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# Classical and multi-marginal optimal transport, with applications


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# Introduction

In the thesis I present the work done during my three years of PhD at Scuola Normale Superiore. The exposition follows the content of four articles ([AST16], [BDS], [CS16] and [CDS]) written in collaboration with Luigi Ambrosio, Elia Bruè, Maria Colombo, Simone Di Marino and Dario Trevisan during this same period. The problems that I have studied belong to the field of optimal transport, both the classical (two-marginal) case and the multi-marginal variant; hence the thesis is sharply divided in two parts presenting two articles each. A fifth article, [AST17], also written during my PhD, does not appear in the thesis because its content is excessively unrelated to the other ones.

Concerning the classical case, I have studied the so called *random matching* problem and an application of optimal transport to the extension of Lipschitz functions defined on metric spaces.

In the random matching problem one is given a reference probability measure $\mu$, for instance the Lebesgue measure in the unit square, from which two families $\{X_i\}_{i=1}^n$ and $\{Y_i\}_{i=1}^n$ of $n$ independent random points each are sampled. Each family of points yields an *empirical* probability measure given by the sum of equal deltas concentrated on such points:

$$\mu_n = \sum_{i=1}^n \delta_{X_i} \qquad \text{and} \qquad \nu_n = \sum_{i=1}^n \delta_{Y_i}.$$

The Wasserstein $W_2$ distance is used to measure how far apart these two random families of points are. Then the question is to determine the rate of convergence to zero of the expected value of this distance as $n \to \infty$. Previous results show that, in the unit square with the Lebesgue measure, $\mathbb{E}\left[W_2^2(\mu_n, \nu_n)\right]$ is asymptotically equivalent to $\frac{\log n}{n}$. This has also been confirmed numerically in [Car+14], where the authors also conjecture the existence of the renormalized limit $\lim_{n\to\infty} \frac{n}{\log n} \mathbb{E}\left[W_2^2(\mu_n, \nu_n)\right]$. Our contribution to the subject in [AST16] is showing that in dimension 2 the actual limit

$$\lim_{n\to\infty} \frac{n}{\log n} \mathbb{E}\left[W_2^2(\mu_n, \nu_n)\right] = \frac{1}{2\pi}$$

exists under quite general assumptions on the domain. The result is obtained through a PDE approach that linearizes the Monge-Ampère equation solved by the transport map and estimates the $W_2$ distance with the Dirichlet energy of solutions to the Laplace equation with random data. This strategy is a formalization of the heuristic idea presented in [Car+14].

The second problem addressed in the classical setting is that of extending Lipschitz functions. Given two metric spaces $X \subset Y$ and a Banach space $B$, the problem is to find a linear extension operator $T : \mathrm{Lip}(X; B) \to \mathrm{Lip}(Y; B)$ with a controlled operator norm. In particular, all the assumptions shall be made on the geometry of $X$ alone and the bound for the norm should be independent of the particular spaces $Y$ and $B$. A result of Lee and Naor in 2005, [LN05], shows that there exists such an operator satisfying $\|T\| \lesssim \log(\lambda_X)$ where $\lambda_X$ is the metric doubling constant of $X$. Our contribution is revisiting their long proof in a spirit closer to the approach followed by Whitney for his $C^1$ extension theorem. The key idea behind our approach is that of *random projection*, a useful concept recently introduced by Ohta in [Oht09] and by Ambrosio and Puglisi in [AP16]: instead of a deterministic projection $P : Y \to X$, for some applications it is sufficient to have a map $\mu : Y \to \mathscr{P}(X)$ with some regularity properties, such as being Lipschitz with respect to the Wasserstein distance $W_1$, induced by the cost equal to the distnce. Given a function $f \in \mathrm{Lip}(Y; B)$, its extension can then be defined as $\tilde{f}(y) = \int_X f(x)\,\mathrm{d}\mu_y(x)$ and the properties of $\mu$ allow to infer regularity properties of such extension. The main portion of our work is to show an elementary construction of a regular random projection, from which interesting consequences can then be derived. With the same tool we are also able to generalize Whitney's extension theorem for $C^1$ functions to the smooth Banach setting.

The second part of the thesis deals with the multi-marginal optimal transport problem. This is a variant of the classical theory which appears naturally in the Density Functional Theory, a computational method used in quantum chemistry to model the electronic structure of atoms and molecules. In this context, the distribution of $N$ indistinguishable electrons is represented by a probability measure $\rho$ in $\mathbb{R}^3$ (the density) and the ground state is obtained as the configuration that minimizes a few energy terms (the functionals). Under some suitable approximations developed by Hohenberg, Kohn and Sham, one of the terms reduces to the minimization of $\int_{(\mathbb{R}^d)^N} \sum_{i<j} \frac{1}{|x_i - x_j|}\,\mathrm{d}\pi(x_1, \dots, x_N)$ among all transport plans $\pi \in \mathscr{P}\big((\mathbb{R}^d)^N\big)$ having $N$ marginals equal to $\rho$. This is a generalization of the two-marginal Kantorovich problem with a singular cost given by the sum of all possible Coulomb interactions.

In the first article on this subject, we disprove a conjecture made by physicists regarding the structure of the optimal transport plan. The conjecture was modeled after the rigid structure of the minimizer in dimension $d = 1$, but unfortunately the analogue in higher dimension turns out to be false in general. Despite this, we are able to show some cases in which the suggested structure is indeed valid and this could be an explanation of the numerical evidence the physicists had while proposing the conjecture.

In a follow-up article on the same subject we address another conjecture, this time regarding the regularity of the dual potentials and the continuity properties of the optimal cost. The main contribution that we provide is a sharp result stating that if the marginal $\rho$ does not concentrate mass too much then the optimal transport cost is finite and locally Lipschitz around $\rho$. The way to reach this conclusion is through an argument which shows that, under the no-concentration assumption on the marginal, the optimal plan is supported far away from the diagonal, that is to say that there are no correlations among electrons which are too close.

# Part I

# Classical optimal transport

# Chapter 1

# Introduction to the classical optimal transport

In this first chapter I introduce the optimal transport problem in its classical formulation and briefly review the theory that is needed in the subsequent parts. This field of research is extremely mature and well established, therefore much more detailed presentations already exist, such as [AGS08], [San15], [Vil01] or [Vil09] for instance.

The original problem posed by Monge in 1780 is as follows. Given two Borel probability measures $\mu$ and $\nu$ in $\mathbb{R}^n$, minimize

$$\int_{\mathbb{R}^n} |T(x) - x| \,\mathrm{d}\mu(x)$$

among all *transport maps* $T : \mathbb{R}^n \to \mathbb{R}^n$ such that $T_\# \mu = \nu$. The notation $T_\# \mu$ denotes the push-forward operation, that is, the measure $T_\# \mu \in \mathscr{M}(\mathbb{R}^n)$ such that $T_\# \mu(A) = \mu\big(T^{-1}(A)\big)$ for every Borel set $A \in \mathscr{B}(\mathbb{R}^n)$.

This optimization problem can be generalized to a Polish space[1] $X$ with two Borel probabilities $\mu$ and $\nu$ and a lower semi-continuous cost function $c : X \times X \to \mathbb{R}$ bounded from below. The transport maps are

$$\mathcal{T}(\mu, \nu) = \{T : X \to X : T_\# \mu = \nu\}$$

and the Monge problem is then the minimization

$$(M) = \inf_{T \in \mathcal{T}(\mu,\nu)} \int_X c\big(x, T(x)\big) \,\mathrm{d}\mu(x).$$

This formulation is hard to treat because of the difficulty to prove the existence of optimal maps. Moreover, in some circumstances the problem can be ill posed simply because there are no admissible transport maps. For these reasons, Kantorovich introduced a relaxed version of the problem that under very general

[1]Separable and completely metrizable.

assumptions guarantees the existence of optimal solutions. His formulation is as follows.

First of all, notice that a transport map $T$ induces a measure $\pi_T = (\mathrm{Id}, T)_\# \mu \in \mathscr{P}(X \times X)$ which has marginals $\mu$ and $\nu$. The idea of Kantorovich is then to consider all admissible *transport plans*

$$\Pi(\mu, \nu) = \left\{ \pi \in \mathscr{P}(X \times X) : P^1_\# \pi = \mu,\ P^2_\# \pi = \nu \right\},$$

where $P^i : X \times X \to X$ are the projections, and minimize the cost

$$(K) = \min_{\pi \in \Pi(\mu,\nu)} \int_{X \times X} c(x, y) \, \mathrm{d}\pi(x, y).$$

Thanks to compactness properties of probability measures and the linearity of the problem (both in the cost and the constraint) with respect to the unknown $\pi$, the existence of minimizers is easier to obtain under very general assumptions. The question is then whether these minimizers are induced by suitable transport maps as described before.

Another advantage of posing the optimal transport as a linear problem is that it unlocks a tool called *duality*. In the field of linear programming it is well known that every linear minimization problem is closely linked to a corresponding maximization problem that shares the same optimal value. The same happens for the Kantorovich's problem, in which the minimum of $(K)$ is equal to the *dual problem*

$$(D) = \sup_{\substack{(\varphi,\psi) \in C_b(X) \times C_b(X) \\ \varphi(x) + \psi(y) \le c(x,y)}} \int_X \varphi(x) \, \mathrm{d}\mu(x) + \int_X \psi(y) \, \mathrm{d}\nu(y).$$

The pair of functions $(\varphi, \psi)$ satisfying the given constraint are called dual potentials.

