\xi](x) \right\|^s d\xi \\ &\leq C^s \int_\Omega \|V(\xi, \cdot)\|_{L^p(D \setminus B_n(0), \boldsymbol{\mu}[\xi])}^s \cdot \|1 + \|x\|^{q-1}\|_{L^{p'}(D, \boldsymbol{\mu}[\xi])}^s d\xi \\ &\leq C^s \left\| \|V(\xi, \cdot)\|_{L^p(D \setminus B_n(0), \boldsymbol{\mu}[\xi])}^{p/q} \right\|_{L^q(\Omega)} \cdot \left\| \left(1 + \|x\|^{q-1}\|_{L^{p'}(D, \boldsymbol{\mu}[\xi])} \right)^s \right\|_{L^{q'}(\Omega)} \\ &\leq (2C)^s \left(\int_{\Omega \times (D \setminus B_n(0))} \|V\|^p d\boldsymbol{\mu} \right)^{1/q} \left(1 + \left\| \|x\|^{q-1}\|_{L^{p'}(D, \boldsymbol{\mu}[\xi])}^s \right\|_{L^{q'}(\Omega)} \right). \end{aligned}$$

If $q = 1$, then $\left\| \left\| \|x\|^0 \right\|_{L^{p'}(D, \mu[\xi])}^s \right\|_{L^\infty(\Omega)} \leq 1$, otherwise $p' \leq q' < \infty$ and

$$\begin{aligned} \left\| \left\| \|x\|^{q-1} \right\|_{L^{p'}(D, \mu[\xi])}^s \right\|_{L^{q'}(\Omega)}^{q'} &= \int_{\Omega} \left(\int_D \|x\|^{(q-1)p'} d\mu[\xi](x) \right)^{sq'/p'} d\xi \\ &\leq \int_{\Omega \times D} \|x\|^{(q-1)sq'} d\mu(\xi, x) = \int_{\Omega \times D} \|x\|^p d\mu(\xi, x) < \infty \end{aligned}$$

(here we used that $\frac{sq'}{p'} = \frac{sq(p-1)}{(q-1)p} = \frac{p-1}{q-1} \geq 1$ and $(q-1)sq' = sq = p$). Thus,

$$\int_{\Omega} \left\| \int_D (1 - f_n(x)) \nabla_{\xi} \varphi(\xi, x) d\mu[\xi](x) \right\|^s d\xi \rightarrow 0 \text{ as } n \rightarrow \infty.$$

The last term can be estimated as follows:

$$\begin{aligned} &\int_{\Omega} \left\| \int_D \varphi(\xi, x) V(\xi, x) \nabla f_n(x) d\mu[\xi](x) \right\|^s d\xi \\ &\leq C^s \int_{\Omega} \left(\int_{B_{3n}(0) \setminus B_n(0)} \|V(\xi, x)\| \frac{1 + \|x\|^q}{n} d\mu[\xi](x) \right)^s d\xi \\ &\leq C^s \int_{\Omega} \|V(\xi, \cdot)\|_{L^p(D \setminus B_n(0), \mu[\xi])}^s \cdot \left\| \frac{1}{n} + 3\|x\|^{q-1} \right\|_{L^{p'}(D, \mu[\xi])}^s d\xi \rightarrow 0 \text{ as } n \rightarrow \infty. \end{aligned}$$

Therefore, $\|v - \nabla g_n\|_{L^s} \rightarrow 0$, hence $g \in W^{1,s}(\Omega)$ and $\nabla g = v$. \square

Lemma 6.3.2. *Let $\mu \in W^{1,p}(\Omega, \mathcal{P}_p(D))$ for some $1 < p < m$. Then there exists a Borel map $\mu^*: \Omega \rightarrow \mathcal{P}(D)$ and a Borel set $A \subset \Omega$ such that $\text{Cap}_p(A) = 0$, $\mu^* = \mu$ a.e., and for any $\xi \in \Omega \setminus A$*

$$W_p \left(\int_{B_r(\xi)} \mu[\zeta] d\zeta, \mu^*[\xi] \right) \rightarrow 0 \text{ as } r \rightarrow 0$$

and, more than that,

$$\int_{B_r(\xi)} W_p^{p^*}(\mu[\zeta], \mu^*[\xi]) d\zeta \rightarrow 0 \text{ as } r \rightarrow 0. \quad (6.3)$$

Proof. First of all, note that due to the σ -subadditivity of the p -capacity, it is enough to consider Ω equal to a ball. Then any function from $W^{1,p}(\Omega)$ can be extended to \mathbb{R}^m , and we can apply results from Section 4.8 in [EG15]. Since we are interested only in local properties, this does not spoil the results.

Step 1: narrow convergence. Let $\{\varphi_n\}_{n \in \mathbb{N}}$ be a dense countable subset of $C_c^1(\mathbb{R}^d)$. Since for each n the function $g_n(\xi) := \int_D \varphi_n d\mu[\xi]$ belongs to $W^{1,p}(\Omega)$, by Theorem 4.8.1 in [EG15] (obviously, it works if \mathbb{R}^m is replaced with an open Ω as well) there exists a Borel function $g_n^*: \Omega \rightarrow \mathbb{R}$ and a Borel set $A_n \subset \Omega$ such that $\text{Cap}_p(A_n) = 0$ and for any $\xi \in \Omega \setminus A_n$

$$\int_D \varphi_n d\mu_r[\xi] = \int_{B_r(\xi)} \varphi_n \rightarrow g_n^*(\xi) \text{ as } r \rightarrow 0, \quad (6.4)$$

where $\mu_r[\xi] := \int_{B_r(\xi)} \mu$. In the same way, take $g_0(\xi) := m_1(\mu[\xi]) := \int_D \|x\| d\mu[\xi](x)$, then by Definition 6.2 $g_0 \in W^{1,p}(\Omega)$, thus there is a corresponding function g_0^* and a Borel set A_0 such that $\text{Cap}_p(A_0) = 0$ and

$$g_0(\mu_r[\xi]) = \int_{B_r(\xi)} g_0 \rightarrow g_0^*(\xi) \text{ as } r \rightarrow 0, \quad \forall \xi \in \Omega \setminus A_0.$$

Now we define $A := \bigcup_{n \in \mathbb{N}_0} A_n$, $\text{Cap}_p(A) = 0$. From the above equation we get that for any $\xi \in \Omega \setminus A$ the family $\{\mu_r[\xi]\}_{r < r_0}$ is tight for small enough $r_0 = r_0(\xi)$. Therefore, there is a

weak partial limit $\mu^*[\xi]$ as $r \rightarrow 0$, and due to (6.4) $g_n^*(\xi) = \int_D \varphi_n d\mu^*[\xi]$, hence it is unique, and $\mu_r[\xi] \rightarrow \mu^*[\xi]$ as $r \rightarrow 0$. Moreover, $g_n^* = g_n$ a.e. for all n , thus $\mu^* = \mu$ a.e. in Ω .

Step 2: Wasserstein convergence. For any $R > 0$ take smooth nonnegative function ψ_R on \mathbb{R}^d such that $\psi_R \equiv 0$ in $B_R(0)$, $\psi_R(x) \leq \|x\|^p$ in $B_{2R}(0) \setminus B_R(0)$, $\psi_R(x) = \|x\|^p$ outside $B_{2R}(0)$, and $\|\nabla \psi_R\| \leq 3p\psi_R^{1/p'}$. Define the corresponding functions

$$f_R(\xi) := \int_D \psi_R d\mu[\xi] \quad \text{and} \quad h_R(\xi) := \left(\frac{1}{R} + f_R(\xi) \right)^{1/p}, \quad \xi \in \Omega.$$

$f_R \in W^{1,1}(\Omega)$ by Lemma 6.3.1, hence $h_R \in W^{1,1}(\Omega)$ and $\nabla h_R = \frac{\nabla f_R}{(1/R + f_R)^{1-1/p}}$. Note that

$$\begin{aligned} \|\nabla f_R(\xi)\|^p &= \left\| \int_{D \setminus B_R(0)} V(\xi, x) \nabla \psi_R(x) d\mu[\xi](x) \right\|^p \\ &\leq \left(\int_{D \setminus B_R(0)} \|\nabla \psi_R\|^{p'} d\mu[\xi] \right)^{p/p'} \int_{D \setminus B_R(0)} \|V(\xi, x)\|^p d\mu[\xi](x) \\ &\leq \left(\int_D (3p)^{p'} \psi_R d\mu[\xi] \right)^{p-1} \int_{D \setminus B_R(0)} \|V(\xi, x)\|^p d\mu[\xi](x) \\ &= (3p)^p f_R^{p-1} \int_{D \setminus B_R(0)} \|V(\xi, x)\|^p d\mu[\xi](x), \end{aligned}$$

hence

$$\int_\Omega \|\nabla h_R\|^p = \int_\Omega \frac{\|\nabla f_R\|^p}{(1/R + f_R)^{p-1}} \leq (3p)^p \int_{\Omega \times (D \setminus B_R(0))} \|V\|^p d\mu.$$

Furthermore,

$$\int_\Omega h_R^p = \frac{|\Omega|}{R} + \int_\Omega \left(\int_D \psi_R d\mu[\xi] \right) d\xi \leq \frac{|\Omega|}{R} + \int_{\Omega \times (D \setminus B_R(0))} \|x\|^p d\mu(\xi, x),$$

thus $h_R \in W^{1,p}(\Omega)$. Recall that w.l.o.g. we assumed Ω is a ball, thus one can extend h_R to \mathbb{R}^m in such way that $h_R \geq 0$ and

$$\|\nabla h_R\|_{L^p(\mathbb{R}^m)}^p \leq C \left(\frac{1}{R} + \int_{\Omega \times (D \setminus B_R(0))} [\|x\|^p + \|V\|^p] d\mu \right),$$

where C is a constant depending on Ω and p . Since $\|\nabla h_R\|_{L^p(\mathbb{R}^m)} \rightarrow 0$ as $R \rightarrow \infty$, one can find a sequence $\{R_n\}_{n \in \mathbb{N}}$ such that $\|\nabla h_{R_n}\|_{L^p(\mathbb{R}^m)} \leq 4^{-n}$. By Lemma 4.8.1 in [EG15]

$$\text{Cap}_p(E_n) \leq C 2^{np} \int_{\mathbb{R}^m} \|\nabla h_{R_n}\|^p \leq C 2^{-np},$$

where C is some constant depending on p and m , and

$$E_n := \left\{ \xi \in \mathbb{R}^m : \sup_{r>0} \int_{B_r(\xi)} h_{R_n} > 2^{-n} \right\}.$$

Note that E_n is a Borel set. Then the Borel–Cantelli lemma yields that $\text{Cap}_p(E) = 0$ for $E := \bigcap_{k \in \mathbb{N}} \bigcup_{n \geq k} E_n$. Using again Theorem 4.8.1 in [EG15] take a Borel set $F \subset \mathbb{R}^m$ such that $\text{Cap}_p(F) = 0$ and for all $n \in \mathbb{N}$ and $\xi \in \mathbb{R}^m \setminus F$ it holds that

$$\int_{B_r(\xi)} h_{R_n} \rightarrow h_{R_n}^*(\xi) \quad \text{and} \quad \int_{B_r(\xi)} |h_{R_n}(\zeta) - h_{R_n}^*(\xi)|^{p^*} d\zeta \rightarrow 0 \quad \text{as } r \rightarrow 0. \quad (6.5)$$

Now fix an arbitrary $\xi \in \mathbb{R}^m \setminus (A \cup E \cup F)$ with the set A defined in Step 1. There is $k = k(\xi) \in \mathbb{N}$ such that $\xi \notin E_n$ for all $n \geq k$, thus $h_{R_n}^*(\xi) \leq 2^{-n}$. By the Minkowski inequality we get for any $r > 0$

$$\begin{aligned} \int_{\mathbb{R}^m \setminus B_{2R_n}(0)} \|x\|^p d\mu_r[\xi](x) &\leq \int_D \psi_{R_n} d\mu_r[\xi] = \int_{B_r(\xi)} f_{R_n} \leq \int_{B_r(\xi)} h_{R_n}^p \\ &\leq \left[h_{R_n}^*(\xi) + \left(\int_{B_r(\xi)} |h_{R_n}(\zeta) - h_{R_n}^*(\xi)|^p d\zeta \right)^{1/p} \right]^p \\ &\leq \left[2^{-n} + \left(\int_{B_r(\xi)} |h_{R_n}(\zeta) - h_{R_n}^*(\xi)|^p d\zeta \right)^{1/p} \right]^p, \end{aligned}$$

hence due to (6.5)

$$\limsup_{r \rightarrow 0} \int_{\mathbb{R}^m \setminus B_{2R_n}(0)} \|x\|^p d\mu_r[\xi](x) \leq 2^{-np}.$$

Recall that $\mu_r[\xi] \rightharpoonup \mu^*[\xi]$, thus by Theorem 6.9 in [Vil09] we conclude that $W_p(\mu_r[\xi], \mu^*[\xi]) \rightarrow 0$.

Step 3. To prove (6.3), consider a dense countable set $\{\nu_l\}_{l \in \mathbb{N}} \subset \mathcal{P}_p(D)$. Note that any function $d_l(\xi) := W_p(\mu[\xi], \nu_l)$ is Sobolev. Then Theorem 4.8.1 (ii) in [EG15] and the previous steps yield that there is a zero-capacity Borel set $G \subset \Omega$ such that for any $\xi \in \Omega \setminus G$ and for all $n, l \in \mathbb{N}$

$$\begin{aligned} \int_{B_r(\xi)} |d_l(\zeta) - d_l^*(\xi)|^{p^*} d\zeta &\rightarrow 0, \quad \int_{B_r(\xi)} \left| \int_D \varphi_n d\mu[\zeta] - \int_D \varphi_n d\mu^*[\xi] \right|^{p^*} d\zeta \rightarrow 0, \\ \int_{B_r(\xi)} \left| m_p^{1/p}(\mu[\zeta]) - m_p^{1/p}(\mu^*[\xi]) \right|^{p^*} d\zeta &\rightarrow 0 \end{aligned}$$

as $r \rightarrow 0$. The last result follows from the fact that $m_p^{1/p}(\cdot)$ is 1-Lipschitz continuous w.r.t. W_p and

$$\int_{B_r(\xi)} m_p(\mu[\zeta]) d\zeta = m_p(\mu_r[\xi]) \rightarrow m_p(\mu^*[\xi]),$$

hence $(m_p^{1/p} \circ \mu)^*(\xi) = m_p^{1/p}(\mu^*[\xi])$. Assume that $d_l^*(\xi) \neq W_p(\mu^*[\xi], \nu_l)$ for some $l \in \mathbb{N}$. Then there is a sequence $\zeta_k \rightarrow \xi$ such that $d_l(\zeta_k) \rightarrow d_l^*(\xi)$, $m_p(\mu[\zeta_k]) \rightarrow m_p(\mu^*[\xi])$, and $\int_D \varphi_n d\mu[\zeta_k] \rightarrow \int_D \varphi_n d\mu^*[\xi]$ for all n . Thus, $W_p(\mu[\zeta_k], \mu^*[\xi]) \rightarrow 0$ by Proposition 2.3.2, and we obtain a contradiction. Therefore, $d_l^*(\xi) = W_p(\mu^*[\xi], \nu_l)$ for all $l \in \mathbb{N}$.

Finally, for any l

$$\begin{aligned} \int_{B_r(\xi)} W_p^{p^*}(\mu[\zeta], \mu^*[\xi]) d\zeta &\leq 2^{p^*-1} \left(W_p^{p^*}(\mu^*[\xi], \nu_l) + \int_{B_r(\xi)} W_p^{p^*}(\mu[\zeta], \nu_l) d\zeta \right) \\ &\rightarrow 2^{p^*-1} W_p^{p^*}(\mu^*[\xi], \nu_l) \quad \text{as } r \rightarrow 0, \end{aligned}$$

and since $\{\nu_l\}_{l \in \mathbb{N}}$ is dense in $\mathcal{P}_p(D)$, we obtain (6.3). \square

6.4 Convergence

In this section we introduce some notions of convergence in $W^{1,p}(\Omega; \mathcal{P}_p(D))$ allowing us to obtain a stability of precise representatives, which is important to study the regularized optimal transportation problem in the next section.

Let us introduce a truncated p -Wasserstein distance for $1 < p < \infty$:

$$\bar{W}_p^p(\mu, \nu) \stackrel{\text{def}}{=} \inf_{\pi \in \Pi(\mu, \nu)} \min\{\|x - y\|^p, 1\} d\pi(x, y), \quad \mu, \nu \in \mathcal{P}(D).$$

Clearly, it is nothing but the p -Wasserstein distance for the truncated metric $\min\{\|x - y\|, 1\}$, and for $p = 1$ it is equivalent to the Kantorovich–Rubinstein distance (2.1). By Proposition 2.3.2, the convergence w.r.t. \bar{W}_p is equivalent to the narrow convergence since the truncated metric is bounded.

Lemma 6.4.1. *Let $1 < p < \infty$ and $\{\mu_n\}_{n \in \mathbb{N}} \subset W^{1,p}(\Omega, \mathcal{P}_p(D))$ be such that $\text{Dir}_p(\mu_n) \leq C$ for all n with some constant $C < \infty$. If*

$$\mu_n \rightharpoonup \nu \in \mathcal{M}_+(\Omega \times D),$$

then $\nu = \mu \otimes \mathcal{L}|_\Omega$ for some Borel map $\mu: \Omega \rightarrow \mathcal{P}(D)$, and

$$\int_\Omega \bar{W}_1(\mu[\xi], \mu_n[\xi]) \, d\xi \rightarrow 0. \quad (6.6)$$

Proof. First of all, note that ν is a Young measure, thus $\nu = \mu \otimes \mathcal{L}|_\Omega$ for some Borel map $\mu: \Omega \rightarrow \mathcal{P}(D)$. Like in Step 1 in the proof of Lemma 6.3.2, let $\{\varphi_k\}_{k \in \mathbb{N}}$ be a dense countable subset of $C_c^1(\mathbb{R}^d)$, $g_n^k(\xi) := \int_D \varphi_k \, d\mu_n[\xi]$, $g_n^k \in W^{1,p}(\Omega) \cap L^\infty(\Omega)$, and $g^k(\xi) := \int_D \varphi_k \, d\mu[\xi]$. For any $\eta \in C_c^1(\Omega)$ we have

$$\int_\Omega \eta g_n^k = \int_{\Omega \times D} \eta(\xi) \varphi_k(\xi, x) \, d\mu_n(\xi, x) \rightarrow \int_{\Omega \times D} \eta(\xi) \varphi_k(\xi, x) \, d\nu(\xi, x) = \int_\Omega \eta g^k.$$

This together with the Rellich–Kondrachov theorem yields that $g_n^k \rightarrow g^k$ in $L_{\text{loc}}^p(\Omega)$. Therefore, up to a subsequence, $g_n^k \rightarrow g^k$ a.s. in Ω for all $k \in \mathbb{N}$, hence $\mu_n[\xi] \rightharpoonup \mu[\xi]$ for a.e. ξ . The claim follows by the dominated convergence theorem since $\bar{W}_1 \leq 1$. \square

The first notion of convergence in $W^{1,p}(\Omega, \mathcal{P}_p(D))$ is based on the Radon–Riesz property. This is an analogue of the strong convergence in the standard Sobolev space.