A particularly important case of optimal transport is when the cost function is $c(x, y) = \mathsf{d}(x, y)^p$, where $\mathsf{d}$ is a distance on $X$ and $p \ge 1$. In order to ensure the finiteness of $(K)$ with this particular choice of the cost, it is appropriate to restrict the problem to probabilities with finite $p$-th moment:

$$\mathscr{P}_p(X) = \left\{ \mu \in \mathscr{P}(X) : \int_X \mathsf{d}(x, x_0)^p \, \mathrm{d}\mu < \infty, \text{ for some } x_0 \in X \right\}.$$

By the triangle inequality, it is easy to check that the definition does not depend on the particular choice of the reference point $x_0$, so that the $p$-th moment is either finite or infinite for all points $x_0 \in X$. With this definition, one can introduce the function $W_p : \mathscr{P}_p(X) \times \mathscr{P}_p(X) \to [0, \infty)$ defined as the $p$-th root of the optimal cost:

$$W_p(\mu, \nu) := \min_{\pi \in \Pi(\mu,\nu)} \left( \int_{X \times X} \mathsf{d}(x, y)^p \, \mathrm{d}\pi(x, y) \right)^{1/p}, \qquad \text{for } \mu, \nu \in \mathscr{P}_p(X).$$

It can be shown that $W_p$ is a distance on $\mathscr{P}_p(X)$, called Wasserstein distance, which almost metrizes weak convergence of probabilities: precisely, we have that $W_p(\mu_n, \mu) \to 0$ if and only if $\mu_n \rightharpoonup \mu$ and $\int_X \mathsf{d}(x, x_0)^p \,\mathrm{d}\mu_n \to \int_X \mathsf{d}(x, x_0)^p \,\mathrm{d}\mu_n$.

Of special interest are the cases when $p = 1$ or $p = 2$. With $p = 1$ there is a deep connection with Lipschitz functions which will be exploited in Chapter 3 in the context of extension results. In fact, the constraint on the potentials in the dual formulation $(D)$ reads $\varphi(x) + \psi(y) \leq \mathsf{d}(x, y)$. First of all, notice that if $\varphi$ is 1-Lipschitz then $(\varphi, -\varphi)$ is an admissible pair of potentials. Moreover, given two potentials $(\varphi, \psi)$, we can take $\tilde{\psi}(y) = \inf_{x \in X} \mathsf{d}(x, y) - \psi(x)$, which is 1-Lipschitz, and $\tilde{\varphi}(x) = \inf_{y \in Y} \mathsf{d}(x, y) - \tilde{\psi}(y)$, also 1-Lipschitz, and the pair $(\tilde{\varphi}, \tilde{\psi})$ is again admissible and majorizes the initial pair. But $-\tilde{\psi}(x) \leq \inf_{y \in Y} \mathsf{d}(x, y) - \tilde{\psi}(y) \leq -\tilde{\psi}(x)$, therefore $\tilde{\psi} = -\tilde{\varphi}$. This shows that in fact

$$W_1(\mu, \nu) = \sup\left\{ \int_X \varphi \,\mathrm{d}\mu - \int_X \varphi \,\mathrm{d}\nu : \varphi \in \mathrm{Lip}(X),\ \mathrm{Lip}(\varphi) \leq 1 \right\}.$$

In Chapter 2 we will be dealing with the case $p = 2$ in the context of random matching. The duality formula, in the form of (2.2.1), plays an important role also here, especially for providing lower bounds on the optimal cost. As hinted before, one can restrict the maximization in $(D)$ to the pairs $(\varphi, \varphi^c)$, where $\varphi^c(y) = \inf_{x \in X} \mathsf{d}(x, y)^2 - \varphi(x)$ is called the *c-conjugate*. In the chapter we will use a different sign convention and introduce a semigroup performing this operation, but the idea remains the same.

# Chapter 2

# A PDE approach to a 2-dimensional matching problem

## 2.1 Introduction

Optimal matching problems are random variational problems widely investigated in the mathematical and physical literature. Many variants are possible, for instance the monopartite problem, dealing with the optimal coupling of an even number $n$ of i.i.d. points $X_i$, the grid matching problem, where one looks for the optimal matching of an empirical measure $\sum_i \frac{1}{n}\delta_{X_i}$ to a deterministic and "equally spaced" grid, the closely related problem of optimal matching to the common law $\mathfrak{m}$ of $X_i$, and the bipartite problem, dealing with the optimal matching of $\sum_i \frac{1}{n}\delta_{X_i}$ to $\sum_i \frac{1}{n}\delta_{Y_i}$, with $(X_i, Y_i)$ i.i.d. See the monographs [Yuk98] and [Tal14] for more information on this subject. In addition to these problems, one may study the optimal assignment problem [Coh04], where the optimization involves also the weights of the Dirac masses $\delta_{X_i}$, and the closely related problem of transporting Lebesgue measure to a Poisson point process [HS13], which involves in the limit measures with infinite mass.

In this chapter, based on [AST16], we focus on two of these problems, namely optimal matching to the reference measure and the bipartite problem. Denoting by $D$ a $d$-dimensional domain and by $\mathfrak{m} \in \mathscr{P}(D)$ the law of the points $X_i$, $Y_i$, the problem is to estimate the rate of convergence to 0 of

$$\mathbb{E}\left[W_p^p\left(\sum_{i=1}^n \frac{1}{n}\delta_{X_i}, \mathfrak{m}\right)\right], \qquad \mathbb{E}\left[W_p^p\left(\sum_{i=1}^n \frac{1}{n}\delta_{X_i}, \sum_{i=1}^n \frac{1}{n}\delta_{Y_i}\right)\right], \tag{2.1.1}$$

where $p \in [1, \infty)$ is the power occurring in the transportation cost $c = \mathsf{d}^p$ (also the case $p = \infty$ is considered in the literature, see for instance [SY91] and the references therein), by finding tight upper and lower bounds and, possibly, to prove the existence of the limit of the renormalized quantities as $n \to \infty$.

When $\mathfrak{m}$ is the uniform measure, the typical distance between points is expected to be of order $n^{-1/d}$, and therefore it is natural to guess that the quantities

$c_{n,p,d}$ introduced in (2.1.1) behave as $n^{-p/d}$. Indeed, e.g. when $D = [0,1]^d$ and $\mathfrak{m}$ is the uniform measure, the 1-Lipschitz test function $\varphi(x) = \min_i |x - X_i|$ easily provides the deterministic estimate $W_p(\sum_i \frac{1}{n}\delta_{X_i}, \mathfrak{m}) \geq W_1(\sum_i \frac{1}{n}\delta_{X_i}, \mathfrak{m}) \geq c(d)n^{-1/d}$. However, it is by now well known that the scaling $n^{-p/d}$ is correct for $d \geq 3$, while it is false for $d = 1$ and $d = 2$.

Despite plenty of heuristic arguments and numerical results, the following are (as far as we know) the main results that have been rigorously proved to date, not including our current contribution, (we focus here on the model case when $\mathfrak{m}$ is the uniform measure and we do not distinguish between optimal matching to $\mathfrak{m}$ and bipartite matching), denoting $a_n \sim b_n$ if both $\limsup_n a_n/b_n < \infty$ and $\limsup_n b_n/a_n < \infty$:

- when $D = [0,1]$ or $D = \mathbb{T}^1$, then $c_{n,p,1}/n^{-p} \sim n^{p/2}$ and, when $p = 2$, $\lim_{n\to\infty} nc_{n,2,1}$ can be explicitly computed, see [CS15];
- when $D = [0,1]^2$, then $c_{n,p,2}/n^{-p/2} \sim (\log n)^{p/2}$, see [AKT84];
- when $D = [0,1]^d$ with $d \geq 3$, then $c_{n,1,d}/n^{-1/d} \sim 1$ and the limit exists [BM02; DY95], for $p \in [1, d/2)$ one has $c_{n,p,d}/n^{-p/d} \sim 1$ and the limit exists [BB13], it is not known whether the limit exists for $p \in [d/2, \infty)$. In the more recent paper [FG15] also non-asymptotic upper bounds have been provided.

In particular, in the case $d = 2$, the convergence of $(\log n)^{-p/2} c_{n,p,2}/n^{-p/2}$ as $n \to \infty$ and the characterization of the limit were still open problems (see for instance [Tal14, Research problem 4.3.3] for the case $p = 1$), and this is specifically the problem we set out to address.

Our interest in this subject has been motivated by the recent work [Car+14] where, on the basis of an ansatz, very specific predictions on the expansion of

$$n^{-p/d}\,\mathbb{E}\left[W_p^p\left(\sum_{i=1}^n \frac{1}{n}\delta_{X_i}, \sum_{i=1}^n \frac{1}{n}\delta_{Y_i}\right)\right]$$

have been made on the torus $\mathbb{T}^d$, for all ranges of dimensions $d$ and powers $p$. See also [CS15] for the analysis of correlations. In brief, the ansatz of [Car+14] is based on a linearisation ($\rho_i \sim 1$ in $C^1$ topology, $\psi \sim \frac{1}{2}|x|^2 + f$ in $C^2$ topology) of the Monge-Ampère equation

$$\rho_1(\nabla\psi)\det\nabla^2\psi = \rho_0$$

(which describes the optimal transport map $T = \nabla\psi$ from the measures having probability densities $\rho_0$ to $\rho_1$), leading to Poisson's equation $-\Delta f = \rho_1 - \rho_0$.

This ansatz is very appealing, but on the mathematical side it poses several challenges, because the energies involved are infinite for $d \geq 2$ (the measures being Dirac masses), because this procedure does not provide an exact matching between the measures (due to the linearization) and because the necessity of giving lower bounds persists, as matchings provide only upper bounds. While we are still very far from justifying rigorously all predictions of [Car+14], see also Section 2.6 for a discussion on this topic, we have been able to use this idea to prove existence of the limit and compute it explicitly in the case $p = d = 2$, in agreement with [Car+14]:

**Theorem 2.1.1** (Main result)**.** *Assume that either $D = [0,1]^2$ or that $D$ is a compact 2-dimensional Riemannian manifold with no boundary, let $\mathfrak{m}$ be its volume measure, and set $\mu^n = \sum_i \frac{1}{n}\delta_{X_i}$ and $\nu^n = \sum_i \frac{1}{n}\delta_{Y_i}$, $X_i$ and $Y_i$ being i.i.d. with law $\mathfrak{m}_D = \mathfrak{m}/\mathfrak{m}(D)$. Then,*

$$\lim_{n\to\infty} \frac{n}{\log n} \mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m}_D)\right] = \frac{\mathfrak{m}(D)}{4\pi}. \tag{2.1.2}$$

*In the bipartite case, if either $D = [0,1]^2$ or $D = \mathbb{T}^2$, one has*

$$\lim_{n\to\infty} \frac{n}{\log n} \mathbb{E}\left[W_2^2(\mu^n, \nu^n)\right] = \frac{1}{2\pi}. \tag{2.1.3}$$

*Finally, in the case $D = [0,1]^2$, if $T^{\mu^n}$ denotes the optimal transport map from $\mathfrak{m}$ to $\mu^n$, one has*

$$\lim_{n\to\infty} \frac{n}{\log n} \int_D \left|\mathbb{E}\left[T^{\mu^n}(x) - x\right]\right|^2 \mathrm{d}\mathfrak{m}(x) = 0. \tag{2.1.4}$$

Figure 2.1 demonstrates some random matching samples. Notice in particular the appearance of long range couplings in a significant portion of the domain. The logarithmic correction (with respect to the higher dimensional asympotic rate) is there to account for this phenomenon.

By the invariance of the statements under rescaling of the measure, we always assume in the sequel that $\mathfrak{m}(D) = 1$. Using the spectral gap, standard results related to the phenomenon of concentration of measure (see [GM83; Led01; BL16]) also yield that the random variables $n(\log n)^{-1}W_2^2(\mu^n, \mathfrak{m})$ converge in law to the Dirac mass at $1/(4\pi)$, more precisely (2.1.2) and exponential concentration yield

$$\lim_{n\to\infty} \mathbb{E}\left[F\left(\frac{n}{\log n} W_2^2(\mu^n, \mathfrak{m})\right)\right] = F\left(\frac{1}{4\pi}\right) \tag{2.1.5}$$

for any $F : \mathbb{R} \to \mathbb{R}$ bounded and continuous. See Remark 2.4.7 for more precise results, whose proof can also be adapted to cover the bipartite case.

In our proof, the geometry of the domain $D$ enters only through the (asymptotic) properties of the spectrum of the Laplacian with homogeneous Neumann boundary conditions; for this reason we are able to cover also abstract manifolds, as the two-dimensional sphere or the two-dimensional nonflat torus embedded in $\mathbb{R}^3$. Even though in dimension $d = 1$ (but mostly for the case $D = [0,1]$) a much

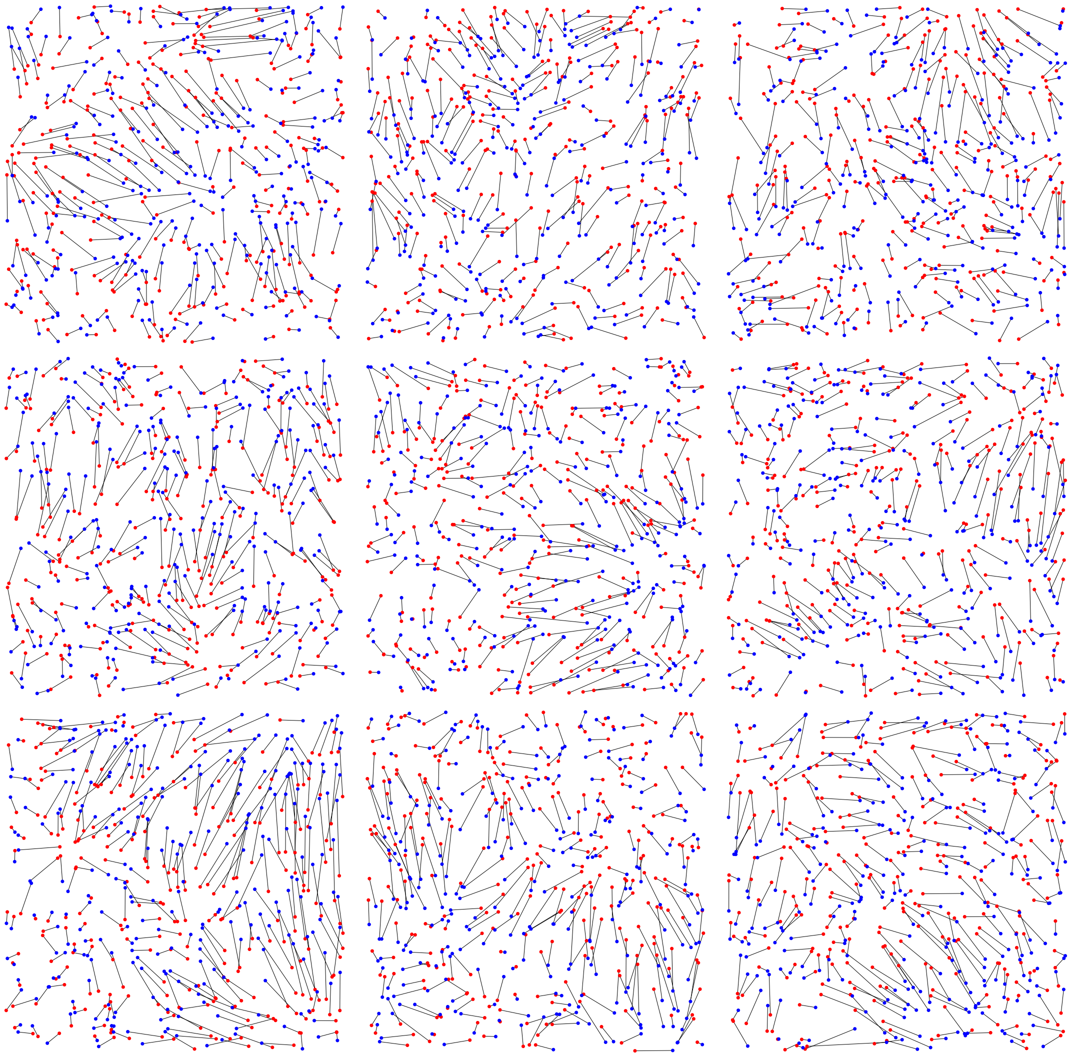


Figure 2.1: Some random matching samples, highlighting that there tend to alwyas be some long range couplings in a significant portion of the domain. This is the fact responsible for the logarithmic correction in 2D with respect to the higher dimensional asymptotic rate.

more detailed analysis can be made, see Remark 2.4.2 and [BL16] for much more on the subject, we include proofs and statements of the 1-dimensional case, to illustrate the flexibility of our synthetic method.

Let us give some heuristic ideas on the strategy of proof, starting from the upper bound. In order to obtain finite energy solutions to Poisson's equation we study the regularized PDE

$$-\Delta f^{n,t} = u^{n,t} - 1 \tag{2.1.6}$$

where $u^{n,t}$ is the density of $P_t^* \mu^n$ and $P_t^*$ is the heat semigroup with Neumann boundary conditions, acting on measures. Then, choosing $t = \gamma n^{-1} \log n$ with $\gamma$ small, we have a small error in the estimation from above of $c_{n,2,2}$ if we replace $\mu^n$ by its regularization $P_t^* \mu^n$. Eventually, we use Dacorogna-Moser's technique (see Proposition 2.2.3) to provide an exact coupling between $P_t^* \mu^n$ and $\mathfrak{m}$, leading to an estimate of the form

$$W_2^2(P_t^* \mu^n, \mathfrak{m}) \leq \int_D \left( \int_0^1 \frac{1}{(1-s) + s u^{n,t}} \, \mathrm{d}s \right) |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}.$$

To conclude, we have to estimate very carefully how much the factor in front of $|\nabla f^{n,t}|^2$ differs from 1; this requires in particular higher integrability estimates on $|\nabla f^{n,t}|$.

Let us consider now the lower bound. The duality formula

$$\frac{1}{2} W_2^2(\mu, \nu) = \sup_{\psi(y) - \varphi(x) \leq \mathsf{d}^2(x,y)/2} \left( - \int_D \varphi \, \mathrm{d}\mu + \int_D \psi \, \mathrm{d}\nu \right)$$

is the standard way to provide lower bounds on $W_2$; given $\varphi$, the best possible $\psi = Q_1 \varphi$ compatible with the constraint is given by the Hopf-Lax formula (2.2.2). Choosing again $\varphi = f^{n,t}$ the solution of (2.1.6), we are led to estimate carefully

$$\frac{1}{2} \int |\nabla f^{n,t}|^2 - \left( - \int_D f^{n,t} u^{n,t} \, \mathrm{d}\mathfrak{m} + \int_D Q_1 f^{n,t} \, \mathrm{d}\mathfrak{m} \right)$$

in events of the form $\{\sup_D |u^{n,t} - 1| \leq \eta\}$ (whose probabilities tend to 1). We do this using Laplacian estimates and the viscosity approximation of the Hopf-Lax semigroup provided by the Hopf-Cole transform; in these estimates, lower bound on the Ricci curvature play an important role.

In the bipartite case, the result can be obtained from the previous ones playing with independence. Heuristically, the random "vectors" pointing from $\mathfrak{m}$ to $\mu^n$ and from $\mathfrak{m}$ to $\nu^n$ are independent and almost centered, and since $\mathscr{P}(D)$ is "Riemannian" on small scales when endowed with the distance $W_2$, we obtain a factor 2, as in the identity $\mathbb{E}[(X - Y)^2] = 2 \operatorname{Var}(X)$ when $X$, $Y$ are i.i.d. random variables. Interestingly, the rigorous proof of this fact provides also the information (2.1.4) on the mean displacement as function of the position.

The paper is organized as follows. In Section 2.2 we first recall preliminary results on the Wasserstein distance and the main tools (Dacorogna-Moser interpolation, duality, Hopf-Lax semigroup) involved in the proof of the upper and lower bounds. Then, we provide moment estimates for $\sqrt{n}(\mu^n - \mathfrak{m})$.

In Section 2.3 we introduce the heat semigroup $P_t$ and, in a quantitative way, the regularity properties of $P_t$ needed for our scheme to work. We also provide estimates on the canonical regularization of the Hamilton-Jacobi equation provided by the Hopf-Cole transform $-\sigma \log P_t e^{-f/\sigma}$. The most delicate part of our proof involves bounds on the probability of the events

$$\left\{ \sup_{x \in D} |u^{n,t}(x) - 1| > \eta \right\}, \qquad \text{for } \eta > 0,$$

which ensure that the probability of these events has a power-like decay as $n \to \infty$ if $t = \gamma n^{-1} \log n$, with $\gamma$ sufficiently large (this plays a role in the proof of the lower bound). Finally, in light of the ansatz of [Car+14], we provide a formula for

$$\mathbb{E}\left[ \int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m} \right],$$

where $f^{n,t}$ solves the random PDE (2.1.6), and prove convergence of the renormalized quantity as $n \to \infty$, if $t \sim n^{-1} \log n$.