Proposition 6.4.2. *Let $\mu \in W^{1,p}(\Omega, \mathcal{P}(D))$ for some $1 < p < \infty$, and a sequence $\{\mu_n\}_{n \in \mathbb{N}} \subset W^{1,p}(\Omega, \mathcal{P}(D))$ be such that $\mu_n \rightharpoonup \mu$ and*

$$\text{Dir}_p(\mu_n) \rightarrow \text{Dir}_p(\mu).$$

Then

$$\int_\Omega \int_{D^2} \|V(\xi, x) - V_n(\xi, x')\|^p \, d\pi_n[\xi](x, x') \, d\xi \rightarrow 0, \quad (6.7)$$

where $\pi_n[\xi] \in \Pi_o(\mu[\xi], \mu_n[\xi])$ is any measurable selection of optimal transport plans for the cost function $\min\{\|x - y\|, 1\}$, and V, V_n are the velocity fields of μ and μ_n , respectively.

Proof. If $\text{Dir}_p(\mu) = 0$, then the claim holds trivially. Now assume w.l.o.g. that $\text{Dir}_p(\mu) = 1$. Since $\mu_n \rightharpoonup \mu$ and $\text{Dir}_p(\mu_n) \leq C$ with some constant C for all $n \in \mathbb{N}$, we have by the Prokhorov theorem that, up to a subsequence,

$$V_n \mu_n \rightharpoonup W \mu$$

with $W \in L^p(\Omega \times D, \mu; \mathbb{R}^{m \times d})$. Clearly, W satisfies the continuity equation for μ : $\nabla_\xi \mu + \nabla_x(W \mu) = 0$, and due to the lower semicontinuity of the Benamou–Brenier functional $(V \mu, \mu) \mapsto \int \|V\|^p \, d\mu$ we have

$$\|W\|_{L^p(\mu)} \leq \liminf \|V_n\|_{L^p(\mu_n)} = \|V\|_{L^p(\mu)},$$

thus $W = V$ as V is the unique minimizer of $\|V\|_{L^p(\mu)}$ satisfying (6.2).

Now fix $U \in C_c^1(\Omega \times D; \mathbb{R}^{m \times d})$. Denote $\pi_n := \pi_n \otimes \mathcal{L}|_\Omega \in \mathcal{M}_+(\Omega \times D^2)$. One has

$$\begin{aligned} \int_{\Omega \times D} \langle V, U \rangle \, d\mu &= \lim \int_{\Omega \times D} \langle V_n, U \rangle \, d\mu_n \\ &= \lim \int_{\Omega \times D^2} \langle V_n(\xi, x'), U(\xi, x') \rangle \, d\pi_n(\xi, x, x') \\ &= \lim \int_{\Omega \times D} \langle \bar{V}_n, U \rangle \, d\mu + \lim \int_{\Omega \times D^2} \langle V_n(\xi, x'), U(\xi, x') - U(\xi, x) \rangle \, d\pi_n(\xi, x, x'), \end{aligned}$$

where $\bar{V}_n(\xi, x) := \int_D V_n d\pi_n[\xi] \Big|_x$ is the barycentric projection of V_n . The last term in the above inequality can be estimated as follows:

$$\begin{aligned}
& \left| \int_{\Omega \times D^2} \langle V_n(\xi, x'), U(\xi, x') - U(\xi, x) \rangle d\pi_n(\xi, x, x') \right| \\
& \leq \int_{\Omega} \int_{D^2} \|V_n(\xi, x')\| \cdot \|U(\xi, x') - U(\xi, x)\|_* d\pi_n[\xi](x, x') d\xi \\
& \leq C \int_{\Omega} \int_{D^2} \|V_n(\xi, x')\| \min\{\|x' - x\|, 1\} d\pi_n[\xi](x, x') d\xi \\
& \leq C \int_{\Omega} \|V_n(\xi, \cdot)\|_{L^p(\mu_n[\xi])} \left(\int_{D^2} \min\{\|x' - x\|, 1\}^{p'} d\pi_n[\xi](x, x') \right)^{1/p'} d\xi \\
& \leq C \|V_n\|_{L^p(\mu_n)} \left(\int_{\Omega} \bar{W}_1(\mu[\xi], \mu_n[\xi]) d\xi \right)^{1/p'} \\
& = C \text{Dir}_p(\mu_n) \left(\int_{\Omega} \bar{W}_1(\mu[\xi], \mu_n[\xi]) d\xi \right)^{1/p'} \rightarrow 0,
\end{aligned}$$

where $C = 2 \max\|U\|_* + \max\|D_x U\|$ and the last line follows from Lemma 6.4.1. Combining the above equations we obtain

$$\int_{\Omega \times D} \langle \bar{V}_n, U \rangle \mu \rightarrow \int_{\Omega \times D} \langle V, U \rangle \mu. \quad (6.8)$$

Since

$$\int_{\Omega \times D} \|\bar{V}_n\|^p d\mu \leq \int_{\Omega \times D} \|V_n\|^p d\mu_n \rightarrow \int_{\Omega \times D} \|V\|^p d\mu,$$

we conclude that $\|\bar{V}_n\|_{L^p(\mu)} \rightarrow \|V\|_{L^p(\mu)}$. Thus, $\bar{V}_n \rightarrow V$ in $L^p(\mu)$ according to (6.8), and $\bar{V}_n \rightarrow V$ in $L^p(\Omega \times D, \mu; \mathbb{R}^{m \times d})$ due to the uniform convexity.

Define $v_n := \|V_n\|$ and $\bar{v}_n := \|\bar{V}_n\|$. Hanner's inequalities [Han56] yield that if $p \geq 2$, then

$$\begin{aligned}
\|v_n + \bar{v}_n\|_{L^p(\pi_n)}^p + \|v_n - \bar{v}_n\|_{L^p(\pi_n)}^p & \leq (\|v_n\|_{L^p(\pi_n)} + \|\bar{v}_n\|_{L^p(\pi_n)})^p + \left| \|v_n\|_{L^p(\pi_n)} - \|\bar{v}_n\|_{L^p(\pi_n)} \right|^p \\
& \rightarrow 2^p \|v\|_{L^p(\mu)}^p = 2^p \text{Dir}_p(\mu).
\end{aligned}$$

On the other hand, by Jensen's inequality

$$\|v_n + \bar{v}_n\|_{L^p(\pi_n)} \geq \|V_n + \bar{V}_n\|_{L^p(\pi_n)} \geq 2\|\bar{V}_n\|_{L^p(\pi_n)} \rightarrow 2\|V\|_{L^p(\mu)} = 2\|v\|_{L^p(\mu)}, \quad (6.9)$$

thus $\|v_n - \bar{v}_n\|_{L^p(\pi_n)}^p \rightarrow 0$. If $1 < p < 2$, then

$$\begin{aligned}
& (\|v_n + \bar{v}_n\|_{L^p(\pi_n)} + \|v_n - \bar{v}_n\|_{L^p(\pi_n)})^p + \left| \|v_n + \bar{v}_n\|_{L^p(\pi_n)} - \|v_n - \bar{v}_n\|_{L^p(\pi_n)} \right|^p \\
& \leq 2^p \left(\|v_n\|_{L^p(\pi_n)}^p + \|\bar{v}_n\|_{L^p(\pi_n)}^p \right) \rightarrow 2^{p+1} \|v\|_{L^p(\mu)}^p
\end{aligned}$$

and by (6.9)

$$\begin{aligned}
& \limsup \left(\|v_n + \bar{v}_n\|_{L^p(\pi_n)} + \|v_n - \bar{v}_n\|_{L^p(\pi_n)} \right)^p + \left| \|v_n + \bar{v}_n\|_{L^p(\pi_n)} - \|v_n - \bar{v}_n\|_{L^p(\pi_n)} \right|^p \\
& \geq (2\|v\|_{L^p(\mu)} + \limsup \|v_n - \bar{v}_n\|_{L^p(\pi_n)})^p + (2\|v\|_{L^p(\mu)} - \limsup \|v_n - \bar{v}_n\|_{L^p(\pi_n)})_+^p,
\end{aligned}$$

thus $\|v_n - \bar{v}_n\|_{L^p(\pi_n)} \rightarrow 0$ due to the strict convexity of the function $t \mapsto (a+t)^p + (a-t)_+^p$. Therefore, in both cases we obtain that

$$\|v_n - \bar{v}_n\|_{L^p(\pi_n)}^p \rightarrow 0. \quad (6.10)$$

Furthermore, the strict convexity of the norm on $\mathbb{R}^{m \times d}$ implies that there exists a monotone function $\delta: [0, 2] \rightarrow [0, 1]$ strictly positive outside $\{0\}$ such that

$$\left\| \frac{X+Y}{2} \right\| \leq \max\{\|X\|, \|Y\|\} \left[1 - \delta \left(\frac{\|X-Y\|}{\max\{\|X\|, \|Y\|\}} \right) \right] \quad \forall X, Y \in \mathbb{R}^{m \times d}.$$

Then

$$\begin{aligned} \int \left\| \frac{V_n + \bar{V}_n}{2} \right\|^p d\pi_n &\leq \int \max\{v_n, \bar{v}_n\}^p \left[1 - \delta \left(\frac{\|V_n - \bar{V}_n\|}{\max\{v_n, \bar{v}_n\}} \right) \right]^p d\pi_n \\ &\leq \int \max\{v_n, \bar{v}_n\}^p d\pi_n - \int \max\{v_n, \bar{v}_n\}^p \delta \left(\frac{\|V_n - \bar{V}_n\|}{\max\{v_n, \bar{v}_n\}} \right) d\pi_n. \end{aligned}$$

Due to (6.9) and (6.10)

$$\lim \int \max\{v_n, \bar{v}_n\}^p d\pi_n = \lim \int \left\| \frac{V_n + \bar{V}_n}{2} \right\|^p d\pi_n = \int \|V\|^p d\mu,$$

thus

$$\int \max\{v_n, \bar{v}_n\}^p \delta \left(\frac{\|V_n - \bar{V}_n\|}{\max\{v_n, \bar{v}_n\}} \right) d\pi_n \rightarrow 0.$$

obviously, for any $\varepsilon > 0$ there is $C_\varepsilon > 0$ such that $t^p \leq \varepsilon + C_\varepsilon \delta(t)$ for all $t \in [0, 2]$, hence

$$\begin{aligned} \int \|V_n - \bar{V}_n\|^p d\pi_n &= \int \max\{v_n, \bar{v}_n\}^p \left(\frac{\|V_n - \bar{V}_n\|}{\max\{v_n, \bar{v}_n\}} \right)^p d\pi_n \\ &\leq \int \max\{v_n, \bar{v}_n\}^p \left[\varepsilon + C_\varepsilon \delta \left(\frac{\|V_n - \bar{V}_n\|}{\max\{v_n, \bar{v}_n\}} \right) \right] d\pi_n \rightarrow \varepsilon \int \|V\|^p d\mu \quad \text{as } n \rightarrow \infty. \end{aligned}$$

Since $\|\bar{V}_n - V\|_{L^p(\pi_n)} = \|\bar{V}_n - V\|_{L^p(\mu)} \rightarrow 0$, the claim follows. \square

Corollary 6.4.3. *Under the assumptions of Proposition 6.4.2 for any $\varphi \in C_b^1(\mathbb{R}^d)$ (i.e. such that $\varphi \in C_b(\mathbb{R}^d)$ and $\nabla\varphi \in C_b(\mathbb{R}^d; \mathbb{R}^d)$) and*

$$g: \xi \mapsto \int_D \varphi d\boldsymbol{\mu}[\xi], \quad g_n: \xi \mapsto \int_D \varphi d\boldsymbol{\mu}_n[\xi],$$

it holds that $g_n \rightarrow g$ in $W^{1,p}(\Omega)$.

Proof. According to Lemma 6.3.1 $g, g_n \in W^{1,p}(\Omega)$ and

$$\begin{aligned} \nabla g(\xi) &= \int_D V(\xi, x) \nabla\varphi(x) d\boldsymbol{\mu}[\xi](x), \\ \nabla g_n(\xi) &= \int_D V_n(\xi, x) \nabla\varphi(x) d\boldsymbol{\mu}_n[\xi](x). \end{aligned}$$

Clearly, $|g(\xi) - g_n(\xi)| \leq C\bar{W}_1(\boldsymbol{\mu}[\xi], \boldsymbol{\mu}_n[\xi])$, thus from (6.6) it follows that $g_n \xrightarrow{L^1(\Omega)} g$. Since g and all g_n are uniformly bounded, we have $g_n \xrightarrow{L^p(\Omega)} g$. Further,

$$\begin{aligned} \nabla g_n(\xi) - \nabla g(\xi) &= \int_{D^2} [V_n(\xi, x') \nabla\varphi(x') - V(\xi, x) \nabla\varphi(x)] d\boldsymbol{\pi}_n[\xi](x, x') \\ &= \int_{D^2} [V_n(\xi, x') - V(\xi, x)] \nabla\varphi(x') d\boldsymbol{\pi}_n[\xi](x, x') \\ &\quad + \int_{D^2} V(\xi, x) [\nabla\varphi(x') - \nabla\varphi(x)] d\boldsymbol{\pi}_n[\xi](x, x'). \end{aligned} \tag{6.11}$$

It follows from (6.7) and the boundedness of $\nabla\varphi$ that

$$\left\| \int_{D^2} [V_n(\xi, x') - V(\xi, x)] \nabla\varphi(x') d\boldsymbol{\pi}_n[\xi](x, x') \right\|_{L^p(\Omega)} \rightarrow 0.$$

Now we estimate the second term: fix $R > 0$, then

$$\begin{aligned} &\left\| \int_{D^2} V(\xi, x) (\nabla\varphi(x') - \nabla\varphi(x)) d\boldsymbol{\pi}_n[\xi](x, x') \right\| \\ &\leq R \int_D \|\nabla\varphi(x') - \nabla\varphi(x)\| d\boldsymbol{\pi}_n[\xi](x, x') + C \int_D (\|V(\xi, x)\| - R)_+ d\boldsymbol{\mu}[\xi](x). \end{aligned}$$

Obviously,

$$\left\| \int_D (\|V(\xi, x)\| - R)_+ d\boldsymbol{\mu}[\xi](x) \right\|_{L^p(\Omega)} \rightarrow 0 \quad \text{as } R \rightarrow \infty.$$

Next, for any compact $K \subset D$ and $\varepsilon > 0$ due to the uniform continuity of $\nabla\varphi$ on K there exists a constant $C_{K,\varepsilon} > 0$ such that

$$\|\nabla\varphi(x') - \nabla\varphi(x)\| \leq \varepsilon + C_{K,\varepsilon} \min\{\|x' - x\|, 1\}$$

for any $x, x' \in K$. Therefore,

$$\begin{aligned} & \left\| \int_D \|\nabla\varphi(x') - \nabla\varphi(x)\| d\boldsymbol{\pi}_n[\xi](x, x') \right\|_{L^p(\Omega)} \\ & \leq \varepsilon + C_{K,\varepsilon} \left(\int_\Omega \bar{W}_1^p(\boldsymbol{\mu}[\xi], \boldsymbol{\mu}_n[\xi]) d\xi \right)^{1/p} + 2 \max\|\nabla\varphi\| \left(\int_\Omega (\boldsymbol{\pi}_n[\xi](D^2 \setminus K^2))^p d\xi \right)^{1/p} \\ & \leq \varepsilon + C_{K,\varepsilon} \left(\int_\Omega \bar{W}_1(\boldsymbol{\mu}[\xi], \boldsymbol{\mu}_n[\xi]) d\xi \right)^{1/p} + 2 \max\|\nabla\varphi\| \left(\int_\Omega (\boldsymbol{\pi}_n[\xi](D^2 \setminus K^2))^p d\xi \right)^{1/p} \end{aligned}$$

and

$$\int_\Omega (\boldsymbol{\pi}_n[\xi](D^2 \setminus K^2))^p d\xi \leq \int_\Omega (\boldsymbol{\mu}[\xi](D \setminus K) + \boldsymbol{\mu}_n[\xi](D \setminus K)) d\xi.$$

Thus, (6.6) together with tightness of the sequence $\{\boldsymbol{\mu}_n\}_{n \in \mathbb{N}}$ yield that

$$\left\| \int_D \|\nabla\varphi(x') - \nabla\varphi(x)\| d\boldsymbol{\pi}_n[\xi](x, x') \right\|_{L^p(\Omega)} \rightarrow 0.$$

Finally, substituting the above results into (6.11) we obtain

$$\nabla g_n \xrightarrow{L^p(\Omega)} \nabla g.$$

□

Corollary 6.4.4. *Under the assumptions of Proposition 6.4.2 there exist a subsequence $\{\boldsymbol{\mu}_{n_k}\}_{k \in \mathbb{N}}$ and a Borel set $A \subset \Omega$ such that $\text{Cap}_p(A) = 0$ and*

$$\boldsymbol{\mu}_{n_k}^*[\xi] \rightarrow \boldsymbol{\mu}^*[\xi] \quad \text{for all } \xi \in \Omega \setminus A,$$

where $\boldsymbol{\mu}_n^*$ and $\boldsymbol{\mu}^*$ are the precise representatives of $\boldsymbol{\mu}_n$ and $\boldsymbol{\mu}$.

Proof. As in the proof of Lemma 6.3.2, fix a countable family $\{\varphi_k\}_{k \in \mathbb{N}}$ dense in $C_c^1(D)$ and define functions $g_n^k(\xi) := \int_D \varphi_k d\boldsymbol{\mu}_n[\xi]$, $g^k(\xi) := \int_D \varphi_k d\boldsymbol{\mu}[\xi]$. Since $\|g_n^k - g^k\|_{W^{1,p}(\Omega)} \rightarrow 0$ for all $k \in \mathbb{N}$ according to Corollary 6.4.3, there exists a zero-capacity set $A \subset \Omega$ and a subsequence such that (without relabelling) $(g_n^k)^*(\xi) \rightarrow (g^k)^*(\xi)$ for all $\xi \in \Omega \setminus A$. Recall that $(g_n^k)^*(\xi) = \int_D \varphi_k d\boldsymbol{\mu}_n^*[\xi]$ and $(g^k)^*(\xi) = \int_D \varphi_k d\boldsymbol{\mu}^*[\xi]$ up to a zero-capacity set, thus the claim follows. □

The above convergence in the assumptions of Proposition 6.4.2, which is partially a counterpart of the strong convergence in $W^{1,p}(\Omega)$, is sometimes too strong. In particular, it is not clear how to obtain a compactness w.r.t. this to prove the existence of a solution of the regularized Monge–Kantorovich problem. Another approach is based on the Wasserstein convergence of phase measures introduced in Section 6.2. Assume for simplicity that $|\Omega| = 1$. Let $u \in W^{1,p}(\Omega)$. We say $\varrho \in \mathcal{P}(\Omega \times \mathbb{R} \times \mathbb{R}^m)$ is a *phase measure* of u if $\pi_{\#}^1 \varrho = \mathcal{L}|_\Omega$, $\bar{x} = u$, $\bar{v} = \nabla u$, and $\int (|x|^p + \|v\|^p) d\varrho(\xi, x, v) < \infty$. Here $\bar{x}(\xi) := \int_{\mathbb{R} \times \mathbb{R}^m} x d\varrho|_\xi$ and $\bar{v}(\xi) := \int_{\mathbb{R} \times \mathbb{R}^m} v d\varrho|_\xi$ are the barycentric projections. Define the cost function on $(\Omega \times \mathbb{R} \times \mathbb{R}^m)^2$:

$$c((\xi, x, v), (\xi', x', v')) := \min\{\|\xi - \xi'\|, 1\} + |x - x'|^p + \|v - v'\|^p,$$

and the corresponding transportation functional $J_p := J_c$ (see Section 2.2). The next lemma, which can be of independent interest, ensures the convergence of precise representatives once phase measures converge in the transportation topology.