Section 2.4 provides the proof of our main result, together with Theorem 2.4.1 dealing with the simpler case $d = 1$. We first deal with the optimal matching to $\mathfrak{m}$, and then we deal with the bipartite case.

In Section 2.5 we recover the result found in [AKT84] as a consequence of our estimates via a Lipschitz approximation argument.

Finally, Section 2.6 covers extensions to more general classes of domains and open problems, pointing out some potential developments.

## 2.2 Notation and preliminary results

### 2.2.1 Wasserstein distance

Let $(D, \mathsf{d})$ be a complete and separable metric space. We recall (see e.g. [AGS08]) that the quadratic Wasserstein distance $W_2(\mu, \nu)$ between Borel probability measures $\mu$, $\nu$ in $D$ with finite quadratic moments is defined by

$$W_2^2(\mu, \nu) = \min \left\{ \int_{D \times D} \mathsf{d}(x, y)^2 \, \mathrm{d}\Sigma(x, y) : \Sigma \in \Gamma(\mu, \nu) \right\},$$

where $\Gamma(\mu, \nu)$ is the class of transport plans (couplings in probability) between $\mu$ and $\nu$, namely Borel probability measures $\Sigma$ in $D \times D$ having $\mu$ and $\nu$ as first and second marginals, respectively. We say that a Borel map $T$ pushing $\mu$ to $\nu$ is optimal if

$$W_2^2(\mu, \nu) = \int_D \mathsf{d}^2(T(x), x) \, \mathrm{d}\mu(x).$$

This means that the plan $\Sigma = (\mathrm{Id} \times T)_{\#}\mu$ induced by $T$ is optimal.

The following duality formula will play a key role, both in the proof of the upper and lower bound of the matching cost:

$$\frac{1}{2}W_2^2(\mu,\nu) = \sup_{\varphi\in \mathrm{Lip}_b(D)} \left( -\int_D \varphi \,\mathrm{d}\mu + \int_D Q_1\varphi \,\mathrm{d}\nu \right). \tag{2.2.1}$$

In (2.2.1) above, $\mathrm{Lip}_b(D)$ stands for the class of bounded Lipschitz functions on $D$ and, for $t > 0$, $Q_t\varphi$ is defined by the Hopf-Lax formula

$$Q_t\varphi(y) = \inf_{x\in D} \left( \varphi(x) + \frac{1}{2t}\mathsf{d}(x,y)^2 \right). \tag{2.2.2}$$

This formula also provides a semigroup if $(X, \mathsf{d})$ is a length space, and $Q_t\varphi \uparrow \varphi$ as $t \downarrow 0$.

We recall a few basic properties of $Q_t$, whose proof is elementary: if $\varphi \in \mathrm{Lip}_b(D)$ then $\inf \varphi \le Q_t\varphi \le \sup \varphi$ and (where Lip stands for the Lipschitz constant)

$$\mathrm{Lip}(Q_t\varphi) \le 2\,\mathrm{Lip}(\varphi), \qquad \left\| \frac{\mathrm{d}}{\mathrm{d}t} Q_t\varphi(x) \right\|_\infty \le 2\big[\mathrm{Lip}(\varphi)\big]^2 \quad \text{for all } x \in D.$$

In particular $\mathrm{Lip}_b(D)$ is invariant under the action of $Q_t$. For $\varphi \in \mathrm{Lip}_b(D)$, the key property of $Q_t\varphi$ is

$$\frac{\mathrm{d}}{\mathrm{d}t}Q_t\varphi + \frac{1}{2}|\nabla Q_t\varphi|^2 \le 0 \quad \mathfrak{m}\text{-a.e. in } X, \text{ for all } t > 0, \tag{2.2.3}$$

with equality if $(D, \mathsf{d})$ is a length space (but we will only need the inequality). In (2.2.3), $|\nabla Q_t\varphi|$ is the metric slope of $Q_t\varphi$, which corresponds to the norm of the gradient in the Riemannian setting.

It is a classic fact that $W_2^2$ is jointly convex, namely if $\mu_i, \nu_i \in \mathscr{P}(D)$, $t_i \ge 0$, $\sum_{i=1}^k t_i = 1$,

$$\mu = \sum_{i=1}^k t_i\mu_i, \qquad \nu = \sum_{i=1}^k t_i\nu_i$$

then

$$W_2^2(\mu,\nu) \le \sum_{i=1}^k t_i W_2^2(\mu_i,\nu_i). \tag{2.2.4}$$

This easily follows by the linear dependence w.r.t. $\Sigma$ in the cost function, and by the linearity of the marginal constraint. More generally, the same argument shows that, for a generic index set $I$,

$$W_2^2\left( \int_I \mu_i \,\mathrm{d}\Theta(i), \int_I \nu_i \,\mathrm{d}\Theta(i) \right) \le \int_I W_2^2(\mu_i,\nu_i)\,\mathrm{d}\Theta(i) \tag{2.2.5}$$

with $\mu_i$, $\nu_i$ and $\Theta$ probability measures, under appropriate measurability assumptions that are easily checked in all the cases in which we are going to apply this formula.

The following result is by now well known, we detail for the reader's convenience some steps of the proof from [AGS08] (see also [Tue93] for more refined results).

**Proposition 2.2.1** (Existence and stability of optimal maps). *Let $D \subset \mathbb{R}^d$ be a compact set, $\mu, \nu \in \mathscr{P}(D)$ with $\mu$ absolutely continuous w.r.t. Lebesgue d-dimensional measure. Then:*

*(a) there exists a unique optimal transport map $T_\mu^\nu$ from $\mu$ to $\nu$.*

*(b) if $\nu_h \to \nu$ weakly in $\mathscr{P}(D)$, then $T_\mu^{\nu_h} \to T_\mu^\nu$ in $L^2(D, \mu; D)$.*

*Proof.* Statement *(a)* is a simple generalization of Brenier's theorem, see for instance [AGS08, Theorem 6.2.4] for a proof. The proof of statement *(b)* is typically obtained by combining the stability w.r.t. weak convergence of the optimal plans $\nu \mapsto (\mathrm{Id} \times T_\mu^\nu)$ (see [AGS08, Proposition 7.1.3]) with a general criterion (see [AGS08, Lemma 5.4.1]) which allows to deduce convergence in $\mu$-measure of the maps $T_h$ to $T$ from the weak convergence of the plans $(\mathrm{Id} \times T_h)_\# \mu$ to $(\mathrm{Id} \times T)_\# \mu$. □

### 2.2.2 Transport estimate

Assume in this section that $D$ is a compact connected Riemannian manifold, possibly with boundary, whose finite Riemannian volume measure is denoted by $\mathfrak{m}$, with $\mathsf{d}$ equal to the Riemannian distance. The estimate from above on $W_2^2$ provided by Proposition 2.2.3 below is closely related to the Benamou-Brenier formula [BB00] (also [AGS08, Theorem 8.3.1]), which provides a representation of $W_2^2$ in terms of the minimization of the action $\int_0^1 \int_D |\mathbf{b}_t|^2 \, \mathrm{d}\mu_t \, \mathrm{d}t$, among all solutions to the continuity equation $\frac{\mathrm{d}}{\mathrm{d}t}\mu_t + \mathrm{div}(\mathbf{b}_t \mu_t) = 0$. It is also related to the Dacorogna-Moser scheme, which provides constructively, under suitable smoothness assumptions, a (not necessarily optimal) transport map between $\mu_0 = u_0 \mathfrak{m}$ and $\mu_1 = u_1 \mathfrak{m}$ by solving the PDE

$$\begin{cases} \Delta f = u_1 - u_0 & \text{in } D, \\ \nabla f \cdot n_D = 0 & \text{on } \partial D \end{cases} \tag{2.2.6}$$

and then using the flow of the vector field $\mathbf{b}_t = u_t^{-1} \nabla f$ at time 1, with $u_t = (1-t)u_0 + t u_1$, to yield the map. We provide here the estimate without building explictly a coupling, in the spirit of [Kuw10] (see also, in an abstract setting [AMS15, Theorem 6.6]), using the duality formula (2.2.1). This has the advantage to avoid smoothness issues and, moreover, uses (2.2.6) only in the weak sense, namely

$$-\int_D \langle \nabla \varphi, \nabla f \rangle \, \mathrm{d}\mathfrak{m} = \int_D \varphi (u_1 - u_0) \, \mathrm{d}\mathfrak{m} \qquad \forall \varphi \in \mathrm{Lip}_b(D).$$

Notice that uniqueness (up to an additive constant) of $f$ in (2.2.6) is obvious. Existence is guaranteed for $u_i \in L^2(\mathfrak{m})$ with $\int_D (u_1 - u_0)\,\mathrm{d}\mathfrak{m} = 0$ under a spectral gap assumption, thanks to the variational interpretation provided by Lax-Milgram theorem. Notice also that with the choice $\mathbf{b}_t = u_t^{-1}\nabla f$ the continuity equation $\frac{\mathrm{d}}{\mathrm{d}t}u_t + \mathrm{div}(\mathbf{b}_t u_t) = 0$ holds, in weak form.

We will also need this definition.

**Definition 2.2.2** (Logarithmic mean)**.** Given $a, b > 0$, we define the logarithmic mean

$$M(a,b) = \frac{a-b}{\log a - \log b} = \left( \int_0^1 \frac{1}{(1-s)a + sb}\,\mathrm{d}s \right)^{-1}.$$

This can be extended to $a, b \geq 0$ by continuity, so that $M(a,0) = M(0,b) = M(0,0) = 0$.

**Proposition 2.2.3.** *Let $u_0, u_1 \in L^2(\mathfrak{m})$ be probability densities with $u_0 > 0$ $\mathfrak{m}$-a.e. in $X$ and let $f \in H^{1,2}(D,\mathfrak{m})$ be any solution to (2.2.6). Then*

$$W_2^2(u_0\mathfrak{m}, u_1\mathfrak{m}) \leq \int_0^1 \int_D \frac{|\nabla f|^2}{(1-s)u_0 + su_1}\,\mathrm{d}\mathfrak{m}\,\mathrm{d}s = \int_D \frac{|\nabla f|^2}{M(u_0,u_1)}\,\mathrm{d}\mathfrak{m}.$$

*Proof.* Let $\varphi \in \mathrm{Lip}_b(D)$, set $u_s = (1-s)u_0 + su_1$ and notice that $u_s > 0$ $\mathfrak{m}$-a.e. in $X$ for all $s \in [0,1)$. We interpolate, then use Leibniz's rule and (2.2.3) to get

$$\begin{aligned}
\int_D (u_1 Q_1\varphi - u_0\varphi)\,\mathrm{d}\mathfrak{m} &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s} \int_D u_s Q_s\varphi\,\mathrm{d}\mathfrak{m}\,\mathrm{d}s \\
&= \int_0^1 \int_D u_s \frac{\mathrm{d}}{\mathrm{d}s} Q_s\varphi + (u_1 - u_0) Q_s\varphi\,\mathrm{d}\mathfrak{m}\,\mathrm{d}s \\
&\leq \int_0^1 \int_D -\frac{1}{2}|\nabla Q_s\varphi|^2 u_s - \langle \nabla f, \nabla Q_s\varphi \rangle\,\mathrm{d}\mathfrak{m}\,\mathrm{d}s \\
&\leq \frac{1}{2}\int_0^1 \int_D \frac{|\nabla f|^2}{u_s}\,\mathrm{d}\mathfrak{m}\,\mathrm{d}s.
\end{aligned}$$

Since $\varphi$ is arbitrary, the statement follows from the duality formula (2.2.1). □

### 2.2.3 Bounds for moments and tails

In this subsection $(D, \mathsf{d})$ is a complete and separable metric space equipped with a Borel probability measure $\mathfrak{m}$. We assume $\mathrm{diam}\, D < \infty$.

For $n \in \mathbb{N}^*$, let $X_1, \ldots, X_n$ be independent and uniformly distributed random variables in $D$, whose common law is $\mathfrak{m}$. Let $\mu^n = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$ be the random empirical measure. We define the measures $r^n = \sqrt{n}(\mu^n - \mathfrak{m})$, where we use the natural scaling provided by the central limit theorem. Our goal is to derive upper bounds for the exponential moments $\exp(\lambda \int_D f\,\mathrm{d}r^n)$ and, as a consequence, tail estimates for $\int_D f\,\mathrm{d}r^n$, related to classical concentration inequalities (Bernstein inequality), see e.g. [Tal14, Lemma 4.3.4]. For the reader's convenience, we provide a complete proof in the form that we need for our purposes.

**Definition 2.2.4.** For $k \in \mathbb{N}$ and $f \in C_b(D)$, define the $k$-moments $[\![ \cdot ]\!]_k \in [0, \infty]$ by

$$[\![ f ]\!]_k^k = \int_D \left( f(x) - \int_D f \, \mathrm{d}\mathfrak{m} \right)^k \mathrm{d}\mathfrak{m}(x)$$

and

$$[\![ f ]\!]_\infty = \left\| f - \int_D f \, \mathrm{d}\mathfrak{m} \right\|_{L^\infty(\mathfrak{m})}.$$

Notice that $[\![ f ]\!]_0 = 1$, $[\![ f ]\!]_1 = 0$, $[\![ f ]\!]_2 \leq \|f\|_2$ and $\left| [\![ f ]\!]_{k+2}^{k+2} \right| \leq [\![ f ]\!]_2^2 [\![ f ]\!]_\infty^k$. Moreover, $[\![ \cdot ]\!]_2^2$ is a quadratic form, therefore we introduce also the associated bilinear form

$$m_2(f, g) = \int_D \left( f(x) - \int_D f \, \mathrm{d}\mathfrak{m} \right) \left( g(x) - \int_D g \, \mathrm{d}\mathfrak{m} \right) \mathrm{d}\mathfrak{m}(x).$$

Analogously, we consider also the following quantity

$$m_4(f, g) = \int_D \left( f(x) - \int_D f \, \mathrm{d}\mathfrak{m} \right)^2 \left( g(x) - \int_D g \, \mathrm{d}\mathfrak{m} \right)^2 \mathrm{d}\mathfrak{m}(x),$$

so that $m_4(f, f) = [\![ f ]\!]_4^4$.

**Lemma 2.2.5** (Moment generating function)**.** *Let $f \in C_b(D)$ and $\lambda \in \mathbb{R}$. Then*

$$\begin{aligned} \mathbb{E}\left[ \exp\left( \lambda \int_D f \, \mathrm{d}r^n \right) \right] &= \left\{ \int_D \exp\left[ \frac{\lambda}{\sqrt{n}} \left( f(x) - \int_D f \, \mathrm{d}\mathfrak{m} \right) \right] \mathrm{d}\mathfrak{m}(x) \right\}^n \\ &= \left( 1 + \sum_{k=2}^\infty \frac{\lambda^k [\![ f ]\!]_k^k}{k! n^{k/2}} \right)^n. \end{aligned}$$

*As a consequence*

$$\mathbb{E}\left[ \exp\left( \lambda \int_D f \, \mathrm{d}r^n \right) \right] \leq \exp\left[ \frac{\lambda^2 [\![ f ]\!]_2^2}{2} \exp\left( \frac{|\lambda| [\![ f ]\!]_\infty}{\sqrt{n}} \right) \right]. \tag{2.2.7}$$

*Proof.* It is sufficient to show the result for $\lambda = 1$; the general statement then follows by taking $\lambda f$ in place of $f$. By the definition of empirical measure we have

$$\begin{aligned}
\mathbb{E}\left[\exp\left(\int_D f\,\mathrm{d}r^n\right)\right] &= \mathbb{E}\left[\exp\left(\frac{1}{\sqrt{n}}\sum_{i=1}^n f(X_i) - \sqrt{n}\int_D f\,\mathrm{d}\mathfrak{m}\right)\right] \\
&= \mathbb{E}\left[\exp\left(\sum_{i=1}^n \frac{1}{\sqrt{n}}\left\{f(X_i) - \int_D f\,\mathrm{d}\mathfrak{m}\right\}\right)\right] \\
&= \mathbb{E}\left[\exp\left(\frac{1}{\sqrt{n}}\left\{f(X_1) - \int_D f\,\mathrm{d}\mathfrak{m}\right\}\right)\right]^n \\
&= \left\{\int_D \sum_{k=0}^\infty \frac{1}{k!}\left[\frac{1}{\sqrt{n}}\left(f(x) - \int_D f\,\mathrm{d}\mathfrak{m}\right)\right]^k \mathrm{d}\mathfrak{m}(x)\right\}^n.
\end{aligned}$$

The equality above gives

$$\begin{aligned}
\mathbb{E}\left[\exp\left(\int_D f\,\mathrm{d}r^n\right)\right] &= \left\{1 + \sum_{k=2}^\infty \frac{[\![f]\!]_k^k}{k!n^{k/2}}\right\}^n = \left\{1 + \sum_{k=0}^\infty \frac{[\![f]\!]_{k+2}^{k+2}}{(k+2)!n^{k/2+1}}\right\}^n \\
&\le \left\{1 + \frac{[\![f]\!]_2^2}{2n}\sum_{k=0}^\infty \frac{[\![f]\!]_\infty^k}{k!n^{k/2}}\right\}^n = \left\{1 + \frac{[\![f]\!]_2^2}{2n}\exp\left(\frac{[\![f]\!]_\infty}{\sqrt{n}}\right)\right\}^n \\
&\le \exp\left[\frac{[\![f]\!]_2^2}{2}\exp\left(\frac{[\![f]\!]_\infty}{\sqrt{n}}\right)\right].
\end{aligned}$$

□

**Lemma 2.2.6.** *Let $f, g \in C_b(D)$. Then*

$$\mathbb{E}\left[\left(\int_D f\,\mathrm{d}r^n\right)^2\right] = [\![f]\!]_2^2, \qquad \mathbb{E}\left[\left(\int_D f\,\mathrm{d}r^n\right)\left(\int_D g\,\mathrm{d}r^n\right)\right] = m_2(f,g), \quad (2.2.8)$$

*and*

$$\begin{aligned}
\mathbb{E}\left[\left(\int_D f\,\mathrm{d}r^n\right)^2\left(\int_D g\,\mathrm{d}r^n\right)^2\right] &= \frac{n-1}{n}\left[[\![f]\!]_2^2[\![g]\!]_2^2 + 2m_2(f,g)^2\right] + \frac{1}{n}m_4(f,g) \\
&\le 3\frac{n-1}{n}[\![f]\!]_2^2[\![g]\!]_2^2 + \frac{1}{n}[\![f]\!]_4^2[\![g]\!]_4^2.
\end{aligned}$$

*Proof.* Since

$$\mathbb{E}\left[\exp\left(\lambda\int_D f\,\mathrm{d}r^n\right)\right] = \sum_{k=0}^\infty \frac{\lambda^k}{k!}\,\mathbb{E}\left[\left(\int_D f\,\mathrm{d}r^n\right)^k\right],$$

it is sufficient to compute the second and fourth derivatives with respect to $\lambda$ at $\lambda = 0$ in the expression for $\mathbb{E}\left[\exp\left(\lambda\int_D f\,\mathrm{d}r^n\right)\right]$ provided by Lemma 2.2.5 to obtain, respectively, the first identity in (2.2.8) and

$$\mathbb{E}\left[\left(\int_D f\,\mathrm{d}r^n\right)^4\right] = 3\frac{n-1}{n}[\![f]\!]_2^4 + \frac{1}{n}[\![f]\!]_4^4.$$

The remaining two identities follow by polarization. □

For $c, \eta > 0$, define the function

$$F(c,\eta) = \sup_{\lambda>0}\left\{\lambda\eta - \frac{\lambda^2}{2}\exp(c\lambda)\right\} > 0. \tag{2.2.9}$$

Notice that $F(c,\eta)$ is decreasing in $c$, increasing in $\eta$ and that the formula

$$cF(c,\eta) = \sup_{\lambda>0}\left\{c\lambda\eta - c\frac{\lambda^2}{2}\exp(c\lambda)\right\} = \sup_{\lambda'>0}\left\{\lambda'\eta - \frac{(\lambda')^2}{2c}\exp(\lambda')\right\}$$

shows that $cF(c,\eta)$ is increasing in $c$. We will use the function $F$ to estimate the tails of $\int_D f\,\mathrm{d}r^n$.