Lemma 6.4.5. *Take $\mu \in \mathcal{P}(\Omega)$ such that $\mu \ll \text{Cap}_p$. Let $u, u_n \in W^{1,p}(\Omega)$, $n \in \mathbb{N}$, and $\varrho, \varrho_n \in \mathcal{P}(\Omega \times \mathbb{R} \times \mathbb{R}^m)$ be their phase measures such that $J_p(\varrho_n, \varrho) \rightarrow 0$. Then $u_n^* \rightarrow u^*$ in μ , i.e. for any $\varepsilon > 0$*

$$\mu(\{\xi \in \mathbb{R}^m : |u_n^*(\xi) - u^*(\xi)| > \varepsilon\}) \rightarrow 0.$$

Proof. Note that since $\mu(\Omega) = 1$, for any $\varepsilon > 0$ there is a compact $K(\varepsilon) \subset \Omega$ such that $\mu(K(\varepsilon)) \geq 1 - \varepsilon$. Therefore, it is enough to consider the case where $\text{supp } \mu \subset \subset \Omega$.

The case of singular μ . Assume that $\mu \perp \mathcal{L}$. The idea of the proof is as follows. We are going to show that for any $\varepsilon > 0$ there are sets $S(\varepsilon), E_n(\varepsilon)$ such that $\mu(S(\varepsilon)) \geq 1 - \varepsilon$,

$$\{\xi \in S(\varepsilon) : u_n^*(\xi) - u^*(\xi) > 1\} \subset E_n(\varepsilon),$$

and one has $\limsup_{n \rightarrow \infty} \text{Cap}_p(E_n(\varepsilon)) \rightarrow 0$ as $\varepsilon \rightarrow 0$. Since $\mu \ll \text{Cap}_p$, this implies that

$$\mu(\{x \in \Omega : u_n^* - u^* > 1\}) \rightarrow 0.$$

We conclude multiplying functions u_n and u by an arbitrary constant.

Step 1. The proof is partially based on the ideas from Lemma 4.8.1 in [EG15]. Fix an open set Ω' such that $\text{supp } \mu \subset \Omega' \subset \subset \Omega$. Take $\varepsilon > 0$ and an open set $U = U(\varepsilon) \subset \Omega'$ with $\mu(U) = 1$, $|U| \leq \varepsilon$ (it is possible since $\mu \perp \mathcal{L}$). Now choose $0 < r_0 = r_0(\varepsilon) \leq \min\{1, d(\Omega', \partial\Omega)/2\}$ satisfying $\mu(U^{-3r_0}) \geq 1 - \varepsilon$, and denote $S = S(\varepsilon) := U^{-3r_0}$, where

$$U^{-r} := \{\xi \in U : d(\xi, \partial U) > r\}, \quad r > 0,$$

is an open subset of U .

Define $w_n := u_n - u$ and $w_n^* := u_n^* - u^*$ (slightly abusing notation). Due to Theorem 4.8.1 in [EG15] there exists an open set $V_n = V_n(\varepsilon) \subset S$ such that $\text{Cap}_p(V_n) < \varepsilon$, w_n^* is continuous on $S \setminus V_n$, and

$$\int_{B_r(\xi)} w_n \xrightarrow{r \rightarrow 0} w_n^*(\xi) \quad \forall \xi \in S \setminus V_n.$$

In particular, one can find a nonnegative function $f_n = f_n(\varepsilon) \in W^{1,p}(\mathbb{R}^m)$ such that $V_n \subset \text{int}\{f_n \geq 1\}$ and $\int_{\mathbb{R}^m} \|\nabla f_n\|^p < \varepsilon$.

Now define

$$A_n = A_n(\varepsilon) := \{\xi \in S \setminus V_n : w_n^*(\xi) > 1\}.$$

Note that $E_n := A_n \cup V_n$ is open. Also consider a family of balls

$$\mathcal{F}_n = \mathcal{F}_n(\varepsilon) := \left\{ B = \bar{B}_r(\xi) : \xi \in A_n, r < r_0, \left| \int_B w_n - w_n^*(\xi) \right| < w_n^*(\xi) - 1 \right\}.$$

By Besicovitch's covering theorem [EG15] there exist $N = N(m)$ countable families of disjoint balls $\{B_{ij}\}_{j \in \mathbb{N}} \subset \mathcal{F}_n$, $i = 1, \dots, N$, satisfying

$$A_n \subset \bigcup_{i=1}^n \bigcup_{j=1}^{\infty} B_{ij} \subset U^{-2r_0}. \quad (6.12)$$

Consider $B_{ij} = \bar{B}_r(\xi)$; the Sobolev extension theorem and Poincaré's inequality for balls [EG15, Theorem 4.5.2] yield that there is a function $f_{ij} \in W^{1,p}(\mathbb{R}^m)$ such that $f_{ij}|_{B_{ij}} = \left(\int_{B_{ij}} w_n - w_n \right)_+$ and

$$\|f_{ij}\|_{W^{1,p}} \leq C \|\nabla w_n\|_{L^p(B_{ij})}. \quad (6.13)$$

Finally, define $g_n = g_n(\varepsilon) := (\tilde{w}_n)_+ + f_n + \sup_{i,j} f_{ij}$, with a Sobolev function \tilde{w}_n such that $\tilde{w}_n \geq w_n$ on any ball B_{ij} . Note that for any $\xi \in B_{ij}$ one has

$$g_n(\xi) \geq w_n(\xi) + f_{ij}(\xi) \geq \int_{B_{ij}} w_n > 1,$$

and $f_n(\xi) \geq 1$ for any $\xi \in V_n$, thus $E_n = A_n \cup V_n \subset \{g_n \geq 1\}$. Since E_n is open we have $E_n \subset \text{int}\{g_n \geq 1\}$, therefore

$$\text{Cap}_p(E_n) \leq \int \|\nabla g_n\|^p \leq C \int \left(\|\nabla \tilde{w}_n\|^p + \|\nabla f_n\|^p + \|\nabla \sup_{i,j} f_{ij}\|^p \right). \quad (6.14)$$

Step 2. Now we are going to estimate the r.h.s. of (6.14). Recall that $\int \|\nabla f_n\|^p \leq \varepsilon$. Furthermore, due to (6.13), (6.12), and Lemma 4.7.2 in [EG15]

$$\begin{aligned} \int \|\nabla \sup_{i,j} f_{ij}\|^p &\leq \int \sup_{i,j} \|\nabla f_{ij}\|^p \leq \sum_{i=1}^N \sum_{j=1}^{\infty} \int \|f_{ij}\|_{W^{1,p}}^p \\ &\leq \sum_{i=1}^N \sum_{j=1}^{\infty} \int_{B_{ij}} \|\nabla w_n\|^p \leq CN \int_{U^{-2r_0}} (\|\nabla u_n\|^p + \|\nabla u\|^p). \end{aligned}$$

Let π_n be an optimal transport plan between ϱ_n and ϱ . Then using Jensen's inequality we get

$$\begin{aligned} \int_{U^{-2r_0}} \|\nabla u_n\|^p &\leq \int \|v_n\|^p \mathbb{1}_{\xi_n \in U^{-2r_0}} d\varrho_n(\xi_n, x_n, v_n) \\ &\leq C \int (\|v\|^p + \|v_n - v\|^p) \mathbb{1}_{\xi_n \in U^{-2r_0}} d\pi_n \\ &\leq C \left(J_p(\varrho_n, \varrho) + \int \|v\|^p \mathbb{1}_{\xi_n \in U^{-2r_0}} d\pi_n \right). \end{aligned}$$

Since $\int \|v\|^p d\varrho < \infty$, there exists a monotone function $\delta: \mathbb{R}_+ \rightarrow \mathbb{R}_+$ such that $\delta(t) \rightarrow 0$ as $t \rightarrow 0$, and for any measurable $\psi: \Omega \rightarrow [0, 1]$ one has

$$\int \psi(\xi) \|v\|^p d\varrho(\xi, x, v) \leq \delta \left(\int_{\Omega} \psi \right).$$

Therefore, using that $\pi_{\#}^1 \varrho = \pi_{\#}^1 \varrho_n = \mathcal{L}|_{\Omega}$ we get

$$\begin{aligned} \int_{U^{-2r_0}} \|\nabla u\|^p &\leq \int \|v\|^p \mathbb{1}_{\xi \in U^{-2r_0}} d\varrho \leq \delta(|U^{-2r_0}|) \leq \delta(|U|) \leq \delta(\varepsilon), \\ \int \|v\|^p \mathbb{1}_{\xi_n \in U^{-2r_0}} d\pi_n &\leq \delta(|U^{-2r_0}|) \leq \delta(\varepsilon). \end{aligned}$$

Combining these bound together, we obtain from (6.14) that

$$\text{Cap}_p(E_n) \leq C \left(\int \|\nabla \tilde{w}_n\|^p + \varepsilon + J_p(\varrho_n, \varrho) + \delta(\varepsilon) \right). \quad (6.15)$$

Note that there is no guarantee that $\int_{\Omega} \|\nabla w_n\|^p$ is small, thus we cannot just take $\tilde{w}_n = w_n$, even despite the fact that w_n in general does not vanish on $\partial\Omega$. Instead, we will construct $\tilde{w}_n = \tilde{w}_n(\varepsilon) \in W_0^{1,p}(\Omega)$ such that $\tilde{w}_n \equiv w_n$ on U^{-2r_0} , and $\int_{\Omega} \|\nabla \tilde{w}_n\|^p$ is small enough. First, take $\varkappa = \varkappa(\varepsilon) \in C^\infty(\mathbb{R}^m)$ such that $\varkappa|_{U^{-2r_0}} \equiv 0$, $\varkappa|_{\mathbb{R}^m \setminus U^{-r_0}} \equiv 1$, and a mollifier $\eta \in C^\infty(\mathbb{R}^m)$, $\text{supp } \eta = B_1(0)$. Fix $0 < h = h(\varepsilon) < \max \left\{ r_0, \frac{1}{2 \max \|\nabla \varkappa\|} \right\}$. Consider

$$w_n^h(\xi) := \int_{B_1(0)} \eta(e) w_n(\xi + h\varkappa(\xi)e) de, \quad \xi \in \Omega^{-r_0}.$$

Note that $w_n^h \equiv w_n$ on U^{-2r_0} and $w_n^h \equiv \eta_h * w_n$ on $\Omega^{-r_0} \setminus U^{-r_0}$. Moreover, $w_n^h \in W^{1,p}(\Omega^{-r_0})$ and

$$\int_{U^{-r_0}} \|\nabla w_n^h\|^p \leq \int_{B_1(0)} \eta(e) \int_{U^{-r_0}} \|\nabla w_n(\xi + h\varkappa(\xi)e)\|^p d\xi de \leq C \int_U \|\nabla w_n\|^p$$

because $\xi \mapsto \xi + h\chi(\xi)e$ is a bilipschitz map for any $e \in B_1(0)$. Again,

$$\int_U \|\nabla w_n\|^p \leq C(J_p(\varrho_n, \varrho) + \delta(|U|)) \leq C(J_p(\varrho_n, \varrho) + \delta(\varepsilon)). \quad (6.16)$$

Furthermore, for any $\zeta \in \Omega^{-r_0}$

$$\begin{aligned} \nabla(\eta_h * w_n)(\zeta) &= (\eta_h * \nabla w_n)(\zeta) \\ &= \int_{\Omega} \eta_h(\zeta - \xi)(\nabla u_n(\xi) - \nabla u(\xi)) \, d\xi \\ &= \int \eta_h(\zeta - \xi_n) v_n \, d\varrho_n(\xi_n, x_n, v_n) - \int \eta_h(\zeta - \xi) v \, d\varrho(\xi, x, v) \\ &= \int [\eta_h(\zeta - \xi_n)(v_n - v) + (\eta_h(\zeta - \xi_n) - \eta_h(\zeta - \xi))v] \, d\pi_n, \end{aligned}$$

hence for any $t \in (0, 1)$

$$\begin{aligned} \|\nabla(\eta_h * w_n)(\zeta)\| &\leq C_h \int (\|v_n - v\| + \min\{\|\xi_n - \xi\|, 1\}\|v\|) \, d\pi_n \\ &\leq C_h \int (\|v_n - v\| + t\|v\| + \mathbb{1}\{\|\xi_n - \xi\| > t\} \cdot \|v\|) \, d\pi_n \\ &\leq C_h \left(J_p^{1/p}(\varrho_n, \varrho) + t \int \|v\| \, d\varrho(\xi, x, v) + \delta^{1/p}(\pi_n\{\|\xi_n - \xi\| > t\}) \right). \end{aligned}$$

By Markov's inequality $\pi_n\{\|\xi_n - \xi\| > t\} \leq \frac{1}{t} J_p(\varrho_n, \varrho)$, thus

$$\int_{\Omega^{-r_0} \setminus U^{-r_0}} \|\nabla w_n^h\|^p = \int_{\Omega^{-r_0} \setminus U^{-r_0}} \|\nabla(\eta_h * w_n)\|^p \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

Combining this bound with (6.16) we obtain that

$$\limsup_{n \rightarrow \infty} \int_{\Omega^{-r_0}} \|\nabla w_n^h\|^p \leq C\delta(\varepsilon).$$

Finally, fix a cut-off function $\theta \in C_c^\infty(\mathbb{R}^m)$ (depending only on Ω, Ω') such that $\theta|_{\Omega'} \equiv 1$, $\theta|_{\mathbb{R}^m \setminus \Omega^{-t}} \equiv 0$, with $t := d(\Omega', \partial\Omega)/2 \geq r_0$. Note that $\Omega^{-t} \subset \Omega^{-r_0}$ and $U \subset \Omega'$. Define $\tilde{w}_n := w_n^h \theta$. In the same way as above one can obtain

$$\sup_{\zeta \in \Omega^{-r_0}} |\eta_h * w_n(\zeta)| \rightarrow 0 \quad \text{as } n \rightarrow \infty$$

henceforth

$$\begin{aligned} \limsup_{n \rightarrow \infty} \int_{\mathbb{R}^m} \|\nabla \tilde{w}_n\|^p &\leq C \limsup_{n \rightarrow \infty} \left(\int_{\Omega^{-t}} \|\nabla w_n^h\|^p + \max \|\nabla \theta\|^p \int_{\Omega^{-t} \setminus \Omega'} |w_n^h|^p \right) \\ &\leq C \limsup_{n \rightarrow \infty} \left(\int_{\Omega^{-r_0}} \|\nabla w_n^h\|^p + \max \|\nabla \theta\|^p \int_{\Omega^{-r_0} \setminus \Omega'} |\eta_h * w_n|^p \right) \leq C\delta(\varepsilon). \end{aligned}$$

Substitution of this bound into (6.15) gives us

$$\limsup \text{Cap}_p(E_n) \leq C(\varepsilon + \delta(\varepsilon)).$$

Since

$$\{\xi \in \Omega : u_n^*(\xi) - u^*(\xi) > 1\} \subset E_n \cup (\Omega \setminus S),$$

$\mu(\mathbb{R}^m \setminus S) \leq \varepsilon$, and $\mu \ll \text{Cap}_p$, the claim follows.

The case of general μ . Now take a general μ and consider the Lebesgue decomposition $\mu = \mu_{ac} + \mu_s$: $\mu_s \perp \mathcal{L}$ and $\mu_{ac} \ll \mathcal{L}$. Take $\Omega' \subset \Omega$ with smooth boundary such that $\text{supp } \mu \subset \Omega'$. Since $\int_{\Omega'} \varphi u_n \rightarrow \int_{\Omega'} \varphi u$ for any $\varphi \in C_b(\mathbb{R}^m)$, the Rellich–Kondrachov theorem yields that $u_n \rightarrow u$ in $L^p(\Omega')$. Furthermore, $u_n = u_n^*$ and $u = u^*$ a.e. in Ω' , thus $u_n^* \rightarrow u^*$ in μ_{ac} . The claim follows. \square

Corollary 6.4.6. *Take $\mu \in \mathcal{P}(\Omega)$ such that $\mu \ll \text{Cap}_q$ for some $1 < q < p$. Let $\{u_n\}_{n \in \mathbb{N}}$ be a bounded sequence in $W^{1,p}(\Omega)$. Then, up to a subsequence, there is $u \in W^{1,p}(\Omega)$ such that $u_n^* \rightarrow u^*$ μ -a.e.*

Proof. Take the phase measures $\varrho_n := (\text{id}, u_n, \nabla u_n)_{\#} \mathcal{L}|_{\Omega}$. Since $\int (\|x\|^p + \|v\|^p) d\varrho_n(\xi, x, v)$ are bounded, there is a subsequence and a measure ϱ such that $J_q(\varrho_n, \varrho) \rightarrow 0$ (without relabelling). Obviously, $\int (\|x\|^p + \|v\|^p) d\varrho(\xi, x, v) < \infty$, ϱ is a Young measure and satisfies the continuity equation, thus this is a phase measure of $u := \int x d\varrho|_{\xi} \in W^{1,p}(\Omega)$. According to the above lemma, $u_n^* \rightarrow u^*$ in μ , thus one can extract a subsequence converging μ -a.e. \square

Corollary 6.4.7. *Let $\mu \in \mathcal{P}(\Omega)$ be as in Lemma 6.4.5, $\gamma, \gamma_n \in W^{1,p}(\Omega, \mathcal{P}_p(D))$, ϱ_n and ϱ be their phase measures, and $J(\varrho_n, \varrho) \rightarrow 0$. Then, up to a subsequence,*

$$\gamma_n^*[\xi] \rightarrow \gamma^*[\xi] \text{ for } \mu\text{-a.e. } \xi.$$

Proof. As in the proof of Lemma 6.4.1 take a countable set $\{\varphi_k\}_{k \in \mathbb{N}} \subset C_c^\infty(\mathbb{R}^d)$ dense in $C_c(\mathbb{R}^d)$ and define functions $g_n^k := \int \varphi_k d\gamma_n[\xi]$, $g^k := \int \varphi_k d\gamma[\xi]$. Lemma 6.3.1 implies that $\varrho_n^k := (\xi, \varphi_k(x), V\nabla\varphi(x))_{\#} \varrho_n$ and $\varrho^k := (\xi, \varphi_k(x), V\nabla\varphi(x))_{\#} \varrho$ are phase measures of g_n^k and g^k , respectively. In the same way as in the proof of Corollary 6.4.3 one can show that $J(\varrho_n^k, \varrho^k) \rightarrow 0$ for any $k \in \mathbb{N}$. Using the above lemma we obtain that there is a subsequence such that $(g_n^k)^*(\xi) \rightarrow (g^k)^*(\xi)$ for μ -a.e. ξ (without relabelling). Since $(g_n^k)^*(\xi) = \int \varphi_k d\gamma_n^*[\xi]$ and $(g^k)^*(\xi) = \int \varphi_k d\gamma^*[\xi]$ outside a zero-capacity set, hence μ -a.e., the claim follows from the diagonal extraction argument. \square

6.5 Regularized Monge–Kantorovich problem

Now let us move to the announced regularized optimal transportation problem. Fix a cost function $c: \Omega \times D \rightarrow \mathbb{R}_+$ and an exponent $1 < p < m$. Take a source measure $\mu \in \mathcal{P}(\Omega)$ and a target measure $\nu \in \mathcal{P}(D)$ and consider the following regularized Monge–Kantorovich problem:

$$\inf \left\{ \int_{\Omega} \left[\int_D c(\xi, x) d\gamma^*[\xi](x) \right] d\mu(\xi) + \text{Dir}_p(\gamma) \mid \gamma \in W^{1,p}(\Omega, \mathcal{P}_p(D)), \int_{\Omega} \gamma^*[\xi] d\mu(\xi) = \nu \right\}. \quad (6.17)$$

In terms of phase measures it can be rewritten as

$$\inf \left\{ \int_{\Omega} \left[\int_D c(\xi, x) d\gamma^*[\xi](x) \right] d\mu(\xi) + \int \|V\|^p d\varrho(\xi, x, V) \mid \gamma \in W^{1,p}(\Omega, \mathcal{P}_p(D)), \int_{\Omega} \gamma^*[\xi] d\mu(\xi) = \nu, \varrho \in \mathcal{M}_+(\Omega \times D \times \mathbb{R}^{m \times d}) \text{ is a phase measure of } \gamma \right\}.$$

which also is an (infinite-dimensional) LP problem, like the standard Monge–Kantorovich problem.