**Lemma 2.2.7** (Tail bound)**.** *Let $X$ be a real random variable such that, for some $c_1, c_2 > 0$,*

$$\mathbb{E}[\exp(\lambda X)] \le \exp\left[\frac{\lambda^2 c_1}{2}\exp(|\lambda|c_2)\right] \qquad \forall \lambda \in \mathbb{R}.$$

*Then for every $\eta \ge 0$ we have*

$$\mathbb{P}(|X| > \eta) \le 2\exp\left[-\frac{1}{c_1}F\left(\frac{c_2}{c_1},\eta\right)\right].$$

*Proof.* We have $\mathbb{P}(|X| > \eta) \le \mathbb{P}(X > \eta) + \mathbb{P}(X < -\eta)$. For the first term and $\lambda > 0$

$$\begin{aligned}\mathbb{P}(X > \eta) &= \mathbb{P}\big(\exp(\lambda X) > \exp(\lambda\eta)\big)\\ &\le \mathbb{E}[\exp(\lambda X)]\exp(-\lambda\eta) \le \exp\left[\frac{\lambda^2 c_1}{2}\exp(\lambda c_2) - \lambda\eta\right].\end{aligned}$$

Hence

$$\begin{aligned}\mathbb{P}(X > \eta) &\le \exp\left[\inf_{\lambda>0}\left(\frac{\lambda^2 c_1}{2}\exp(\lambda c_2) - \lambda\eta\right)\right]\\ &= \exp\left[\frac{1}{c_1}\inf_{\lambda>0}\left\{\frac{\lambda^2}{2}\exp\left(\lambda\frac{c_2}{c_1}\right) - \lambda\eta\right\}\right].\end{aligned}$$

For the other term, we use the fact that $\mathbb{P}(X < -\eta) = \mathbb{P}(-X > \eta)$ and $-X$ satisfies the same hypothesis. □

## 2.3 Heat semigroup

In this section we add more structure to $D$, assuming that $(D, \mathsf{d})$ is a compact connected Riemannian manifold (possibly with boundary) endowed with the Riemannian distance, and that $D$ has finite diameter and volume. Then, we can and will normalize $(D, \mathsf{d})$ in such a way that the volume is unitary, and let $\mathfrak{m}$ be the volume measure of $(D, \mathsf{d})$. The typical examples we have in mind are the flat $d$-dimensional torus $\mathbb{T}^d$ and the $d$-dimensional cube $[0,1]^d$, see also Section 2.6 for more general setups.

We denote by $P_t$ the heat semigroup associated to $(D, \mathsf{d}, \mathfrak{m})$, with Neumann boundary conditions. In one of the many equivalent representations, it can be viewed as the $L^2(\mathfrak{m})$ gradient flow of the Dirichlet energy $\frac{1}{2}\int_D |\nabla f|^2 \,\mathrm{d}\mathfrak{m}$. Standard results (see for instance [Wan14]) ensure that $P_t$ is a Markov semigroup, so that it is a contraction semigroup in all $L^p \cap L^2(\mathfrak{m})$ spaces, $1 \le p \le \infty$; thanks to this property it has a unique extension to all $L^p(\mathfrak{m})$ spaces even when $p \in [1,2)$. Moreover, the finiteness of volume and boundary conditions ensure that $P_t$ is mass-preserving, i.e. $t \mapsto \int_D P_t f \,\mathrm{d}\mathfrak{m}$ is constant in $[0,\infty)$ for all $f \in L^1(\mathfrak{m})$ and thus it can be viewed as an operator in the class of probability densities (which correspond to the measures absolutely continuous w.r.t. $\mathfrak{m}$). More generally, we can use the Feller property (i.e. that $P_t$ maps $C_b(D)$ into $C_b(D)$) to define the adjoint semigroup $P_t^*$ on the class $\mathcal{M}$ of Borel measures in $D$ with finite total variation by

$$\int_D f \,\mathrm{d}P_t^*\mu = \int_D P_t f \,\mathrm{d}\mu$$

and to regularize with the aid of $P_t^*$ singular measures to absolutely continuous measures, under appropriate additional assumptions on $P_t$. Since $P_t$ is selfadjoint, the operator $P_t^*$ can also be viewed as the extension of $P_t$ from $L^1(\mathfrak{m})$ to $\mathcal{M}$; occasionally, when there is no risk of confusion, with a slight abuse of notation we consider also $P_t^*$, $t > 0$, as an operator from $\mathcal{M}$ to $L^1(\mathfrak{m})$.

We denote by $p_t(x,y)$ the transition probabilities of the semigroup, characterized by the formula

$$P_t f(x) = \int_D p_t(x,y) f(y) \,\mathrm{d}\mathfrak{m}(y),$$

so that

$$P_t^*\delta_{x_0} = p_t(x_0, \cdot\,)\mathfrak{m} \qquad \text{for all } x_0 \in D,\ t > 0.$$

The infinitesimal generator of $P_t$ is nothing but (the extension of) the Laplace-Beltrami operator on $D$, which we denote by $\Delta$. Besides the "qualitative" properties of $P_t$ mentioned above, our proof depends on several quantitative estimates related to $P_t$.

**Quantitative estimates on $P_t$.** We assume throughout the validity of the following properties: there are positive constants $d$, $C_{\mathrm{sg}}$, $C_{\mathrm{uc}}$, $C_{\mathrm{ge}}$, $C_{\mathrm{rt}}$, $C_{\mathrm{dr}}$ and $K$ such that for all $t \ge 0$ one has

(SG) spectral gap: $\|P_t f\|_2 \le e^{-C_{\mathrm{sg}} t}\|f\|_2$ for any $f \in L^2(\mathfrak{m})$ with $\int_D f \, d\mathfrak{m} = 0$,

(UC) ultracontractivity: $|p_t(x, y) - 1| \le C_{\mathrm{uc}} t^{-d/2}$ for all $x, y \in D$,

(GE) gradient estimate: $\mathrm{Lip}\big(p_t(x, \cdot)\big) \le C_{\mathrm{ge}} t^{-(d+1)/2}$ for all $x \in D$,

(RT) Riesz transform bound:

$$\int_D |\nabla f|^4 \, d\mathfrak{m} \le C_{\mathrm{rt}} \int_D \left|(-\Delta)^{1/2} f\right|^4 d\mathfrak{m},$$

(DR) dispersion rate: $\int_D \mathsf{d}^2(x, y) p_t(x, y) \, d\mathfrak{m}(y) \le C_{\mathrm{dr}} t$ for all $x \in D$,

(GC) gradient contractivity: $|\nabla P_t f|(x) \le e^{Kt} P_t |\nabla f|(x)$ for all $x \in D$.

In the sequel, since many parameters and constants will be involved, in some statements we call a constant *geometric* if it depends only on $D$ through $d$, $C_{\mathrm{sg}}$, $C_{\mathrm{uc}}$, $C_{\mathrm{ge}}$, $C_{\mathrm{rt}}$, $C_{\mathrm{dr}}$ and $K$. The validity of these properties on a wide class of compact Riemannian manifolds is known, we refer e.g. to the monograph [Wan14], chapter 1, for a detailed discussion of the case where $D$ has no boundary, and chapter 2 for that with (convex) boundary. Here we notice that (SG) is equivalent to a Poincaré inequality, (GC) is equivalent to a lower bound on Ricci curvature by $-K$, (RT) holds if the Ricci curvature is non-negative [Bak87, Theorem 4.1] or, more generally, using also (SC) and (UC), bounded from below (see Remark 2.3.5 at the end of this section). The assumption (UC) is related to the validity of Sobolev inequalities, see e.g. the abstract equivalence result [VSC08, Theorem II.4.3], taking into account that in the compact case one has to subtract averages, hence the term $-1$ in (UC). Property (DR) follows from an upper bound on the Laplacian of the distance squared from any fixed point, and (GE) is a consequence of the others, see (2.3.4). Let us draw now some easy consequences of these assumptions.

Spectral gap implies that for $f \in L^2(D, \mathfrak{m})$ with $\Delta f \in L^2(D, \mathfrak{m})$ we have the representation

$$f(x) = \int_D f \, d\mathfrak{m} + \int_0^\infty (P_t \Delta f)(x) \, dt. \tag{2.3.1}$$

Ultracontractivity entails that $P_t : L^1 \to L^\infty$ continuously for $t > 0$, because

$$|P_t f(x)| \le \left| \int_D p_t(x, y) f(y) \, d\mathfrak{m}(y) - \int_D f(y) \, d\mathfrak{m}(y) \right| + \|f\|_1 \le (C_{\mathrm{uc}} t^{-d/2} + 1)\|f\|_1.$$

Hence, by interpolation and duality, $P_t : L^p \to L^q$ continuously for any $1 \le p \le q \le \infty$, with $\|P_t\|_{p \to q} \le C(1 + t^{-\frac{d}{2}(\frac{1}{p} - \frac{1}{q})})$, for some geometric constant $C$, possibly depending also on $p$ and $q$. If $p = 1$, by approximation we also get $P_t^* : \mathcal{M} \to L^q$ continuously for $1 \le q \le \infty$, where $\mathcal{M}$ is of course endowed with the total variation norm. Notice also that

$$[\![ p_t(\cdot, y) ]\!]_2^2 \le [\![ p_t(\cdot, y) ]\!]_\infty \le C_{\mathrm{uc}} t^{-d/2} \tag{2.3.2}$$

because

$$\llbracket p_t(\,\cdot\,,y)\rrbracket_2^2 = \int_D \big(p_t(x,y)-1\big)^2 \,\mathrm{d}\mathfrak{m}(x) = \int_D p_t(x,y)\big(p_t(x,y)-1\big)\,\mathrm{d}\mathfrak{m}(x)$$
$$\le \llbracket p_t(\,\cdot\,,y)\rrbracket_\infty \int_D p_t(x,y)\,\mathrm{d}\mathfrak{m}(x) = \llbracket p_t(\,\cdot\,,y)\rrbracket_\infty \le C_{\mathrm{uc}} t^{-d/2}.$$