Notice that if $\nu \in \mathcal{P}_p(D)$, then $\gamma \equiv \nu$ is a competitor in problem (6.17), thus its value is bounded from above by

$$\int_{\Omega} \left[\int_D c(\xi, x) d\nu(x) \right] d\mu(\xi).$$

The next theorem shows that the above problem admits a solution under quite mild assumptions.

Theorem 6.5.1. *Let $c(\xi, \cdot)$ be l.s.c. for all $\xi \in \Omega$ and Ω be bounded and have a Lipschitz boundary. If $\mu \in \mathcal{P}(\Omega)$ is such that $\mu \ll \text{Cap}_q$ for some $1 < q < p$ and the value of the problem (6.17) is finite, then it admits a solution.*

Remark 6.5.2. Notice that γ^* is defined μ -a.e. once $\mu \ll \text{Cap}_p$ but here we need a stronger assumption.

Lemma 6.5.3. *Let Ω and $\mu \in \mathcal{P}(\Omega)$ be as in Theorem 6.5.1, and μ assign positive mass to every connected component of Ω . Then there is a constant C such that for any $u \in L^1(\Omega)$ with $\nabla u \in L^p(\Omega)$*

$$\|u\|_{L^p(\Omega)} \leq C (\|\nabla u\|_{L^p(\Omega)} + \|u^*\|_{L^p(\Omega, \mu)}).$$

Proof. Assume the assertion is false, then there is a sequence $u_n \in L^1(\Omega)$ such that $\|u\|_{L^p(\Omega)} = 1$ but $\|\nabla u\|_{L^p(\Omega)} \rightarrow 0$ and $\|u_n^*\|_{L^p(\Omega, \mu)} \rightarrow 0$. Then by the Rellich–Kondrachov theorem, up to extraction of a subsequence, u_n converge to some u in $L^p(\Omega)$. Clearly, $\|u\|_{L^p(\Omega)} = 1$, $\nabla u \equiv 0$, thus $u \equiv a_k \in \mathbb{R}$ in every connected component Ω_k of Ω and $\|u_n - u\|_{W^{1,p}(\Omega)} \rightarrow 0$. Hence there is a subsequence such that $u_n^* \rightarrow u^*$ μ -a.e. (without relabelling). Therefore,

$$\sum_k \int_{\Omega_k} |a_k|^p d\mu = \int |u^*|^p d\mu \leq \liminf \int_{\Omega} |u_n^*|^p d\mu \rightarrow 0,$$

thus $a_k = 0$ for all Ω_k , i.e. $u \equiv 0$, which leads to a contradiction. \square

Proof of Theorem 6.5.1. Take a minimizing sequence $\{\gamma_n\}_{n \in \mathbb{N}} \subset W^{1,p}(\Omega, \mathcal{P}(D))$ for (6.17) and let V_n be their velocity fields and $\varrho_n = (\text{id}, V_n)_{\#} \gamma_n$ be their phase measures. Note that if Ω_k is a connected component of Ω and $\mu(\Omega_k) = 0$, then w.l.o.g. $\gamma_n \equiv \delta_0$ in Ω_k , hence we can assume that μ assigns positive mass to every connected component of Ω . Lemma 6.5.3 together with Proposition 6.2.1 ensures that

$$\begin{aligned} \int \|x\|^p d\varrho_n(\xi, x, V) &= \int_{\Omega} m_p(\gamma_n[\xi]) d\xi \\ &\leq C \left(\int_{\Omega} g_{\gamma_n}^p(\xi) d\xi + \int_{\Omega} m_p(\gamma_n^*[\xi]) d\mu(\xi) \right) \leq C \left(\int \|V\|^p d\varrho_n(\xi, x, V) + m_p(\nu) \right), \end{aligned}$$

where g_{γ_n} comes from Definition 6.2. Then $\int (\|x\|^p + \|V\|^p) d\varrho_n(\xi, x, V) \leq M < \infty$ for all n , thus, up to a subsequence, ϱ_n converge to some $\varrho \in \mathcal{M}_+(\Omega \times D \times \mathbb{R}^d)$ in the transportation topology induced by the cost function

$$c((\xi, x, v), (\xi', x', v')) := \min\{\|\xi - \xi'\|, 1\} + |x - x'|^q + \|v - v'\|^q.$$

Clearly, $\int (\|x\|^p + \|V\|^p) d\varrho(\xi, x, V) \leq M$ and ϱ is a phase measure of some $\gamma \in W^{1,p}(\Omega, \mathcal{P}_p(D))$. By Corollary 6.4.7 there is a subsequence such that $\gamma_n^*[\xi] \rightarrow \gamma^*[\xi]$ for μ -a.e. ξ (without relabelling). Therefore, for any test function $\varphi \in C_b(D)$ the dominated convergence theorem yields that

$$\int_{\Omega} \left[\int_D \varphi d\gamma^*[\xi] \right] d\mu(\xi) = \lim \int_{\Omega} \left[\int_D \varphi d\gamma_n^*[\xi] \right] d\mu(\xi) = \int_D \varphi d\nu,$$

thus $\int_{\Omega} \gamma^*[\xi] d\mu(\xi) = \nu$, i.e. γ is a competitor in (6.17). By Fatou's lemma and the lower semicontinuity of $c(\xi, \cdot)$

$$\int_{\Omega} \left[\int_D c(\xi, x) d\gamma^*[\xi](x) \right] d\mu(\xi) \leq \liminf \int_{\Omega} \left[\int_D c(\xi, x) d\gamma_n^*[\xi](x) \right] d\mu(\xi).$$

Since

$$\text{Dir}_p(\gamma) \leq \int \|V\|^p d\varrho(\xi, x, V) \leq \liminf \int \|V\|^p d\varrho_n(\xi, x, V) = \liminf \text{Dir}_p(\gamma_n),$$

we conclude that γ is a solution of (6.17). \square

6.5.1 Open questions

Finally, let us mention that there is a lot of directions for further research concerning the considered problem.

- The existence of a solution if $\mu \ll \text{Cap}_p$ but $\mu \not\ll \text{Cap}_q$ for any $q < p$.

- The stability of solutions of (6.17) w.r.t. change of μ and ν (cf. Propositions 2.2.8 and 3.3.5).
- The relation of this problem to the regularized Monge problem (6.1): do their values coincide and when is a solution of (6.17) induced by a transport map?
- The asymptotic behavior of

$$\inf \left\{ \int_{\Omega} \left[\int_D c(\xi, x) d\gamma^*[\xi](x) \right] d\mu(\xi) + \lambda \text{Dir}_p(\gamma) \mid \gamma \in W^{1,p}(\Omega, \mathcal{P}_p(D)), \int_{\Omega} \gamma^*[\xi] d\mu(\xi) = \nu \right\}$$

as $\lambda \rightarrow +0$. When does it converge to the standard Monge–Kantorovich problem?

Chapter 7

Analysis of iterative Bregman projections

7.1 Introduction

Our focus in this chapter is on the computational aspects of OT-related problems for the case of discrete probability measures. The state-of-the-art approach for the Monge–Kantorovich problem in this setting proposed by M. Cuturi in 2013 [Cut13] is to apply Sinkhorn’s matrix scaling algorithm [Sin74] to the entropy-regularized optimization problem. In [Ben+15] Benamou et al. proposed the iterative Bregman projections (IBP) algorithm for a wide range of OT problems including the multimarginal optimal transport and the Wasserstein (or Fréchet) barycenters. This method can be considered in some cases as an alternating projections (w.r.t. the Kullback–Leibler divergence) algorithm and also as a generalization of the Sinkhorn algorithm.

Here we provide theoretical iteration complexity bounds on IBP applied to the multimarginal OT problem and to the Fréchet barycenter problem in terms of the accuracy ε . Let us also mention that there is a lot of works proposing various algorithms for the considered problems and some of them provide theoretical complexity bounds which are better than the ones we obtain in this chapter (see Section 1.4). However, here we stick to the IBP algorithm because of its simplicity and clarity, which makes it favorable from the practical point of view.

Notations. We define the probability simplex in \mathbb{R}^N as $\Delta^{N-1} := \{x \in \mathbb{R}_+^N : \sum_{i=1}^N x_i = 1\}$. For $x \in \mathbb{R}_+^N$ we denote the negative entropy as

$$H(x) := \sum_{i=1}^N x_i (\log x_i - 1) = \langle x, \log x - \mathbf{1} \rangle.$$

Here $\mathbf{1} = \mathbf{1}_N \in \mathbb{R}^N$ is the vector of ones. The term $-\langle x, \mathbf{1} \rangle$ is added to simplify calculations if the mass of x is not preserved. Here and further by $\log(x)$ ($\exp(x)$) we denote the element-wise logarithm (exponent) of matrix or vector x , and $\langle A, B \rangle := \sum_{i,j=1}^{n,m} A_{ij} B_{ij}$ for any $A, B \in \mathbb{R}^{n \times m}$. For two matrices A and B we also define element-wise multiplication and element-wise division as $A \odot B$ and $\frac{A}{B}$ respectively. The Kullback–Leibler divergence for $x, y \in \mathbb{R}_+^N$ is defined as the Bregman divergence associated with H :

$$KL(x|y) := \sum_{i=1}^N \left(x_i \log \frac{x_i}{y_i} - x_i + y_i \right) = \langle x, \log x - \log y \rangle + \langle y - x, \mathbf{1} \rangle \geq 0.$$

By $[n]$ we denote the set $\{1, \dots, n\}$. If $x \in \mathbb{R}^N$, then we sometimes refer to its j -th component as $[x]_j$.

The chapter is organized as follows. In Section 7.2 we formulate the general problem and formulate the dual version of the IBP algorithm. In Section 7.3 we study the convergence of dual IBP in the abstract setting. Section 7.4 is devoted to the multimarginal optimal transport

problem. In Section 7.5 we consider the application of IBP to the barycenter problem. Finally, Section 7.6 provides some numerical results concerning the convergence of dual IBP.

7.2 Problem statement and preliminaries

Consider the following LP problem:

$$\langle x, c \rangle \rightarrow \min_{x \in \mathbb{R}_+^N \cap \mathcal{C}_1 \cap \dots \cap \mathcal{C}_m}, \quad (7.1)$$

where each \mathcal{C}_i is an affine subspace of \mathbb{R}^N . For simplicity we assume that $c \in [0, 1]^N$. Following [Cut13; Ben+15], add an entropy penalization:

$$\langle x, c \rangle + \lambda H(x) \rightarrow \min_{x \in \mathbb{R}_+^N \cap \mathcal{C}_1 \cap \dots \cap \mathcal{C}_m}, \quad (7.2)$$

where $\lambda > 0$ is a penalization parameter. The problem (7.2) is sometimes called an entropy-linear programming problem [Gas+16]. The idea of IBP is to notice that this is equivalent to minimization of $KL(x|e^{-c/\lambda})$ and use alternating projections on the sets $\mathcal{C}_1, \dots, \mathcal{C}_m$ w.r.t. the Kullback–Leibler divergence: at the step t we choose $i_t \in [m] := \{1, \dots, m\}$ and set

$$x_{t+1} := \operatorname{argmin}_{x \in \mathcal{C}_{i_t}} KL(x|x_t), \quad (7.3)$$

with $x_0 := e^{-c/\lambda}$. Let us remark that if \mathcal{C}_i is not an affine set, then one must add a correction term to ensure the convergence of this algorithm to the solution of (7.2). Actually, IBP can be considered as Dykstra’s algorithm in the non-Euclidean setting [BL00] and, as we will see later, it is equivalent to alternating minimization in the dual problem. However, in all the Monge–Kantorovich problem, the multimarginal OT, and the Wasserstein barycenter problems the sets \mathcal{C}_i are affine. Moreover, in the case of the Monge–Kantorovich problem this is exactly the Sinkhorn algorithm.

Set

$$\mathcal{C}_i = \{x \in \mathbb{R}^N : A_i x = b_i\}, \quad A_i \in \mathbb{R}^{n_i \times N}, \quad b_i \in \mathbb{R}^{n_i}.$$

By the min-max theorem (see [BV04])

$$\begin{aligned} & \min_{x \in \mathbb{R}_+^N \cap \mathcal{C}_1 \cap \dots \cap \mathcal{C}_m} \langle x, c \rangle + \lambda H(x) \\ &= \min_{x \in \mathbb{R}_+^N} \left[\langle x, c + \lambda \log x - \lambda \mathbf{1} \rangle + \lambda \sum_{i=1}^m \sup_{u_i \in \mathbb{R}^{n_i}} \langle u_i, b_i - A_i x \rangle \right] \\ &= \sup_{u_1, \dots, u_m} \left[\lambda \sum_{i=1}^m \langle u_i, b_i \rangle + \inf_{x \in \mathbb{R}_+^N} \left(\langle x, c + \lambda \log x - \lambda \mathbf{1} \rangle - \lambda \sum_{i=1}^m \sup_{u_i \in \mathbb{R}^{n_i}} \langle x, A_i^\top u_i \rangle \right) \right] \\ &= \lambda \sup_{u_1, \dots, u_m} \left[\sum_{i=1}^m \langle u_i, b_i \rangle - \left\langle \exp \left(\sum_{i=1}^m A_i^\top u_i - \frac{c}{\lambda} \right), \mathbf{1} \right\rangle \right], \end{aligned}$$

thus the dual problem to (7.2) (up to a multiple $-\lambda$) is

$$\psi(\mathbf{u}) := \langle x(\mathbf{u}), \mathbf{1} \rangle - \sum_{i=1}^m \langle u_i, b_i \rangle \rightarrow \min_{\mathbf{u} \in \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_m}}, \quad (7.4)$$

where $\mathbf{u} = (u_1, \dots, u_m) \in \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_m}$ and

$$x(\mathbf{u}) := \exp \left(\sum_{i=1}^m A_i^\top u_i - \frac{c}{\lambda} \right).$$

Note that

$$\nabla_{u_i} \psi(\mathbf{u}) = A_i x(\mathbf{u}) - b_i.$$

Let x_λ^* be the unique solution of the primal problem, then \mathbf{u} is a solution of the dual problem (which can not be unique) iff $x(\mathbf{u}) = x_\lambda^*$. In particular, note that (7.3) is equivalent to solving (7.2) with only one set \mathcal{C}_{i_t} instead of $\mathcal{C}_1, \dots, \mathcal{C}_m$ and $-\lambda \log x_t$ instead of c , thus

$$x_{t+1} = \exp(A_{i_t}^\top v_t + \log x_t),$$

where

$$v_t = \operatorname{argmin}_{v \in \mathbb{R}^{n_{i_t}}} \langle \exp(A_{i_t}^\top v + \log x_t), \mathbf{1} \rangle - \langle v, b_{i_t} \rangle.$$

Since $x_0 := e^{-c/\lambda} = x(0)$, we conclude that IBP is equivalent to alternating minimization in the dual problem (7.4), like Dykstra's algorithm [GM89]. In particular, $x_t = x(\mathbf{u}^t)$, where $\mathbf{u}^0 = 0$ and at each step we update $u_{i_t}^{t+1} := u_{i_t} + v_t$. This brings us to the dual version of IBP (Algorithm 1). The operators π_i are defined as follows: $\pi_i(\mathbf{u}) = \mathbf{u}' = (u'_1, \dots, u'_m)$, where

$$u'_i := \operatorname{argmin}_{u \in \mathbb{R}^{n_i}} \psi(u_1, \dots, u, \dots, u_m), \quad u'_j := u_j \quad \text{for } j \in [m] \setminus \{i\}. \quad (7.5)$$

Notice that it is a bit more general than IBP since we allow any starting points u_1^0, \dots, u_m^0 , not only zero. For now, we do not specify the stopping criterion and the way we choose indices i_t . Clearly, if $m = 2$ (e.g. in the Sinkhorn algorithm), then i_t are uniquely defined by i_0 . If $m > 2$, then there are three main possibilities to take i_t :

- in a fixed cyclic order;
- randomly;
- greedily, optimizing some criterion at every step.

It is known from the theory of alternating optimization that a fixed order can lead to a slower convergence, thus in this work we consider the other options.

Algorithm 1 Dual iterative Bregman projections

Input: $c, A_1, \dots, A_m, b_1, \dots, b_m, \lambda > 0$, starting points u_1^0, \dots, u_m^0 .

- 1: Set $t := 0$.
- 2: **repeat**
- 3: Choose $i_t \in [m] \setminus \{i_{t-1}\}$.
- 4: $\mathbf{u}^{t+1} := \pi_{i_t}(\mathbf{u}^t)$.
- 5: $t := t + 1$.
- 6: **until** A stopping criterion is fulfilled.

Output: $x(\mathbf{u}^t)$.

To obtain an admissible point for the initial problem (7.1) we apply a ‘‘rounding procedure’’ to the output $x(\mathbf{u}^t)$ of the above algorithm. In the subsequent sections, we show that to solve the non-regularized problem 7.1 with accuracy ε , in the considered cases, it is enough to take $\lambda \propto \varepsilon$ and run (dual) IBP for $O(\frac{1}{\varepsilon^2})$ iterations (with constants depending on N).