Writing $\mu = \int_D \delta_x \,\mathrm{d}\mu(x)$ and (DR) in the form $W_2^2(P_t^*\delta_x,\delta_x) \le C_{\mathrm{dr}} t$, from the joint convexity of $W_2^2$ (2.2.5) we obtain

$$W_2^2(P_t^*\mu,\mu) \le C_{\mathrm{dr}} t.$$

By duality, see [Kuw10], the gradient contractivity property leads to contractivity w.r.t. $W_2$ distance

$$W_2^2(P_t^*\mu,P_t^*\nu) \le e^{2Kt} W_2^2(\mu,\nu).$$

Moreover, it implies that for some geometric constant $C$ we have

$$\|\nabla f\|_\infty \le C\|\Delta f\|_\infty \tag{2.3.3}$$

for every $f \in L^2(D,\mathfrak{m})$ with $\Delta f \in L^\infty(D,\mathfrak{m})$. Indeed, from Bakry's work (see [BGL14] and [Wan11]), it is known that (GC) implies the reverse Poincaré inequality

$$|\nabla P_t g|^2 \le \frac{K}{e^{2Kt}-1}\left[P_t(g^2)-(P_t g)^2\right] \le \frac{K}{e^{2Kt}-1}\|g\|_\infty^2,$$

hence the bound $\|\nabla P_t g\|_\infty \le c t^{-1/2}\|g\|_\infty$ for $t \in (0,1]$ and some geometric constant $c$. Using the representation formula (2.3.1) and the previous estimate with $g = \Delta f$ and $g = P_{t-1}\Delta f$ we obtain (2.3.3) as

$$\|\nabla f\|_\infty \le \int_0^\infty \|\nabla P_t \Delta f\|_\infty \,\mathrm{d}t = \int_0^2 \|\nabla P_t\Delta f\|_\infty \,\mathrm{d}t + \int_2^\infty \|\nabla P_1(P_{t-1}\Delta f)\|_\infty \,\mathrm{d}t$$
$$\le c\left(\|\Delta f\|_\infty \int_0^2 t^{-1/2}\,\mathrm{d}t + \|P_1\|_{L^2\to L^\infty}\int_2^\infty \|P_{t-2}\Delta f\|_2 \,\mathrm{d}t\right)$$
$$\le c\left(2\sqrt{2} + \|P_1\|_{L^2\to L^\infty}\int_2^\infty e^{-C_{\mathrm{sg}}(t-2)}\,\mathrm{d}t\right)\|\Delta f\|_\infty.$$

Using the same bound, we also have, for $x \in D$, $t \in (0,1]$,

$$\mathrm{Lip}\big(p_t(x,\,\cdot\,)\big) = \|\nabla P_t^*\delta_x\|_\infty \le c(t/2)^{-1/2}\|P_{t/2}^*(\delta_x - \mathfrak{m})\|_\infty \le c\, C_{\mathrm{uc}}(t/2)^{-(d+1)/2}, \tag{2.3.4}$$

which shows that (GE) above is actually a consequence of (SG), (UC) and (GC) (for $t > 1$, one uses (SG) to obtain even exponential decay).

In the following lemma we collect some further consequences of the gradient contractivity assumption (GC).

**Lemma 2.3.1.** *For every $s \geq 0$ and $g \in C_b(D)$ one has*

$$\min g \leq -\log\left(P_s e^{-g}\right) \leq \max g, \quad \textit{hence} \quad \|-\log\left(P_s e^{-g}\right)\|_\infty \leq \|g\|_\infty, \tag{2.3.5}$$

$$\|\nabla \log\left(P_s e^{-g}\right)\|_\infty \leq e^{K^+ s}\|\nabla g\|_\infty. \tag{2.3.6}$$

*Proof.* Write $G = e^{-g}$. Inequality (2.3.5) follows from the fact that $P_s$ is Markov and the inequalities $e^{-\max g} \leq G \leq e^{-\min g}$. In order to prove (2.3.6) we use (GC) to get

$$|\nabla \log\left(P_s e^{-g}\right)| = \frac{|\nabla P_s e^{-g}|}{P_s e^{-g}} \leq e^{K^+ s}\frac{P_s\left(|\nabla g| e^{-g}\right)}{P_s e^{-g}} \leq e^{K^+ s}\|\nabla g\|_\infty. \qquad \square$$

**Lemma 2.3.2** (Viscous Hamilton-Jacobi)**.** *Assume that $D$ is a compact Riemannian manifold without boundary. Let $\sigma > 0$, $f \in C(D)$, and define, for $t \geq 0$,*

$$\varphi_t^\sigma = -\sigma \log\left(P_{(\sigma t)/2} e^{-f/\sigma}\right).$$

*Then $\varphi_t^\sigma \in C\big([0, +\infty) \times D\big) \cap C^\infty\big((0, +\infty) \times D\big)$ solves*

$$\begin{cases} \partial_t \varphi_t^\sigma = -\dfrac{|\nabla \varphi_t^\sigma|^2}{2} + \dfrac{\sigma}{2}\Delta \varphi_t^\sigma & \textit{in } (0, +\infty) \times D, \\ \varphi_0^\sigma = f & \textit{in } D. \end{cases} \tag{2.3.7}$$

*Moreover*

$$\min f \leq \varphi_t^\sigma \leq \max f, \qquad \|\varphi_t^\sigma\|_\infty \leq \|f\|_\infty, \tag{2.3.8}$$

$$\|\nabla \varphi_t^\sigma\|_\infty \leq e^{K^+ \sigma t}\|\nabla f\|_\infty, \tag{2.3.9}$$

$$\|(\Delta \varphi_t^\sigma)^+\|_\infty \leq \|(\Delta f)^+\|_\infty + \frac{e^{2K^+ t} - 1}{2}\|\nabla f\|_\infty^2, \tag{2.3.10}$$

$$\varphi_1^\sigma(y) - \varphi_0^\sigma(x) \leq \frac{\mathsf{d}(x,y)^2}{2} + \frac{\sigma}{2}\|(\Delta f)^+\|_\infty + \frac{\sigma}{4}(e^{2K^+} - 1)\|\nabla f\|_\infty^2, \tag{2.3.11}$$

$$\int_D (\varphi_0^\sigma - \varphi_1^\sigma)\, d\mathfrak{m} \leq \exp\left(\|(\Delta f)^+\|_\infty + \frac{1}{2}(e^{2K^+} - 1)\|\nabla f\|_\infty^2\right)\int_D \frac{|\nabla f|^2}{2}\, d\mathfrak{m}. \tag{2.3.12}$$

*Proof.* The smoothness of $\varphi_t^\sigma$ for positive times follows by the chain rule and standard (linear) parabolic theory. To check that $\varphi^\sigma$ solves (2.3.7), it is sufficient to compare

$$\partial_t \varphi_t^\sigma = -\frac{\sigma^2}{2}\frac{\Delta P_{(\sigma t)/2} e^{-f/\sigma}}{P_{(\sigma t)/2} e^{-f/\sigma}}$$

with the terms arising from the application of the diffusion chain rule

$$\begin{aligned}\frac{\sigma}{2}\Delta\varphi_t^\sigma &= -\frac{\sigma^2}{2}\Delta\log\left(P_{(\sigma t)/2}e^{-f/\sigma}\right)\\ &= -\frac{\sigma^2}{2}\frac{\Delta P_{(\sigma t)/2}e^{-f/\sigma}}{P_{(\sigma t)/2}e^{-f/\sigma}}+\frac{\sigma^2}{2}\left|\frac{\nabla P_{(\sigma t)/2}e^{-f/\sigma}}{P_{(\sigma t)/2}e^{-f/\sigma}}\right|^2\\ &= \partial_t\varphi_t^\sigma+\frac{1}{2}|\nabla\varphi_t^\sigma|^2.\end{aligned}\tag{2.3.13}$$

Inequalities (2.3.8) and (2.3.9) follow in a straightforward way, respectively from (2.3.5) and (2.3.6) of Lemma 2.3.1, with $s=(\sigma t)/2$ and $g=f/\sigma$.

To prove (2.3.10) we use Bochner's inequality

$$\Delta\frac{|\nabla\varphi_t^\sigma|^2}{2}\geq -K|\nabla\varphi_t^\sigma|^2+\langle\nabla\varphi_t^\sigma,\nabla\Delta\varphi_t^\sigma\rangle,$$

which encodes the bound from below on Ricci curvature, and, setting $\xi_t=\Delta\varphi_t^\sigma$, we get

$$\partial_t\xi_t\leq K|\nabla\varphi_t^\sigma|^2-\langle\nabla\varphi_t^\sigma,\nabla\xi_t\rangle+\frac{\sigma}{2}\Delta\xi_t\leq K^+e^{2K^+t}\|\nabla f\|_\infty^2-\langle\nabla\varphi_t^\sigma,\nabla\xi_t\rangle+\frac{\sigma}{2}\Delta\xi_t$$

which, by the maximum principle (here we use that $D$ has no boundary), leads to (2.3.10).

To prove (2.3.11), let $\gamma\in C^1([0,1],D)$, with $\gamma(0)=x$, $\gamma(1)=y$, and compute

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t^\sigma(\gamma(t)) &= \left(\partial_t\varphi_t^\sigma\right)(\gamma(t))+\langle\left(\nabla\varphi_t^\sigma\right)(\gamma(t)),\dot\gamma(t)\rangle\\ &= -\frac{1}{2}|\nabla\varphi_t^\sigma(\gamma(t))|^2+\frac{\sigma}{2}\Delta\varphi_t^\sigma(\gamma(t))+\langle\left(\nabla\varphi_t^\sigma\right)(\gamma(t)),\dot\gamma(t)\rangle\\ &\leq \frac{1}{2}|\dot\gamma(t)|^2+\frac{\sigma}{2}\|(\Delta\varphi_t^\sigma)^+\|_\infty.\end{aligned}\tag{2.3.14}$$

Integrating over $t\in(0,1)$ and using (2.3.10), we obtain

$$\varphi_1^\sigma(y)-\varphi_0^\sigma(x)\leq\frac{1}{2}\int_0^1|\dot\gamma(t)|^2\,\mathrm{d}t+\frac{\sigma}{2}\|(\Delta f)^+\|_\infty+\frac{\sigma}{4}(e^{2K^+}-1)\|\nabla f\|_\infty^2,$$

which yields (2.3.11) after we take the infimum with respect to $\gamma$.