7.3 Convergence of dual IBP

Here we provide complexity bounds on IBP based on a refinement of the analysis from [AWR17] and general results for Dykstra's algorithm and alternating minimization.

First of all, we have to decide which kind of convergence is needed to obtain an approximate solution of the initial problem (7.1). In [AWR17] it is shown that for the Sinkhorn algorithm it is enough to obtain

$$\sum_{i=1}^m \|x(\mathbf{u}) - x(\pi_i(\mathbf{u}))\|_1 \leq \varepsilon' \quad (7.6)$$

for a suitable ε' depending on ε . In the next sections we will see that this approach works for the multimarginal OT and the barycenter problem as well.

Let $\mathbf{u}^* = (u_1^*, \dots, u_m^*)$ be some solution of (7.4), $\psi^* := \psi(\mathbf{u}^*)$, and

$$\tilde{\psi}(\mathbf{u}) := \psi(\mathbf{u}) - \psi^*, \quad \mathbf{u} \in \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_m}.$$

Further analysis of dual IBP convergence is based on the following simple observation (cf. [AWR17]): if $\mathbf{u}' := \pi_i(\mathbf{u})$, then

$$\begin{aligned} \psi(\mathbf{u}) - \psi(\mathbf{u}') &= \langle x(\mathbf{u}) - x(\mathbf{u}'), \mathbf{1} \rangle + \sum_{j=1}^n \langle u'_j - u_j, b_j \rangle \\ &= \langle x(\mathbf{u}) - x(\mathbf{u}'), \mathbf{1} \rangle + \langle u'_i - u_i, A_i x(\mathbf{u}') \rangle \\ &= \langle x(\mathbf{u}) - x(\mathbf{u}'), \mathbf{1} \rangle + \langle \log x(\mathbf{u}') - \log x(\mathbf{u}), x(\mathbf{u}') \rangle \\ &= KL(x(\mathbf{u}') | x(\mathbf{u})). \end{aligned}$$

If $x(\mathbf{u}), x(\mathbf{u}') \in \Delta^{N-1}$, then Pinsker's inequality yields

$$\psi(\mathbf{u}) - \psi(\mathbf{u}') \geq \frac{1}{2} \|x(\mathbf{u}') - x(\mathbf{u})\|_1^2. \quad (7.7)$$

Remark 7.3.1. Notice that in the general case, the inequality $t \log \frac{t}{s} - t + s \geq \frac{(t-s)^2}{2 \max\{s, t\}}$ following from the Taylor's theorem for all $s, t \in \mathbb{R}_+$, implies that

$$KL(x|y) \geq \frac{\|x - y\|_1^2}{2\langle x + y, \mathbf{1} \rangle},$$

for all $x, y \in \mathbb{R}_+^N$, thus

$$\psi(\mathbf{u}) - \psi(\mathbf{u}') \geq \frac{\|x(\mathbf{u}') - x(\mathbf{u})\|_1^2}{2\langle x(\mathbf{u}) + x(\mathbf{u}'), \mathbf{1} \rangle}.$$

This inequality can be used to analyze the case where the total mass of $x(\mathbf{u}^t)$ is not preserved, but this is outside of the scope of the current work.

The gradient inequality for the convex function ψ gives us

$$\begin{aligned} \tilde{\psi}(\mathbf{u}) &\leq \sum_{i=1}^m \langle \nabla_{u_i} \psi(\mathbf{u}), u_i - u_i^* \rangle = \sum_{i=1}^m \langle A_i x(\mathbf{u}) - b_i, u_i - u_i^* \rangle \\ &= \sum_{i=1}^m \langle A_i x(\mathbf{u}) - A_i x(\pi_i(\mathbf{u})), u_i - u_i^* \rangle = \sum_{i=1}^m \langle x(\mathbf{u}) - x(\pi_i(\mathbf{u})), A_i^\top (u_i - u_i^*) \rangle. \end{aligned}$$

Now we need an additional assumption which allows us to use (7.7) and relates it to the above inequality.

Assumption 7.1. Suppose that there is $R = R(\lambda) > 0$ such that for all $t \geq 0$ one has

$$\sum_{i=1}^m \langle x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t)), A_i^\top (u_i^t - u_i^*) \rangle \leq R \sum_{i=1}^m \|x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t))\|_1$$

and $x(\pi_i(\mathbf{u}^t)) \in \Delta^{N-1}$ for any $i \in [m]$.

7.3.1 Greedy strategy

Consider a *greedy strategy*: for each t choose i_t which maximizes $\|x(\pi_{i_t}(\mathbf{u}^t)) - x(\mathbf{u}^t)\|_1$, and stop once (7.6) holds for \mathbf{u}^t . Otherwise, if the stopping criterion is not fulfilled and $t \geq 1$, then due

to (7.7)

$$\begin{aligned} \psi(\mathbf{u}^t) - \psi(\mathbf{u}^{t+1}) &\geq \frac{1}{2} \|x(\mathbf{u}^{t+1}) - x(\mathbf{u}^t)\|_1^2 \geq \frac{1}{2} \left(\frac{1}{m-1} \sum_{i=1}^m \|x(\pi_i(\mathbf{u})) - x(\mathbf{u})\|_1 \right)^2 \\ &\geq \frac{1}{2(m-1)^2} \max \left\{ \left(\frac{\tilde{\psi}(\mathbf{u})}{R} \right)^2, (\varepsilon')^2 \right\} = \frac{1}{2(m-1)^2 R^2} \max \left\{ \tilde{\psi}^2(\mathbf{u}), (\varepsilon' R)^2 \right\}. \end{aligned} \quad (7.8)$$

Here we used that $\mathbf{u}^t = \pi_{i_{t-1}}(\mathbf{u}^t)$. To study the sequence $\{\tilde{\psi}(\mathbf{u}^t)\}_{t \in \mathbb{N}_0}$ we need the next technical lemma.

Lemma 7.3.2. *Let $\{\delta_t\}_{t \in \mathbb{N}_0} \subset \mathbb{R}_+$ be a nonincreasing sequence. Take $\beta > 0$ and define for any $t \geq 0$*

$$\alpha_t := \frac{\delta_t - \delta_{t+1}}{\max\{\delta_t^2, \beta^2\}} \geq 0. \quad (7.9)$$

Then

$$\sum_{t=0}^{\infty} \alpha_t \leq \frac{3}{\beta}.$$

Proof. According to (7.9)

$$\alpha_t = \frac{\delta_t - \delta_{t+1}}{\max\{\delta_t^2, \beta^2\}} \leq \min \left\{ \frac{1}{\delta_t}, \frac{\delta_t}{\beta^2} \right\} \leq \frac{1}{\beta}. \quad (7.10)$$

Furthermore,

$$\frac{1}{\delta_{t+1}} \geq \frac{1}{\delta_t} \frac{1}{1 - \alpha_t \delta_t} \geq \frac{1}{\delta_t} + \alpha_t.$$

Define $S_t := \sum_{\tau=0}^{t-1} \alpha_\tau$. The above inequality yields

$$\frac{1}{\delta_t} \geq \frac{1}{\delta_0} + S_t. \quad (7.11)$$

On the other hand, $\delta_{t+1} \leq \delta_t - \alpha_t \beta^2$, hence for any $s \geq t$

$$\delta_t - \delta_s \geq \beta^2 (S_s - S_t). \quad (7.12)$$

To combine the two estimates above we consider a switching strategy parametrized by a number $h \in (0, \delta_0]$. Let $t \geq 0$ be the last moment where $\delta_t \geq h$. Then for any $0 \leq s \leq t$ by (7.11)

$$S_s \leq S_t \leq \frac{1}{\delta_t} - \frac{1}{\delta_0} \leq \frac{1}{h} - \frac{1}{\delta_0}$$

and for $s \geq t$ by (7.12) and (7.10)

$$S_s \leq S_{t+1} + \frac{\delta_{t+1} - \delta_s}{\beta^2} \leq \alpha_t + S_t + \frac{h}{\beta^2} \leq \frac{1}{\beta} + \frac{1}{h} + \frac{h}{\beta^2} - \frac{1}{\delta_0}.$$

Minimizing the sum of these two estimates w.r.t. $h \in (0, \delta_0]$, we conclude that

$$S_s \leq \inf_{0 < h \leq \delta_0} \left(\frac{1}{\beta} + \frac{1}{h} + \frac{h}{\beta^2} - \frac{1}{\delta_0} \right) = \begin{cases} \frac{1}{\beta} + \frac{\delta_0}{\beta^2}, & \delta_0 < \beta, \\ \frac{3}{\beta} - \frac{1}{\delta_0}, & \text{otherwise.} \end{cases}$$

In both cases, we have $S_s \leq \frac{3}{\beta}$. □

Theorem 7.3.3. *Under Assumption 7.1 Algorithm 1 with greedy strategy stops after at most*

$$6(m-1)^2 \frac{R}{\varepsilon'} + 2$$

iterations.

Proof. Bound (7.8) yields that

$$\alpha_t := \frac{\tilde{\psi}(\mathbf{u}^t) - \tilde{\psi}(\mathbf{u}^{t+1})}{\max\{\tilde{\psi}^2(\mathbf{u}^t), (\varepsilon'R)^2\}} \geq \frac{1}{2(m-1)^2R^2}$$

for all $t \geq 1$, thus by Lemma 7.3.2 it can hold for no more than

$$2(m-1)^2R^2 \frac{3}{\varepsilon'R} = \frac{6(m-1)^2R}{\varepsilon'}$$

iterations. Therefore, stopping criterion (7.6) is fulfilled for the first time at iteration

$$t \leq 1 + 6(m-1)^2 \frac{R}{\varepsilon'}.$$

The claim follows. \square

7.3.2 Randomized strategy

A drawback of the greedy strategy is that at every step we have to compute $x(\pi_i(\mathbf{u}^t))$ for all i . In some cases (e.g. for both problems we deal with in this chapter) $\|x(\pi_i(\mathbf{u}^t)) - x(\mathbf{u}^t)\|_1 = \|A_i x(\mathbf{u}^t) - b_i\|_1$, but computing of $A_i x(\mathbf{u}^t)$ and $x(\pi_i(\mathbf{u}^t))$ has the same complexity, so it is m times more expensive than just to make a step of IBP. Another way is to use a randomized strategy and pick up each i_t randomly and uniformly from $[m] \setminus \{i_{t-1}\}$. Nontrivial issue is the choice of a stopping criterion, since computing of $\sum_{i=1}^m \|x(\pi_i(\mathbf{u}^t)) - x(\mathbf{u}^t)\|_1$ at each iteration is too expensive. Instead, we suggest for any $t = km$, $k \in \mathbb{N}_0$, to draw random $\tau_k \sim U([t, t+m-1])$ and stop whenever

$$\sum_{i=1}^m \|x(\pi_i(\mathbf{u}^{\tau_k})) - x(\mathbf{u}^{\tau_k})\|_1 \leq \varepsilon'.$$

Theorem 7.3.4. *Under Assumption 7.1 Algorithm 1 with randomized strategy stops with probability at least $1 - \delta$ for any $\delta \in (0, \frac{1}{2})$ after at most*

$$\frac{12(m-1)^2R}{\varepsilon'} + 6m \log \frac{2}{\delta} + m$$

iterations.

Proof. Step 1. Assume for now that we run IBP infinitely. Let $N \in \mathbb{N}_0 \cup \{\infty\}$ be the (random) number of iterations $t \geq 1$ where (7.6) fails, and $\{T_n\}_{n \in \mathbb{N}}$ be the sequence of these iterations. If N is finite, then we continue it with ∞ . First, we are going to obtain a bound on N . Define random variables

$$Z_n := \begin{cases} \frac{\|x(\mathbf{u}^{T_n+1}) - x(\mathbf{u}^{T_n})\|_1^2}{\sum_{i=1}^m \|x(\pi_i(\mathbf{u}^{T_n})) - x(\mathbf{u}^{T_n})\|_1^2} - \frac{1}{m-1}, & n \leq N, \\ 0, & \text{otherwise.} \end{cases}$$

Obviously, $-\frac{1}{m-1} \leq Z_n \leq 1 - \frac{1}{m-1}$ a.s. Let \mathcal{F}_n be the sigma-algebra of events induced by T_1, \dots, T_n and i_0, \dots, i_{T_n-1} . Then $\mathbb{E}[Z_n | \mathcal{F}_n] = 0$ and, if $n \leq N$,

$$\text{Var}[Z_n | \mathcal{F}_n] \leq \frac{1}{m-1} \sum_{j \neq i_{T_n-1}} \frac{\|x(\pi_j(\mathbf{u}^{T_n})) - x(\mathbf{u}^{T_n})\|_1^4}{\left(\sum_{i=1}^m \|x(\pi_i(\mathbf{u}^{T_n})) - x(\mathbf{u}^{T_n})\|_1^2\right)^2} \leq \frac{1}{m-1},$$

otherwise $\text{Var}[Z_n | \mathcal{F}_n] = 0$. Therefore, in the same way as in Proposition 2 from [Yin04] one can prove that for any $s \in \mathbb{N}$ and $h > 0$

$$\mathbb{P}\left\{\sum_{n=1}^s Z_n \leq -h\right\} \leq \exp\left(-\frac{h^2}{2(s/(m-1) + h/3)}\right). \quad (7.13)$$

Due to (7.7) for all $n \leq N$

$$\begin{aligned} \psi(\mathbf{u}^{T_n}) - \psi(\mathbf{u}^{T_{n+1}}) &\geq \frac{1}{2} \left(Z_n + \frac{1}{m-1} \right) \sum_{i=1}^m \|x(\pi_i(\mathbf{u}^{T_n})) - x(\mathbf{u}^{T_n})\|_1^2 \\ &\geq \frac{1}{2(m-1)} \left(Z_n + \frac{1}{m-1} \right) \left(\sum_{i=1}^m \|x(\pi_i(\mathbf{u}^{T_n})) - x(\mathbf{u}^{T_n})\|_1 \right)^2 \\ &\geq \frac{1}{2(m-1)} \left(Z_n + \frac{1}{m-1} \right) \left(\max \left\{ \frac{\tilde{\psi}(\mathbf{u}^{T_n})}{R}, \varepsilon' \right\} \right)^2 \end{aligned}$$

(here we used that $\pi_{i_{T_n-1}}(\mathbf{u}^{T_n}) = \mathbf{u}^{T_n}$, thus

$$\alpha_{T_n} := \frac{\tilde{\psi}(\mathbf{u}^{T_n}) - \tilde{\psi}(\mathbf{u}^{T_{n+1}})}{\max \left\{ \tilde{\psi}^2(\mathbf{u}^{T_n}), (\varepsilon' R)^2 \right\}} \geq \frac{1}{2(m-1)R^2} \left(Z_n + \frac{1}{m-1} \right).$$

By Lemma 7.3.2

$$\frac{3}{\varepsilon' R} \geq \sum_{t=0}^{\infty} \alpha_t \geq \sum_{n=1}^N \alpha_{T_n} \geq \frac{1}{2(m-1)R^2} \sum_{n=1}^N \left(Z_n + \frac{1}{m-1} \right),$$

hence

$$\sum_{n=1}^s \left(Z_n + \frac{1}{m-1} \right) \leq \frac{6(m-1)R}{\varepsilon'} \quad \forall 0 \leq s \leq N.$$

Consequently, for any $s \in \mathbb{N}_0$

$$\mathbb{P}\{N \geq s\} \leq \mathbb{P}\left\{ \sum_{n=1}^s \left(Z_n + \frac{1}{m-1} \right) \leq \frac{6(m-1)R}{\varepsilon'} \right\} = \mathbb{P}\left\{ \sum_{n=1}^s Z_n \leq \frac{6(m-1)R}{\varepsilon'} - \frac{s}{m-1} \right\}.$$

Set

$$s := \left\lceil \frac{12(m-1)^2 R}{\varepsilon'} + 5(m-1) \log \frac{2}{\delta} \right\rceil,$$

then $h := \frac{s}{m-1} - \frac{6(m-1)R}{\varepsilon'} \geq \frac{s}{2(m-1)} > 0$ and bound (7.13) yields that

$$\mathbb{P}\{N \geq s\} \leq \exp\left(-\frac{h^2}{2(s/(m-1) + h/3)}\right) \leq \exp\left(-\frac{h^2}{2(2h + h/3)}\right) \leq \exp\left(-\frac{3h}{14}\right) \leq \frac{\delta}{2}.$$

Step 2. Now fix $n \in \mathbb{N}$ and consider independent random variables $\tau_0, \dots, \tau_{n-1}$ such that $\tau_k \sim U([km, (k+1)m - 1])$. Obviously, they are independent with i_0, i_1, \dots . Let l_k be the number of iterations $km \leq t < (k+1)m$ such that (7.6) does not hold. Denote by \mathbf{E}_n the event where (7.6) fails at all τ_k . Then

$$\mathbb{P}(\mathbf{E}_n | l_0, \dots, l_{n-1}) \leq \prod_{k=0}^{n-1} \frac{l_k}{m} \leq \left(\frac{1}{nm} \sum_{k=0}^{n-1} l_k \right)^n.$$

But $\sum_{k=0}^{n-1} l_k \leq N + 1$, and combining this with Step 1 we obtain that

$$\mathbb{P}(\mathbf{E}_n) \leq \left(\frac{s}{nm} \right)^n + \mathbb{P}\{N \geq s\} \leq \left(\frac{s}{nm} \right)^n + \frac{\delta}{2}.$$

If $nm \geq s + m \log \frac{2}{\delta}$, then due to the concavity of $\log(\cdot)$

$$nm(\log(nm) - \log s) \geq nm - s \geq m \log \frac{2}{\delta},$$

hence

$$\left(\frac{s}{nm}\right)^n \leq \frac{\delta}{2},$$

and $\mathbb{P}(\mathbf{E}_n) \leq \delta$. Thus with probability at least $1 - \delta$ the number of iterations is bounded by

$$\begin{aligned} m \left[\frac{s}{m} + \log \frac{2}{\delta} \right] &\leq s + m \log \frac{2}{\delta} + m \\ &\leq \frac{12(m-1)^2 R}{\varepsilon'} + 5(m-1) \log \frac{2}{\delta} + 1 + m \log \frac{2}{\delta} + m \\ &\leq \frac{12(m-1)^2 R}{\varepsilon'} + 6m \log \frac{2}{\delta} + m. \end{aligned}$$

□

7.4 Multimarginal OT problem

Given a cost tensor $C \in [0, 1]^{n_1 \times \dots \times n_m}$ and vectors $p_i \in \Delta^{n_i-1}$, the discrete multimarginal optimal transport problem is formulated as

$$\min \{ \langle C, X \rangle : X \in \mathbb{R}_+^{n_1 \times \dots \times n_m}, A_i X = p_i \}, \quad (7.14)$$

where X is a multimarginal transport plan and A_i is the projector on the i -th component \mathbb{R}^{n_i} . Clearly, this can be written in the form (7.1).

It is easy to see that the dual function (7.4) in this case equals to

$$\psi(u_1, \dots, u_m) = \sum_{j_1, \dots, j_m} X_{j_1, \dots, j_m}(\mathbf{u}) - \sum_{i=1}^m \langle u_i, p_i \rangle,$$

where

$$X_{j_1, \dots, j_m}(\mathbf{u}) := \exp \left(-\frac{C_{j_1, \dots, j_m}}{\lambda} + \sum_{i=1}^m [u_i]_{j_i} \right).$$

Operators π_i are given by

$$\pi_i(\mathbf{u}) = (u_1, \dots, u'_i, \dots, u_m), \quad u'_i = u_i + \log p_i - \log(A_i X(\mathbf{u})),$$

which in terms of the primal variable X corresponds to the coordinate-wise multiplication by the tensor $\bigotimes_{k=1}^{i-1} \mathbf{1}_{n_k} \otimes \frac{p_i}{A_i X(\mathbf{u})} \otimes \bigotimes_{k=i+1}^m \mathbf{1}_{n_k}$ [Ben+15]. In particular,

$$\|X(\mathbf{u}) - X(\pi_i(\mathbf{u}))\|_1 = \left\| \left(\mathbf{1} - \frac{p_i}{A_i X(\mathbf{u})} \right) A_i X(\mathbf{u}) \right\|_1 = \|A_i X(\mathbf{u}) - p_i\|_1.$$

Let $\text{vec}(X) \in \mathbb{R}^N$ be a vectorized tensor X , where $N := \prod_{i=1}^m n_i$. Abusing notations, we also sometimes suppose $A_i \in \mathbb{R}^{n_i \times N}$.

First, define a rounding map P_b by Algorithm 2. This is a trivial generalization of Algorithm 2 in [AWR17]. Note that

$$A_i \hat{X} = A_i x_m + (1 - \langle x_m, \mathbf{1} \rangle) q_i = A_i x_m + \langle b_i - A_i x_m, \mathbf{1} \rangle q_i = b_i \quad \forall i \in [m],$$

thus \hat{X} is a feasible point for problem 7.14 if $b_i = p_i$.

Lemma 7.4.1. *Let \hat{X} come from Algorithm 2, then*

$$\|\hat{X} - X\|_1 \leq \sum_{i=1}^m \|A_i X - b_i\|_1.$$

Algorithm 2 Rounding to feasible point in MOT

Input: $X \in \mathbb{R}_+^{n_1 \times \dots \times n_m}$ such that $\|X\|_1 = 1$, $b_1 \in \Delta^{n_1-1}, \dots, b_m \in \Delta^{n_m-1}$.

1: $x_0 := \text{vec}(X)$.

2: **for** $i \in [m]$ **do**

3: $x_i := x_{i-1} \odot A_i^\top \left(\frac{b_i}{A_i x_{i-1}} \wedge \mathbf{1} \right)$ (here $a \wedge b$ is the coordinate-wise minimum of a and b).

4: **end for**

5: **for** $i \in [m]$ **do**

6: $q_i := \frac{b_i - A_i x_m}{\langle b_i - A_i x_m, \mathbf{1} \rangle} \in \Delta^{n_i-1}$.

7: **end for**

8: $\hat{X} := \text{vec}^{-1}(x_m) + (1 - \langle x_m, \mathbf{1} \rangle) \otimes_{i=1}^m q_i$.

Output: \hat{X} .

Proof. Consider x_0, \dots, x_m from Algorithm 2. Then $x_i \leq x_{i-1}$ coordinate-wise,

$$\begin{aligned} \|x_i - x_{i-1}\|_1 &= \langle x_{i-1} - x_i, \mathbf{1} \rangle = \left\| x_{i-1} - x_{i-1} \odot A_i^\top \left(\frac{b_i}{A_i x_{i-1}} \wedge \mathbf{1} \right) \right\|_1 \\ &= \left\| A_i x_{i-1} - (A_i x_{i-1}) \odot \left(\frac{b_i}{A_i x_{i-1}} \wedge \mathbf{1} \right) \right\|_1 \\ &= \left\| (A_i x_{i-1}) \odot \left(\frac{b_i}{A_i x_{i-1}} - \mathbf{1} \right) \right\|_+ = \|(A_i x_{i-1} - b_i)_+\|_1, \end{aligned}$$

Therefore,

$$\begin{aligned} \|\hat{X} - X\|_1 &\leq \|x_0 - x_m\|_1 + (1 - \langle x_m, \mathbf{1} \rangle) = 2\langle x_0 - x_m, \mathbf{1} \rangle \\ &= 2 \sum_{i=1}^m \langle (A_i x_{i-1} - b_i)_+, \mathbf{1} \rangle \leq 2 \sum_{i=1}^m \|A_i x_0 - b_i\|_1. \end{aligned}$$

Since $\langle b_i, \mathbf{1} \rangle = \langle A_i x_0, \mathbf{1} \rangle = \|X\|_1 = 1$, then $\langle (A_i x_0 - b_i)_+, \mathbf{1} \rangle = \frac{1}{2} \|A_i x_0 - b_i\|_1$ and

$$\|\hat{X} - X\|_1 \leq \sum_{i=1}^m \|A_i x_0 - b_i\|_1.$$

□

Lemma 7.4.2. Let $\mathbf{u} \in \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_m}$ and $\|X(\mathbf{u})\|_1 = 1$. Then

$$\langle P_{\mathbf{p}}(X(\mathbf{u})), C \rangle \leq \langle X^*, C \rangle + 2 \sum_{i=1}^m \|A_i X(\mathbf{u}) - p_i\|_1 + \lambda \log N,$$

where X^* is any solution of (7.14).

Proof. From the duality it immediately follows that

$$X(\mathbf{u}) = \underset{X \in \mathbb{R}_+^{n_1 \times \dots \times n_m}: A_i X = b_i, i \in [m]}{\text{argmin}} \left(\langle X, C \rangle + \lambda H(X) \right),$$

where $b_i := A_i X(\mathbf{u}) \in \Delta^{n_i-1}$. Then for $X' := P_{\mathbf{b}}(X^*)$ we have

$$\langle X', C \rangle + \lambda H(X') \geq \langle X(\mathbf{u}), C \rangle + \lambda H(X(\mathbf{u})).$$

Using that the values of C belong to $[0, 1]$ and Lemma 7.4.1 we obtain

$$\begin{aligned} \langle P_{\mathbf{p}}(X(\mathbf{u})), C \rangle &\leq \langle X(\mathbf{u}), C \rangle + \|P_{\mathbf{p}}(X(\mathbf{u})) - X(\mathbf{u})\|_1 \\ &\leq \langle X', C \rangle + \lambda H(X') - \lambda H(X(\mathbf{u})) + \|P_{\mathbf{p}}(X(\mathbf{u})) - X(\mathbf{u})\|_1 \\ &\leq \langle X^*, C \rangle + \|X' - X^*\|_1 + \lambda (H(X') - H(X(\mathbf{u}))) + \|P_{\mathbf{b}}(X(\mathbf{u})) - X(\mathbf{u})\|_1 \\ &\leq \langle X^*, C \rangle + 2 \sum_{i=1}^m \|b_i - p_i\|_1 + \lambda (H(X') - H(X(\mathbf{u}))). \end{aligned}$$

The claim follows from the bounds

$$1 \leq -H(x) \leq 1 + \log N \quad \forall x \in \Delta^{N-1}.$$

□

The above lemma justifies the correctness of Algorithm 3.

Algorithm 3 Solving (7.14) by dual IBP

Input: C, p_1, \dots, p_m , accuracy $\varepsilon > 0$.

1: Set $\lambda := \frac{\varepsilon}{2 \log N}$, $\varepsilon' := \frac{\varepsilon}{4}$.

2: Run Algorithm 1 with $u_i^0 := \log p_i$, $i \in [m]$, and obtain $X(\mathbf{u}^t)$ such that

$$\sum_{i=1}^m \|A_i X(\mathbf{u}^t) - p_i\|_1 \leq \varepsilon'.$$

3: Compute \hat{X} by Algorithm 2.

Output: \hat{X} .

The next result provides bounds on \mathbf{u}^t from Algorithm 1 in the seminorm

$$|v| := \max v - \min v,$$

which will be used to ensure Assumption 7.1.

Lemma 7.4.3. Fix $\lambda > 0$ and let $\mathbf{u} \in \mathbb{R}^{n_1 \times \dots \times n_m}$, $\mathbf{u}' = (u_1, \dots, u'_i, \dots, u_m) := \pi_i(\mathbf{u})$ for some $i \in [m]$, where π_i is defined by (7.5) for the regularized multimarginal OT problem. Then

$$|u'_i - \log p_i| \leq \frac{1}{\lambda}. \quad (7.15)$$

In particular, any solution \mathbf{u}^* of the dual problem for the regularized multimarginal OT satisfies (7.15) for all $i \in [m]$

Proof. W.l.o.g. assume that $i = 1$. According to Section 7.2 \mathbf{u}'_1 is characterized by the equation $P_1 X(\mathbf{u}') = p_1$, and $P_1 X(\mathbf{u}^*) = p_1$ as well. From the formula for $X(\mathbf{u})$ we obtain that for any $j \in [n_1]$

$$\begin{aligned} [p_1]_j &= [A_1 X(\mathbf{u}')]_j = [p_1]_j e^{[u'_1 - \log p_1]_j} \sum_{j_2, \dots, j_m} \exp \left(-\frac{C_{j, j_2, \dots, j_m}}{\lambda} + \sum_{i=2}^m [u_i]_{j_i} \right) \\ &\leq [p_1]_j e^{[u'_1 - \log p_1]_j} \sum_{j_2, \dots, j_m} \exp \left(\sum_{i=2}^m [u_i]_{j_i} \right). \end{aligned}$$

In the same way, using that $C_{j, j_2, \dots, j_m} \leq 1$, one gets

$$[p_1]_j \geq [p_1]_j e^{[u'_1 - \log p_1]_j - 1/\lambda} \sum_{j_2, \dots, j_m} \exp \left(\sum_{i=2}^m [u_i]_{j_i} \right),$$

thus

$$-\log \left[\sum_{j_2, \dots, j_m} \exp \left(\sum_{i=2}^m [u_i]_{j_i} \right) \right] \leq [u'_1 - \log p_1]_j \leq \frac{1}{\lambda} - \log \left[\sum_{j_2, \dots, j_m} \exp \left(\sum_{i=2}^m [u_i]_{j_i} \right) \right].$$

The claim follows. □

Theorem 7.4.4. *The iteration complexity of Algorithm 3 is bounded by*

$$48(m-1)^2 \frac{\log N}{\varepsilon^2} + 1 = O\left(\frac{m^2 \log N}{\varepsilon^2}\right)$$

for the greedy strategy and, with probability at least $1 - \delta$, by

$$96(m-1)^2 \frac{\log N}{\varepsilon^2} + 6m \log \frac{2}{\delta} + 1 = O\left(\frac{m^2 \log N}{\varepsilon^2} + m \log \frac{1}{\delta}\right)$$

for the randomized strategy.

Proof. Obviously, if $r_i := A_i X \in \Delta^{n_i-1}$, then $\|X\|_1 = \sum_{j_1, \dots, j_m} X_{j_1, \dots, j_m} = \langle r_i, \mathbf{1} \rangle = 1$, and vice versa. Hence $\|X(\pi_i(\mathbf{u}))\|_1 = 1$ for any \mathbf{u} .

Note that $A_i^\top \mathbf{1}_{n_i} = \mathbf{1}_N$, hence for all $t \geq 1$

$$\begin{aligned} \langle x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t)), A_i^\top (u_i^t - \log p_i) \rangle &= \langle A_i (x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t))), (u_i^t - \log p_i - a\mathbf{1}) \rangle \\ &\leq \|x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t))\|_1 \|u_i^t - \log p_i - a\mathbf{1}\|_\infty \end{aligned}$$

for any $a \in \mathbb{R}$. Taking $a := \frac{\max(u_i^t - \log p_i) + \min(u_i^t - \log p_i)}{2}$, using Lemma 7.4.3 and the fact that $u_i^0 := \log p_i$, we conclude with

$$\begin{aligned} \langle x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t)), A_i^\top (u_i^t - \log p_i) \rangle &\leq \|x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t))\|_1 \frac{|u_i^t - \log p_i|}{2} \\ &\leq \frac{1}{2\lambda} \|x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t))\|_1. \end{aligned}$$

The same bound holds for u_i^* , thus

$$\sum_{i=1}^m \langle x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t)), A_i^\top (u_i^t - u_i^*) \rangle \leq \frac{1}{\lambda} \sum_{i=1}^m \|x(\mathbf{u}^t) - x(\pi_i(\mathbf{u}^t))\|_1.$$

Therefore, Assumption 7.1 is fulfilled with $R = \frac{1}{\lambda} = \frac{2 \log N}{\varepsilon}$. The claim follows from Theorems 7.3.3 and 7.3.4. \square

7.5 Barycenter problem

Now we consider the problem of finding discrete Fréchet barycenter. Given cost matrices $C_1 \in [0, 1]^{n_1, n}, \dots, C_L \in [0, 1]^{n_L, n}$, vectors $p_1 \in \Delta^{n_1-1}, \dots, p_L \in \Delta^{n_L-1}$, and positive weights $(w_1, \dots, w_L) \in \Delta^{L-1}$, it can be written as

$$\min \left\{ \sum_{l=1}^L w_l \langle C_l, X_l \rangle : (X_1, \dots, X_L) \in \mathbb{R}_+^{n_1 \times n} \times \dots \times \mathbb{R}_+^{n_L \times n} \cap \mathcal{C}_u \cap \mathcal{C}_v \right\}, \quad (7.16)$$

where

$$\begin{aligned} \mathcal{C}_u &:= \{(X_1, \dots, X_L) \in \mathbb{R}^{n_1 \times n} \times \dots \times \mathbb{R}^{n_L \times n} : X_l \mathbf{1} = p_l, \forall l \in [L]\}, \\ \mathcal{C}_v &:= \{(X_1, \dots, X_L) \in \mathbb{R}^{n_1 \times n} \times \dots \times \mathbb{R}^{n_L \times n} : \langle X_l \mathbf{1}, \mathbf{1} \rangle = 1, \exists q \in \mathbb{R}^n : X_l^\top \mathbf{1} = q \forall l \in [L]\}. \end{aligned}$$

If we identify $(w_1 X_1, \dots, w_L X_L)$ with a vector $x = \text{vec}(X) \in \mathbb{R}_+^{(n_1 + \dots + n_L)n}$, then this problem can also be written in the form 7.1 with the corresponding matrices

$$\begin{aligned} A_u x &:= (w_1 X_1 \mathbf{1}, \dots, w_L X_L \mathbf{1}) \in \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_L}, \\ A_v x &:= (w_1 (X_1^\top \mathbf{1} - q), \dots, w_L (X_L^\top \mathbf{1} - q)) \in \mathbb{R}^L \times (\mathbb{R}^n)^L, \quad \text{where } q := \sum_{l=1}^L w_l X_l^\top \mathbf{1} \end{aligned}$$

(to simplify the notations we denote them by A_u and A_v instead of A_1 and A_2).

The dual function (7.4) in this case reads as

$$\psi(\mathbf{u}, \boldsymbol{\nu}, \mathbf{s}) = \sum_{l=1}^L w_l \langle X_l(\mathbf{u}, \boldsymbol{\nu}, \mathbf{s}), \mathbf{1}\mathbf{1}^\top \rangle - \sum_{l=1}^L w_l \langle u_l, p_l \rangle - \sum_{l=1}^L w_l s_l,$$

where $\mathbf{u} = (u_1, \dots, u_L) \in \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_L}$ corresponds to the first constraint, $\mathbf{s} \in \mathbb{R}^L$ and $\boldsymbol{\nu} = (\nu_1, \dots, \nu_L) \in (\mathbb{R}^n)^L$ correspond to the second one, and

$$X_l(\mathbf{u}, \boldsymbol{\nu}, \mathbf{s}) := \frac{1}{w_l} \exp \left(-\frac{C_l}{\lambda} + u_l \mathbf{1}^T + \mathbf{1} \left(\nu_l - \sum_{k=1}^L w_k \nu_k \right)^\top + s_l \mathbf{1}\mathbf{1}^\top \right), \quad l \in [L].$$

Let us make the change of variables $v_l := \nu_l - \sum_{k=1}^L w_k \nu_k$ with the additional constraint $\sum_{l=1}^L w_l v_l = 0$. Then

$$\psi(\mathbf{u}, \mathbf{v}, \mathbf{s}) = \sum_{l=1}^L w_l \langle X_l(\mathbf{u}, \mathbf{v}, \mathbf{s}), \mathbf{1}\mathbf{1}^\top \rangle - \sum_{l=1}^L w_l \langle u_l, p_l \rangle - \sum_{l=1}^L w_l s_l$$

and

$$X_l(\mathbf{u}, \mathbf{v}, \mathbf{s}) = X_l(u_l, v_l, s_l) := \frac{e^{s_l}}{w_l} \exp \left(-\frac{C_l}{\lambda} + u_l \mathbf{1}^T + \mathbf{1} v_l^\top \right).$$

According to the previous section the operator π_u is given by

$$\pi_u(\mathbf{u}, \mathbf{v}, \mathbf{s}) = (\mathbf{u}', \mathbf{v}, \mathbf{s}), \quad u'_l = u_l + \log p_l - \log(X_l(\mathbf{u}, \mathbf{v}, \mathbf{s})\mathbf{1}),$$

which in the primal variables corresponds to the multiplication of rows: $X_l \mapsto \text{diag} \left(\frac{p_l}{X_l \mathbf{1}} \right) X_l$. Now consider $(\mathbf{u}, \mathbf{v}', \mathbf{s}') = \pi_v(\mathbf{u}, \mathbf{v}, \mathbf{s})$, then there is $h \in \mathbb{R}^n$ such that for all $l \in [L]$

$$\nabla_{v_l} \psi(\mathbf{u}, \mathbf{v}', \mathbf{s}') = X_l^\top(\mathbf{u}, \mathbf{v}', \mathbf{s}') \mathbf{1} = e^{s'_l - s_l} e^{v'_l - v_l} \odot (X_l^\top(\mathbf{u}, \mathbf{v}, \mathbf{s}) \mathbf{1}) = h$$

and $\partial_{s_l} \psi(\mathbf{u}, \mathbf{v}', \mathbf{s}') = \langle X_l(\mathbf{u}, \mathbf{v}', \mathbf{s}') \mathbf{1}, \mathbf{1} \rangle - 1 = 0$. Thus

$$v'_l = v_l - (s'_l - s_l) \mathbf{1} - \log(X_l^\top(\mathbf{u}, \mathbf{v}, \mathbf{s}) \mathbf{1}) + \log h$$

and since $\sum_{l=1}^L w_l v_l = \sum_{l=1}^L w_l v'_l = 0$,

$$\log h = \sum_{l=1}^L w_l \log(X_l^\top(\mathbf{u}, \mathbf{v}, \mathbf{s}) \mathbf{1}) + \mathbf{1} \sum_{l=1}^L w_l (s'_l - s_l).$$

We can take $s'_l - s_l = d$ for all l , then

$$v'_l = v_l + \sum_{k=1}^L w_k \log(X_k^\top(\mathbf{u}, \mathbf{v}, \mathbf{s}) \mathbf{1}) - \log(X_l^\top(\mathbf{u}, \mathbf{v}, \mathbf{s}) \mathbf{1}) \quad \text{and} \quad s'_l = s_l - \log(\langle q, \mathbf{1} \rangle),$$

where $q := \prod_{l=1}^L (X_l^\top \mathbf{1})^{w_l}$ is the coordinate-wise geometric mean of the marginals $X_1^\top \mathbf{1}, \dots, X_L^\top \mathbf{1}$. In terms of the primal variables this corresponds to $X_l \mapsto \frac{1}{\langle q, \mathbf{1} \rangle} X_l \text{diag} \left(\frac{q}{X_l^\top \mathbf{1}} \right)$. Notice that this step is a bit different then in [Ben+15] or [Kro+19] (where it is just $X_l \mapsto X_l \text{diag} \left(\frac{q}{X_l^\top \mathbf{1}} \right)$ because there is no s_l variables), but it allows to simplify the analysis and obtain the same complexity bounds.

First, define a rounding map by Algorithm 4. Obviously, it returns $(\hat{X}_1, \dots, \hat{X}_L)$ which is a feasible point for problem 7.16 if $b_l = p_l$.

Algorithm 4 Rounding to feasible point in barycenter problem

Input: Matrices $X_1 \in \mathbb{R}_+^{n_1 \times n}, \dots, X_L \in \mathbb{R}_+^{n_L \times n}$ such that $X_1^\top \mathbf{1} = \dots = X_L^\top \mathbf{1} = q \in \Delta^{n-1}$, vectors $b_1 \in \Delta^{n_1-1}, \dots, b_L \in \Delta^{n_L-1}$, weights w_1, \dots, w_L .

1: By Algorithm 2 with $m = 2$ compute $\hat{X}_l \in \mathbb{R}_+^{n_1 \times n}$ such that $\hat{X}_l \mathbf{1} = b_l, \hat{X}_l^\top \mathbf{1} = q$.

Output: $\hat{X}_1, \dots, \hat{X}_L$.

Lemma 7.5.1. Let $\mathbf{u} \in \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_L}$, $\mathbf{v} \in (\mathbb{R}^n)^L$, $\mathbf{s} \in \mathbb{R}^L$, and $X_l^\top(u_l, v_l, s_l) \mathbf{1} = q \in \Delta^{n-1}$ for all $l \in [L]$. Then

$$\sum_{l=1}^L w_l \langle \hat{X}_l, C_l \rangle \leq \sum_{l=1}^L w_l \langle X_l^*, C_l \rangle + 2 \sum_{l=1}^L w_l \|X_l(u_l, v_l, s_l) \mathbf{1} - p_l\|_1 + \lambda \log n,$$

where (X_1^*, \dots, X_L^*) is any solution of (7.16) and $(\hat{X}_l)_{l \in [L]}$ are obtained by Algorithm 4 from $(X_l(u_l, v_l, s_l))_{l \in [L]}$ and vectors p_1, \dots, p_L .

Proof. From the duality we obtain that $x(\mathbf{u}, \mathbf{v}, \mathbf{s})$ is the solution of the regularized barycenter problem with constraints $X_l \mathbf{1} = b_l := X_l(u_l, v_l, s_l) \mathbf{1} \in \Delta^{n_l-1}$. Then for (X'_1, \dots, X'_L) obtained from (X_1^*, \dots, X_L^*) via Algorithm 4 with these b_l we have

$$\sum_{l=1}^L w_l \langle X'_l, C_l \rangle + \lambda H(x') \geq \sum_{l=1}^L w_l \langle X_l(u_l, v_l, s_l), C_l \rangle + \lambda H(x(\mathbf{u}, \mathbf{v}, \mathbf{s})).$$

Note that $X'_l \mathbf{1} = X_l(u_l, v_l, s_l) \mathbf{1}$, thus

$$H(X'_l) - H(X_l(u_l, v_l, s_l)) \leq \log n,$$

and

$$\begin{aligned} H(x') - H(x(\mathbf{u}, \mathbf{v}, \mathbf{s})) &= \sum_{l=1}^L (\langle w_l X'_l, \log(w_l X'_l) - \mathbf{1} \rangle - \langle w_l X_l(u_l, v_l, s_l), \log(w_l X_l(u_l, v_l, s_l)) - \mathbf{1} \rangle) \\ &= \sum_{l=1}^L w_l (H(X'_l) - H(X_l(u_l, v_l, s_l))) \leq \log n. \end{aligned}$$

By Lemma 7.4.1

$$\sum_{l=1}^L w_l \|X'_l - X_l^*\|_1 \leq \sum_{l=1}^L w_l \|(X_l^*)^\top \mathbf{1} - b_l\|_1 = \sum_{l=1}^L w_l \|p_l - b_l\|_1$$

as well as

$$\sum_{l=1}^L w_l \|\hat{X}_l - X_l(u_l, v_l, s_l)\|_1 \leq \sum_{l=1}^L w_l \|X_l^\top(u_l, v_l, s_l) \mathbf{1} - p_l\|_1 = \sum_{l=1}^L w_l \|p_l - b_l\|_1.$$

Thus, using that the values of C belong to $[0, 1]$ we obtain

$$\begin{aligned} \sum_{l=1}^L w_l \langle \hat{X}_l, C_l \rangle &\leq \sum_{l=1}^L w_l \langle X_l(\mathbf{u}, \mathbf{v}), C_l \rangle + \sum_{l=1}^L w_l \|p_l - b_l\|_1 \\ &\leq \sum_{l=1}^L w_l \langle X'_l, C_l \rangle + \lambda (H(x') - H(x(\mathbf{u}, \mathbf{v}, \mathbf{s}))) + \sum_{l=1}^L w_l \|p_l - b_l\|_1 \\ &\leq \langle X^*, C \rangle + 2 \sum_{l=1}^L w_l \|p_l - b_l\|_1 + \lambda \log n. \end{aligned}$$

□

We are going to use the stopping criterion

$$\|x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t) - x(\pi_u(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t))\|_1 + \|x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t) - x(\pi_v(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t))\|_1 \leq \varepsilon'. \quad (7.17)$$

But if we stop after iteration t where $i_t = u$, then possibly $X_l^\top \mathbf{1} \neq X_1^\top \mathbf{1}$ and we cannot apply Algorithm 4 to produce an approximate solution of (7.16). The next lemma shows that in this case we can make one more step of IBP.

Lemma 7.5.2. *Let $(\mathbf{u}, \mathbf{v}', \mathbf{s}') := \pi_u(\mathbf{u}, \mathbf{v}, \mathbf{s})$. Then*

$$\sum_{l=1}^L w_l \|X_l(u_l, v'_l, s'_l) \mathbf{1} - p_l\|_1 \leq \|x(\mathbf{u}, \mathbf{v}, \mathbf{s}) - x(\pi_u(\mathbf{u}, \mathbf{v}, \mathbf{s}))\|_1 + \|x(\mathbf{u}, \mathbf{v}, \mathbf{s}) - x(\pi_v(\mathbf{u}, \mathbf{v}, \mathbf{s}))\|_1.$$

Proof. First, due to the form of π_u one has

$$\|x(\mathbf{u}, \mathbf{v}, \mathbf{s}) - x(\pi_u(\mathbf{u}, \mathbf{v}, \mathbf{s}))\|_1 = \sum_{l=1}^L w_l \|X_l(u_l, v_l, s_l) \mathbf{1} - p_l\|_1. \quad (7.18)$$

Then

$$\begin{aligned} \sum_{l=1}^L w_l \|X_l(u_l, v'_l, s'_l) \mathbf{1} - p_l\|_1 &\leq \sum_{l=1}^L w_l (\|X_l(u_l, v'_l, s'_l) - X_l(u_l, v_l, s_l)\|_1 + \|X_l(u_l, v_l, s_l) \mathbf{1} - p_l\|_1) \\ &= \|x(\mathbf{u}, \mathbf{v}, \mathbf{s}) - x(\pi_v(\mathbf{u}, \mathbf{v}, \mathbf{s}))\|_1 + \|x(\mathbf{u}, \mathbf{v}, \mathbf{s}) - x(\pi_u(\mathbf{u}, \mathbf{v}, \mathbf{s}))\|_1. \end{aligned}$$

□

The above lemmata together with (7.18) justify the correctness of Algorithm 5.

Algorithm 5 Solving (7.16) by dual IBP

Input: Cost matrices C_1, \dots, C_L , vectors p_1, \dots, p_L , weights w_1, \dots, w_L , accuracy $\varepsilon > 0$.

1: Set $\lambda := \frac{\varepsilon}{2 \log n}$, $\varepsilon' := \frac{\varepsilon}{4}$.

2: Run Algorithm 1 with $u_l^0 := \log p_l$, $v_l^0 = 0$, $s_l^0 = 0$, for $l \in [L]$, and obtain $(w_1 X_1, \dots, w_L X_L) := x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t)$ satisfying (7.17).

3: **if** $i_{t-1} = u$ **then**

4: Set $(w_1 X_1, \dots, w_L X_L) := x(\mathbf{u}^{t+1}, \mathbf{v}^{t+1}, \mathbf{s}^{t+1})$.

5: **end if**

6: Compute $\hat{X}_1, \dots, \hat{X}_L$ by Algorithm 2.

Output: $\hat{X}_1, \dots, \hat{X}_L$.

Again, we need the following bounds to ensure Assumption 7.1.

Lemma 7.5.3. *Fix $\lambda > 0$. Let $\mathbf{u} \in \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_L}$, $\mathbf{v} \in (\mathbb{R}^n)^L$, $\mathbf{s} \in \mathbb{R}^L$, and $(\mathbf{u}^*, \mathbf{v}^*, \mathbf{s}^*)$ be any solution of the dual problem. If $(\mathbf{u}', \mathbf{v}, \mathbf{s}) := \pi_u(\mathbf{u}, \mathbf{v}, \mathbf{s})$, then*

$$|u'_l - \log p_l| \leq \frac{1}{\lambda} \quad \forall l \in [L],$$

and if $(\mathbf{u}, \mathbf{v}', \mathbf{s}') := \pi_v(\mathbf{u}, \mathbf{v}, \mathbf{s})$, then

$$|v'_l| \leq \frac{2}{\lambda} \quad \forall l \in [L].$$

In particular, $(\mathbf{u}^*, \mathbf{v}^*, \mathbf{s}^*)$ also satisfies the above bounds.

Proof. In the same way as in the proof of Lemma 7.4.3 we can show that

$$\log w_l - s_l - \log \langle e^{v_l}, \mathbf{1} \rangle \leq \min(u'_l - \log p_l) \leq \max(u'_l - \log p_l) \leq \log w_l - s_l - \log \langle e^{v_l}, \mathbf{1} \rangle + \frac{1}{\lambda},$$

hence $|u'_l - \log p_l| \leq \frac{1}{\lambda}$. Similarly,

$$\begin{aligned} s_l + \log \langle e^{u_l}, \mathbf{1} \rangle - \log w_l - \frac{1}{\lambda} &\leq \min [\log (X_l^\top(u_l, v_l, s_l) \mathbf{1}) - v_l] \\ &\leq \max [\log (X_l^\top(u_l, v_l, s_l) \mathbf{1}) - v_l] \leq s_l + \log \langle e^{u_l}, \mathbf{1} \rangle - \log w_l, \end{aligned}$$

thus $|\log (X_l^\top(u_l, v_l, s_l) \mathbf{1}) - v_l| \leq \frac{1}{\lambda}$ and $|v'_l| \leq \frac{2}{\lambda}$. In particular, the same bounds hold for $(\mathbf{u}^*, \mathbf{v}^*, \mathbf{s}^*)$. \square

Theorem 7.5.4. *The iteration complexity of Algorithm 5 is bounded by*

$$96 \frac{\log n}{\varepsilon^2} + 2 = O\left(\frac{\log N}{\varepsilon^2}\right).$$

Proof. By construction, $X_l(\pi_u(\mathbf{u}, \mathbf{v}, \mathbf{s}))$ and $X_l(\pi_v(\mathbf{u}, \mathbf{v}, \mathbf{s}))$ have unit mass for all $\mathbf{u}, \mathbf{v}, \mathbf{s}$. Hence using Lemma 7.5.3 we can obtain in the same way as in the proof of Theorem 7.4.4 that for all $t \geq 1$

$$\begin{aligned} \langle x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t) - x(\pi_u(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t)), A_u^\top(\mathbf{u}^t - \log \mathbf{p}) \rangle &= \sum_{l=1}^L w_l \langle X_l(u_l^t, v_l^t, s_l^t) \mathbf{1} - p_l, u_l^t - \log p_l \rangle \\ &\leq \frac{1}{2} \sum_{l=1}^L w_l \|X_l(u_l^t, v_l^t, s_l^t) \mathbf{1} - p_l\|_1 |u_l^t - \log p_l| \\ &\leq \frac{1}{2\lambda} \|x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t) - x(\pi_u(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t))\|_1, \end{aligned}$$

and thus

$$\langle x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t) - x(\pi_u(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t)), A_u^\top(\mathbf{u}^t - \mathbf{u}^*) \rangle \leq \frac{1}{\lambda} \|x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t) - x(\pi_u(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t))\|_1.$$

Furthermore,

$$\begin{aligned} \langle x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t) - x(\pi_v(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t)), A_v^\top(\mathbf{s}^t, \mathbf{v}^t) \rangle &= \sum_{l=1}^L w_l [\langle X_l^\top(u_l^t, v_l^t, s_l^t) \mathbf{1} - \hat{q}, v_l^t \rangle + s_l (\langle X_l(u_l^t, v_l^t, s_l^t) \mathbf{1}, \mathbf{1} \rangle - 1)] \\ &= \sum_{l=1}^L w_l \langle X_l^\top(u_l^t, v_l^t, s_l^t) \mathbf{1} - \hat{q}, v_l^t \rangle, \end{aligned}$$

where $\hat{q} := \frac{q}{(q, \mathbf{1})} \in \Delta^{n-1}$, $q := \prod_{l=1}^L (X_l^\top \mathbf{1})^{w_l}$. By the same arguments,

$$\langle x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t) - x(\pi_v(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t)), A_v^\top(\mathbf{s}^t - \mathbf{s}^*, \mathbf{v}^t - \mathbf{v}^*) \rangle \leq \frac{2}{\lambda} \|x(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t) - x(\pi_v(\mathbf{u}^t, \mathbf{v}^t, \mathbf{s}^t))\|_1.$$

Therefore, Assumption 7.1 is fulfilled with $R = \frac{2}{\lambda} = \frac{4 \log N}{\varepsilon}$. The claim follows from Theorem 7.3.3. \square

7.6 Numerical experiments

In this section, we provide a numerical analysis of dual IBP for the computation of approximate Wasserstein barycenters and the solution of the multimarginal optimal transport problem. Let us mention that this is not among the main goals of the thesis and we add it here for illustrative purposes. The algorithm is implemented in Python 3.7 [VD09] using the log-domain stabilization technique to speed up [Chi+18; Sch19].

Multimarginal optimal transport. Let us consider the multimarginal problem (1.6) associated with the 2-Wasserstein barycenter problem. We generated three samples in \mathbb{R}^2 of size 40 from the uniform distributions on the unit discs centered at the points $(0, 0)$, $(0, 1)$, and $(1, 0)$, respectively (Fig. 7.1a). Then we applied Algorithm 3 to solve the corresponding discrete problem (1.6) with equal weights. The push-forward of the obtained approximate solution $\hat{\gamma}$ by the barycenter map $(x_1, x_2, x_3 \mapsto \frac{x_1+x_2+x_3}{3})$, which gives an approximate Wasserstein barycenter, is depicted in Figure 7.1b. Finally, Figure 7.2a shows the dependence of the number of iterations T on the accuracy ε for the greedy, cyclic, and random strategies. As we can see, in the considered range of values ε the complexities of all three strategies are close and the dependence is almost linear in the log–log scale with the slope ≈ -1.2 , i.e. $T \approx \mathcal{C} \left(\frac{1}{\varepsilon}\right)^{1.2}$, which is faster than the theoretical bound $O\left(\frac{1}{\varepsilon}\right)^2$ obtained in Section 7.4.

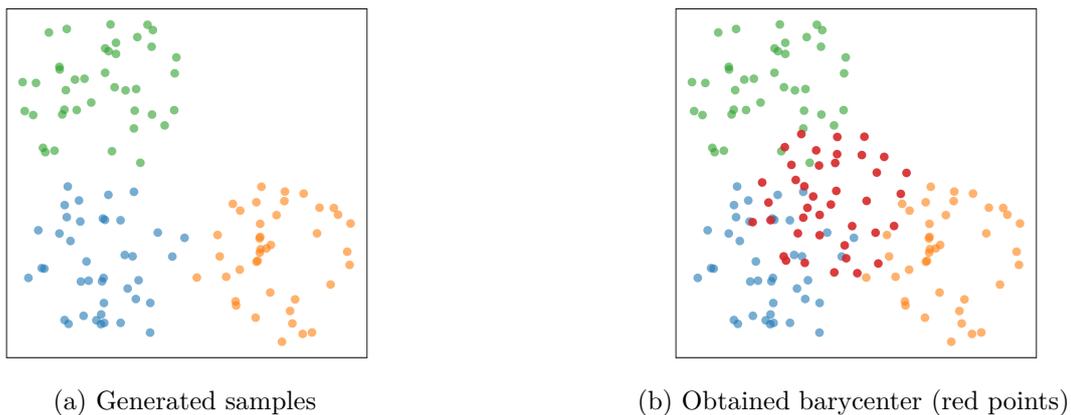


Figure 7.1: The initial data and the output of Algorithm 3

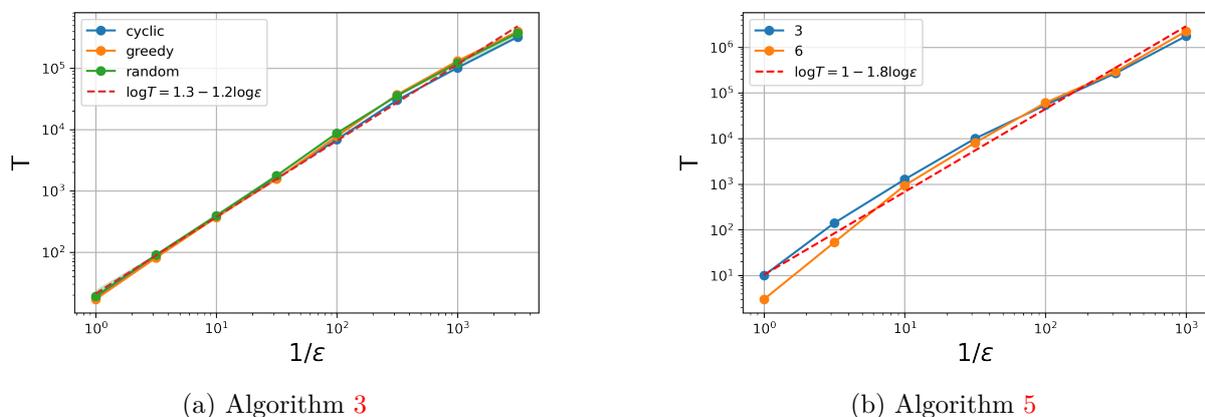


Figure 7.2: Number of iterations T vs. accuracy ε

Wasserstein barycenters. Figure 7.3 depicts two samples of greyscale images of handwritten digits (“3” and “6”, respectively) from the MNIST dataset [LC10]. Considering the images as measures on the 28×28 regular grid (normalized to have the total mass 1), we are looking for the 2-Wasserstein barycenters of these samples with equal weights supported on the same grid. Figure 7.4 shows the output of Algorithm 5 applied to the above images with different accuracy ε after the normalization of the cost matrix to be between 0 to 1. As expected, the higher the accuracy, the sharper the barycenter, and for small ε we observe notable oscillations. Figure 7.2b demonstrates the dependence of the number of iterations T on the accuracy ε . For small ε the complexities for two samples are similar. Moreover, the dependence is almost linear in the log–log scale with the slope ≈ -1.8 , i.e. $T \approx \mathcal{C} \left(\frac{1}{\varepsilon}\right)^{1.8}$, which is faster but close enough to the theoretical bound $O\left(\frac{1}{\varepsilon}\right)^2$ obtained in Section 7.5.



Figure 7.3: Two sample of images from the MNIST dataset: digits “3” (top row) and “6” (bottom row)

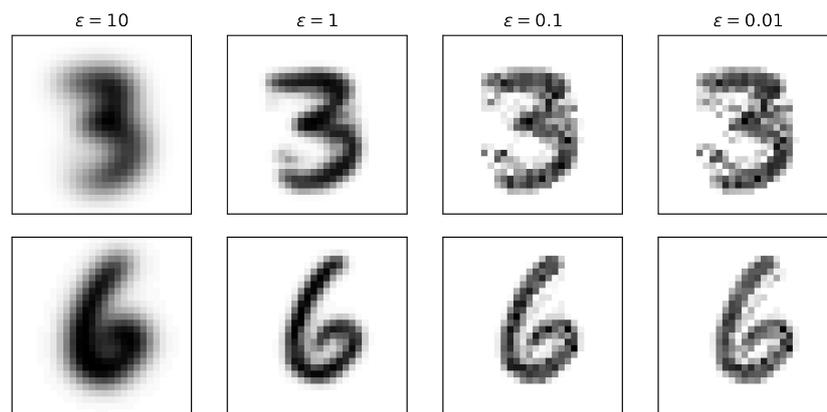


Figure 7.4: Approximate barycenters of the images from Figure 7.3 for different values of ε

As we see, in both cases, the convergence is faster than given by the upper bounds from Sections 7.4 and 7.5. However, for the moment, we are not aware of better theoretical guarantees or lower bounds for IBP.

Chapter 8

Résumé des résultats de la thèse

8.1 Transport optimal

La théorie du transport optimal est aujourd’hui un domaine de recherche populaire. Elle remonte à G. Monge [Mon81], tandis que sa formulation moderne est due à L. Kantorovich [Kan42]. L’objet central est le problème du transport optimal, qui consiste à transformer une distribution de masse μ en une autre ν avec le minimum de travail. Dans la formulation de Kantorovich, connue sous le nom de problème de Monge–Kantorovich, ce problème se lit comme suit : étant donné des mesures de probabilité μ et ν et une *fonction de coût* $c(\cdot, \cdot)$, on veut minimiser le coût total de transport

$$\int c(x, y) \, d\gamma(x, y) \rightarrow \min_{\gamma},$$

où la minimisation se fait parmi les couplages de μ et ν . D’un intérêt particulier est le cas où μ et ν sont des mesures de probabilité sur le même espace métrique (X, ρ) et $c := \rho^p$ pour un certain $1 \leq p < \infty$. On peut alors définir la *distance de p -Wasserstein*

$$W_p(\mu, \nu) := \left(\inf \left\{ \int_{X \times X} \rho^p(x, y) \, d\gamma(x, y) : \gamma \text{ est un couplage de } \mu \text{ et } \nu \right\} \right)^{1/p}.$$

L’espace $\mathcal{P}_p(X)$ de mesures de probabilité sur X avec le moment d’ordre p fini, doté de W_p , est appelé espace de p -Wasserstein sur X . Une propriété importante de la distance de Wasserstein est qu’elle capture la géométrie de l’espace sous-jacent X . En raison de ce fait, elle est largement utilisée dans divers domaines tels que la théorie des probabilités et les statistiques, les processus stochastiques, les EDP, la théorie cinétique, le traitement des images, l’analyse des données et l’apprentissage automatique. Dans cette thèse, on considère certains problèmes variationnels impliquant le transport optimal.

8.2 Topologie des transports

Dans le Chapitre 3, on considère un cadre abstrait avec un espace métrique séparable X et une fonction de coût continue $c: X \times X \rightarrow \mathbb{R}_+$ et définissons la fonction de transport

$$J(\mu, \nu) := \inf \left\{ \int_{X \times X} c(x, y) \, d\gamma(x, y) : \gamma \text{ est un couplage de } \mu \text{ et } \nu \right\}.$$

On suppose que X est un espace de Radon (voir la Définition 2.2) — par exemple, un espace polonais ; la fonction de coût est « cohérente » et satisfait la propriété de Radon–Riesz, c’est-à-dire que $c(x, y) = 0$ si et seulement si $x = y$ et qu’il existe une métrique plus faible ρ_w sur X telle que si $x_n \rightarrow x$, $\rho_w(y_n, y) \rightarrow 0$ et $c(x_n, y_n) \rightarrow c(x, y)$, alors $y_n \rightarrow y$. On suppose également que c satisfait une forme faible de l’inégalité triangulaire : pour certaines constantes $A, B > 0$

$$c(x, y) \leq A + B(\min\{c(x, z), c(z, x)\} + \min\{c(y, z), c(z, y)\}) \quad \forall x, y, z, \in X.$$

En particulier, ces hypothèses sont satisfaites dans le cas de la métrique de Wasserstein. On montre ensuite que J hérite des propriétés ci-dessus de la fonction de coût c . Elle induit une topologie τ_J sur $\mathcal{P}(X)$ avec la base de « boules » $B_r^J(\mu) := \{\nu \in \mathcal{P}(X) : J(\mu, \nu) < r\}$ (on peut donc la considérer comme une généralisation de la métrique de Wasserstein). De plus, sous l'hypothèse supplémentaire de la « complétude » de (X, c) on obtient que tout ensemble $E(\mu) := \{\nu \in \mathcal{P}(X) : J(\mu, \nu) < \infty\}$ doté de τ_J est un espace polonais (Théorème 3.3.9).

Ce chapitre est principalement basé sur le travail [Kro18].

8.3 Barycentres

En 2011, M. Agueh et G. Carlier ont introduit un « élément typique » d'une famille de mesures de probabilité μ_1, \dots, μ_n sur l'espace euclidien \mathbb{R}^d , appelé le barycentre de Wasserstein [AC11] :

$$\nu^* := \operatorname{argmin}_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} \sum_{i=1}^n w_i W_2^2(\mu_i, \nu),$$

où w_1, \dots, w_n sont des poids positifs. Il s'agit d'une instance particulière de la moyenne de Fréchet dans le cas de l'espace de 2-Wasserstein [Fré48]. Il s'avère que le barycentre capture dans une certaine mesure la forme des mesures moyennées μ_1, \dots, μ_n , ce qui le rend favorable par rapport à la moyenne linéaire des mesures et lui vaut une grande attention.

Dans les travaux [BK12; KP17; LL17], le concept de barycentre de Wasserstein a été généralisé au cas d'une distribution de probabilité P sur $\mathcal{P}_p(X)$ et d'un exposant $p \geq 1$:

$$\nu^* := \operatorname{argmin}_{\nu \in \mathcal{P}_p(X)} \int W_p^p(\mu, \nu) dP(\mu).$$

[BK18] et [LL17] montrent la stabilité du barycentre par rapport à P . En particulier, si les mesures μ_1, μ_2, \dots sont tirées indépendamment selon P , alors les barycentres empiriques

$$\nu_n := \operatorname{argmin}_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} \frac{1}{n} \sum_{i=1}^n W_p^p(\mu_i, \nu).$$

convergent vers le barycentre de la population $\nu^* : W_p(\nu_n, \nu^*) \rightarrow 0$, c'est-à-dire qu'il existe la loi des grands nombres (LLN). De plus, J. Bigot, E. Cazelles et N. Papadakis dans [BCP19] ont proposé d'ajouter une pénalisation à la fonctionnelle de variance de Wasserstein ci-dessus pour régulariser le barycentre. Les Chapitres 3, 4 et 5 sont consacrés à des sujets connexes.

Barycentres de Fréchet. Dans le contexte de la Section 8.2, on définit une moyenne dans $\mathcal{P}(X)$ en fonction de J , que l'on appelle le *barycentre de Fréchet* régularisé : étant donné une distribution P sur $\mathcal{P}(X)$ et une pénalité G ,

$$\nu^* := \operatorname{argmin}_{\nu \in \mathcal{P}(X)} \left[\int J(\mu, \nu) dP(\mu) + G(\nu) \right].$$

On prouve qu'un tel barycentre existe lorsque $\int J(\mu, \mu_0) dP(\mu) < \infty$ pour un certain μ_0 , X est localement compact par rapport à ρ_w , G est semi-continu inférieur par rapport à la convergence étroite et borné par le bas par une fonction $\alpha(\nu) = o(J(\mu_0, \nu))$ lorsque $J(\mu_0, \nu) \rightarrow \infty$ (Proposition 3.5.1). Le Théorème 3.5.2 montre que les barycentres de Fréchet sont stables par rapport à P au sens de [LL17]. A savoir, soit

$$\mathcal{J}(P, Q) := \inf \left\{ \int J(\mu, \nu) d\Gamma(\mu, \nu) : \Gamma \text{ est un couplage de } P \text{ et } Q \right\}, \quad P, Q \in \mathcal{P}(X),$$

et $\mathcal{J}(P_n, P) \rightarrow 0$. Étant donnée une suite G_n satisfaisant aux hypothèses ci-dessus avec un même α et Γ -convergeant (localement) vers une fonctionnelle G , si ν_n est un barycentre de P_n , alors il

existe une sous-suite convergeant vers un certain barycentre de P dans la topologie du transport (Théorème 3.5.2). En particulier, dans le cadre stochastique mentionné ci-dessus, on a une loi des grands nombres.

Ces résultats sont principalement basés sur le travail [Kro18].

Barycentres de Bures–Wasserstein. Pour les mesures gaussiennes $\mu = \mathcal{N}(a, Q)$ et $\nu = \mathcal{N}(b, S)$ sur \mathbb{R}^d , il s'avère que

$$W_2^2(\mu, \nu) = \|a - b\|^2 + \operatorname{tr} Q + \operatorname{tr} S - 2 \operatorname{tr} \left(Q^{1/2} S Q^{1/2} \right)^{1/2}.$$

De plus, il est connu que si $P \in \mathcal{P}(\mathcal{P}_2(\mathbb{R}^d))$ est concentré sur des mesures gaussiennes, alors (au moins un de) son barycentre de 2-Wasserstein est aussi gaussien [AC11]. Pour des raisons de simplicité, on ne considère que les mesures centrées, qui sont entièrement décrites par leur matrice de covariance. On peut ensuite généraliser la formule ci-dessus aux matrices semi-définies positives hermitiennes, ce qui permet d'obtenir la métrique dite de *Bures–Wasserstein* d_{BW} sur $\mathbb{H}_+(d)$. Dans le Chapitre 4, basé sur le travail conjoint avec V. Spokoiny et A. Suvorikova [KSS21], on considère les barycentres de Bures–Wasserstein correspondants. On étudie les propriétés différentielles de la métrique de Bures–Wasserstein pour prouver le théorème de la limite centrale :

$$\sqrt{n}(Q_n - Q_*) \xrightarrow{d} \mathcal{N}(0, \Xi),$$

où

$$Q_n := \operatorname{argmin}_{Q \in \mathbb{H}_+(d)} \frac{1}{n} \sum_{i=1}^n d_{BW}^2(S_i, Q), \quad Q_* := \operatorname{argmin}_{Q \in \mathbb{H}_+(d)} \int_{\mathbb{H}_+(d)} d_{BW}^2(S, Q) dP(S)$$

sont les barycentres empiriques et de population, respectivement, et les S_i sont tirés indépendamment selon P . On obtient également des bornes non asymptotiques sur $\|Q_n - Q_*\|$ et $W_2(\nu_n, \nu_*)$ sous l'hypothèse que $\operatorname{tr} S_i$ est une variable aléatoire sous-exponentielle. De plus, pour le cas d'une famille dégénérée d'échelle-localisation (scale-location), on fournit un exemple de taux de convergence plus lent que $\frac{1}{\sqrt{n}}$.

Barycentres entropiques de Wasserstein Dans le Chapitre 5, on considère une distribution P sur l'espace de 2-Wasserstein sur \mathbb{R}^d et, suivant [BCP19], on définit son barycentre de Wasserstein régularisé par l'entropie.

$$\nu^* := \operatorname{argmin}_{\nu \in \mathcal{P}_2(\Omega)} \left[\int W_2^2(\mu, \nu) dP(\mu) + \lambda \operatorname{Ent}(\nu) \right],$$

où $\Omega \subset \mathbb{R}^d$ est un ensemble ouvert de mesure de Lebesgue positive. On prouve l'existence et l'unicité de cet objet, et le caractérisons en termes de potentiels duaux de Kantorovich. En particulier, ν^* est a.c. et sa densité $\bar{\rho}$ satisfait les conditions suivantes

$$\log \bar{\rho}(x) = -\frac{1}{\lambda} \int u_{\bar{\rho}}^{\nu}(x) dP(\nu) \quad \forall x \in \Omega,$$

où $u_{\bar{\rho}}^{\nu}$ est un potentiel de Kantorovich entre $\bar{\rho}$ et ν pour la fonction de coût $\frac{\|x-y\|^2}{2}$ (Théorème 5.3.6). En utilisant cette caractérisation, on étudie les propriétés des barycentres entropiques de Wasserstein : des bornes de moments (Proposition 5.4.2), un principe de maximum (Proposition 5.4.7), une régularité supérieure (Proposition 5.5.2) et une stabilité au sens de [LL17] (Lemma 5.4.6). De plus, si Ω est une boule et que P est concentré sur des mesures sur Ω avec une densité Hölderienne, alors on prouve le théorème de la limite centrale pour les densités des barycentres empiriques dans l'espace de Sobolev H^2 (Théorème 5.6.2).

Ce chapitre est basé sur un travail conjoint avec G. Carlier et K. Eichinger [CEK20].

8.4 Espaces de Sobolev de fonctions à valeur mesures et problème de Monge–Kantorovich régularisé

Le Chapitre 6 est consacré à l'espace de Sobolev $W^{1,p}$ des applications à valeurs dans l'espace de p -Wasserstein sur \mathbb{R}^d . Étant donné un domaine ouvert $\Omega \subset \mathbb{R}^m$, on définit l'espace $W^{1,p}(\Omega, \mathcal{P}_p(\mathbb{R}^d))$ au sens de Reshetnyak [Res97]. Selon Lavenant [Lav19b], celui-ci admet une définition équivalente : $\mu : \Omega \rightarrow \mathcal{P}_p(\mathbb{R}^d)$ est Sobolev s'il existe une mesure de Young ϱ sur $\Omega \times \mathbb{R}^d \times \mathbb{R}^{m \times d}$ (*mesure de phase*) telle que sa projection sur les deux premières composantes $\pi_{\#}^{1,2} \varrho = \mu \otimes \mathcal{L}|_{\Omega}$, $\int \|V\|^p d\varrho(\xi, x, V) < \infty$ et pour tout $\varphi \in C_c^1(\Omega \times \mathbb{R}^d)$

$$\int (\nabla_{\xi} \varphi(\xi, x) + V \nabla_x \varphi(\xi, x)) d\varrho(\xi, x, V) = 0.$$

On étudie les propriétés fines des applications de Sobolev, à savoir, on montre l'existence de représentants précis à un petit ensemble près : pour tout Sobolev μ , il existe un borélien $A \subset \Omega$ et une application $\mu^* : \Omega \rightarrow \mathcal{P}_p(\mathbb{R}^d)$ telle que $\text{Cap}_p(A) = 0$ et

$$W_p \left(\int_{B_r(\xi)} \mu[\zeta] d\zeta, \mu^*[\xi] \right) \rightarrow 0 \text{ lorsque } r \rightarrow 0$$

(Lemma 6.3.2). On donne également deux notions de convergence dans ces espaces : une basée sur la propriété de Radon–Riesz (Proposition 6.4.2) et une sur la convergence des mesures de phase dans une topologie de transport (Corollaire 6.4.7). Les deux assurent la convergence des représentants précis. Enfin, on définit l'énergie de Dirichlet de μ comme suit

$$\text{Dir}_p(\mu) := \inf \left\{ \int \|V\|^p d\varrho : \varrho \text{ est une mesure de phase de } \mu \right\}$$

et on applique la théorie ci-dessus au problème régularisé de Monge–Kantorovich entre $\mu \in \mathcal{P}(\Omega)$ et $\nu \in \mathcal{P}(\mathbb{R}^d)$:

$$\int_{\Omega} \int_{\mathbb{R}^d} c(x, y) d\gamma_x^*(y) d\mu(x) + \text{Dir}_p(\gamma) \rightarrow \min_{\gamma_x \in W^{1,p} : \int \gamma_x^* d\mu(x) = \nu},$$

Où γ_x^* est le représentant précis de la carte $x \mapsto \gamma_x \in \mathcal{P}_p(\mathbb{R}^d)$. Sous des hypothèses assez faibles, on montre l'existence d'une solution du problème ci-dessus (Théorème 6.5.1).

8.5 Analyse des projections itératives de Bregman

Dans le Chapitre 7, on considère l'algorithme itératif des projections de Bregman [Ben+15] pour résoudre le problème

$$\min \{ \langle c, x \rangle + \lambda \text{Ent}(x) : x \in \mathbb{R}_+^N, A_i x = b_i, i = 1, \dots, m \}.$$

Il s'agit d'une généralisation de l'algorithme bien connu de Sinkhorn pour le problème de Monge–Kantorovich discret régularisé par l'entropie, consistant à alterner les projections sur les ensembles affines $\{A_i x = b_i\}$ en fonction de la divergence de Kullback–Leibler. On donne une autre forme de cet algorithme sous la forme d'une minimisation alternée dans le problème dual et suggérons deux stratégies différentes de projections : gloutonne et aléatoire. On fournit un schéma général de la preuve des limites de complexité et l'appliquons à deux problèmes liés au transport optimal : le transport optimal multimarginal et le barycentre de Fréchet. Dans les deux cas, on obtient la complexité d'itération $O\left(\frac{1}{\varepsilon^2}\right)$ pour atteindre la précision ε (dans le problème primal non régularisé), par rapport à la limite précédente la plus connue $O\left(\frac{1}{\varepsilon^3}\right)$ pour l'algorithme de Sinkhorn [AWR17].

Ceci est basé sur et généralise les résultats des travaux conjoints avec A. Gasnikov, P. Dvurechensky et al. [DGK18; Kro+19; Sto+19].

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