To show (2.3.12), we notice first that

$$\begin{aligned}\int_D(\varphi_0^\sigma-\varphi_1^\sigma)\,\mathrm{d}\mathfrak{m} &= -\int_D\int_0^1\partial_t\varphi_t^\sigma\,\mathrm{d}t\,\mathrm{d}\mathfrak{m}\\ &= \frac{1}{2}\int_0^1\int_D|\nabla\varphi_t^\sigma|^2\,\mathrm{d}\mathfrak{m}\,\mathrm{d}t-\frac{\sigma}{2}\int_0^1\int_D\Delta\varphi_t^\sigma\,\mathrm{d}\mathfrak{m}\,\mathrm{d}t\\ &= \frac{1}{2}\int_0^1\int_D|\nabla\varphi_t^\sigma|^2\,\mathrm{d}\mathfrak{m}\,\mathrm{d}t,\end{aligned}\tag{2.3.15}$$

where the second term vanishes because $D$ is without boundary. For $t \in (0,1)$, one has

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_D |\nabla\varphi_t^\sigma|^2 \,\mathrm{d}\mathfrak{m} &= -\frac{\mathrm{d}}{\mathrm{d}t}\int_D (\Delta\varphi_t^\sigma)\,\varphi_t^\sigma \,\mathrm{d}\mathfrak{m} = -2\int_D (\Delta\varphi_t^\sigma)\,\partial_t\varphi_t^\sigma \,\mathrm{d}\mathfrak{m} \\ &= \int_D (\Delta\varphi_t^\sigma)\,|\nabla\varphi_t^\sigma|^2 - \sigma\int_D (\Delta\varphi_t^\sigma)^2 \,\mathrm{d}\mathfrak{m} \\ &\leq \|(\Delta\varphi_t^\sigma)^+\|_\infty \int_D |\nabla\varphi_t^\sigma|^2 \,\mathrm{d}\mathfrak{m}.\end{aligned} \tag{2.3.16}$$

Combining (2.3.15) and (2.3.16) and taking into account the estimate (2.3.10) on $\Delta\varphi_t^\sigma$, inequality (2.3.12) follows by Gronwall's inequality. □

**Corollary 2.3.3** (Dual potential)**.** *Assume that $D$ is a compact Riemannian manifold without boundary. For every Lipschitz function $f$ with $\|(\Delta f)^-\|_\infty < \infty$, there exists $g \in C_b(D)$ such that*

$$f(x) + g(y) \leq \frac{\mathsf{d}(x,y)^2}{2},$$
$$\int_D (f+g)\,\mathrm{d}\mathfrak{m} \geq -\exp\left(\|(\Delta f)^-\|_\infty + \frac{1}{2}(e^{2K^+}-1)\|\nabla f\|_\infty^2\right)\int_D \frac{|\nabla f|^2}{2}\,\mathrm{d}\mathfrak{m}.$$

*Proof.* For $\sigma > 0$, consider the functions $g^\sigma = \varphi_1^\sigma$ solving the initial value problem (2.3.7) with $f$ replaced by $-f$. Inequalities (2.3.5) and (2.3.6) entail that $g^\sigma$ are uniformly bounded in the space of Lipschitz functions: as $\sigma \to 0$, we can extract a subsequence $(g^{\sigma_h})$ pointwise converging to some bounded Lipschitz function $g$. Inequality (2.3.11) gives in the limit the first inequality of the thesis, while (2.3.12) yields the second one, by dominated convergence. □

*Remark* 2.3.4 (On the equality $g = Q_1(-f)$). Recall that the theory of viscosity solutions [CL83; BC97] is specifically designed to deal with equations, as the Hamilton-Jacobi equations, for which the distributional point of view fails. This theory can be carried out also on manifolds, see [Fat08] for a nice presentation of this subject. Since one can prove (using also apriori estimates on the time derivatives, arguing as in Corollary 2.3.3) the existence of a function $\varphi_t$, uniform limit of a subsequence of $\varphi_t^\sigma$, since classical solutions are viscosity solutions and since locally uniform limits of viscosity solutions are viscosity solutions, the function $\varphi_t$ is a viscosity solution to the HJ equation $\partial_t u + \frac{1}{2}|\nabla u|^2 = 0$. Then, if the initial condition is $-f$, the uniqueness theory of first order viscosity solutions applies, and gives that $\varphi_t$ is precisely given by $Q_t(-f)$, as defined in (2.2.2). Setting $t = 1$, this argument proves that actually the function $g$ of Corollary 2.3.3 coincides with $Q_1(-f)$, and that there is full convergence as $\sigma \to 0$ (see also [Cap03] for a proof of the convergence, in Euclidean spaces, based on the theory of large deviations). We preferred a more elementary and self-contained presentation, because the weaker statement $g \leq Q_1(-f)$ provided by the Corollary is sufficient for our purposes, and because our argument works also in the more abstract setting described in Section 2.6 (in which neither large deviations nor theory of viscosity solutions are completely developed), emphasizing the role played by the lower Ricci curvature bounds.

*Remark* 2.3.5 ((RT) and (GC)). As already remarked, if (GC) holds with $K \le 0$, then [Bak87, Theorem 4.1] implies the validity of (RT). For general $K$, the same result yields the bound

$$\|\nabla f\|_4 \le C \left( \|(-\Delta)^{1/2} f\|_4 + \|f\|_4 \right), \tag{2.3.17}$$

for some constant $C$ depending on $K$ only. Below, we prove that, assuming (SG) and (UC), the Poincaré inequality

$$\left\| f - \int_D f \, \mathrm{d}\mathfrak{m} \right\|_4 \le C \|(-\Delta)^{1/2} f\|_4, \tag{2.3.18}$$

holds, with $C$ depending on $C_{\mathrm{sg}}$ and $C_{\mathrm{uc}}$ only, so that (RT) follows also in this case, noticing that one can always replace $\|f\|_4$ with $\|f - \int_D f \, \mathrm{d}\mathfrak{m}\|_4$ in (2.3.17).

To prove (2.3.18), we assume without loss of generality that $\int_D f \, \mathrm{d}\mathfrak{m} = 0$, and introduce the semigroup $R_t$ generated by $(-\Delta)^{1/2}$, which can be explicitly represented via Bochner subordination [BF75, Example 9.23] as

$$R_t f = \int_0^\infty \frac{t}{\sqrt{4\pi} s^{3/2}} e^{-\frac{t^2}{4s}} P_s f \, \mathrm{d}s. \tag{2.3.19}$$

This representation and the bound $\|P_s\|_{4\to4} \le 1$ give that $\|R_t\|_{4\to4} \le 1$. Moreover, using (SC), (UC) and the inequality $\|f\|_2 \le \|f\|_4$, we have

$$\begin{aligned}
\|R_t f\|_4 &\le \int_0^\infty \frac{t}{\sqrt{4\pi} s^{3/2}} e^{-\frac{t^2}{4s}} \|P_s f\|_4 \, \mathrm{d}s \\
&\le \left( \int_0^1 \frac{t}{\sqrt{4\pi} s^{3/2}} e^{-\frac{t^2}{4s}} \, \mathrm{d}s + \int_1^\infty \frac{t}{\sqrt{4\pi} s^{3/2}} e^{-\frac{t^2}{4s}} \|P_1\|_{4\to2} e^{-C_{\mathrm{sg}}(s-1)} \, \mathrm{d}s \right) \|f\|_4.
\end{aligned}$$

Simple estimates on the integrals above show that $\|R_t f\|_4 \le \frac{1}{2}\|f\|_4$, for any $t \ge C$, with $C$ depending on $C_{\mathrm{sg}}$ and $C_{\mathrm{uc}}$ only. On the other hand, the representation $R_t f - f = \int_0^t R_s (-\Delta)^{1/2} f \, \mathrm{d}s$ holds for any $t \ge 0$, hence, if $t \ge C$,

$$\|f\|_4 \le \|R_t f\|_4 + \|R_t f - f\|_4 \le \frac{1}{2}\|f\|_4 + t\|(-\Delta)^{1/2} f\|_4,$$

which yields (2.3.18).

### 2.3.1 Density fluctuation bounds

Recalling the notation $\mu^n = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$, $r^n = \sqrt{n}(\mu^n - \mathfrak{m})$, we now define our regularized empirical measures.

**Definition 2.3.6** (Regularized empirical measures)**.** For $t \geq 0$ define

$$\mu^{n,t} = P_t^* \mu^n, \qquad r^{n,t}\mathfrak{m} = P_t^* r^n = \sqrt{n}(\mu^{n,t} - \mathfrak{m}),$$

so that for $t > 0$ one has

$$r^{n,t}(y) = \int_D (p_t(\cdot, y) - 1)\, \mathrm{d}r^n.$$

The goal of this subsection is to collect apriori estimates on the deviation of $r^{n,t}$ from 0.

**Lemma 2.3.7** (Pointwise bound)**.** *For $y \in D$ and $\eta > 0$ one has*

$$\mathbb{P}\left(\frac{|r^{n,t}(y)|}{\sqrt{n}} > \eta\right) \leq 2\exp\left(-\frac{nt^{d/2}}{2C_{\mathrm{uc}}} F(1,\eta)\right), \tag{2.3.20}$$

*where $F$ is defined in* (2.2.9)*.*

*Proof.* Consider the random variable $X = r^{n,t}(y)/\sqrt{n} = \int_D p_t(\cdot, y)/\sqrt{n}\, \mathrm{d}r^n$. By (2.2.7) with $f = p_t(\cdot, y)/\sqrt{n}$ we have

$$\begin{aligned}\mathbb{E}[\exp(\lambda X)] &\leq \exp\left[\frac{\lambda^2 [\![p_t(\,\cdot\,, y)]\!]_2^2}{2n} \exp\left(|\lambda| \frac{[\![p_t(\,\cdot\,, y)]\!]_\infty}{n}\right)\right] \\ &\leq \exp\left[\frac{\lambda^2}{2} \cdot \frac{C_{\mathrm{uc}}}{nt^{d/2}} \exp\left(|\lambda| \frac{C_{\mathrm{uc}}}{nt^{d/2}}\right)\right],\end{aligned}$$

where in the second inequality we used (2.3.2). Then Lemma 2.2.7 with $c_1 = c_2 = C_{\mathrm{uc}}/(nt^{d/2})$ implies (2.3.20). □

**Lemma 2.3.8** (Deterministic bound)**.** *With probability* 1 *one has*

$$\frac{|r^{n,t}(y) - r^{n,t}(z)|}{\sqrt{n}} \leq \frac{2C_{\mathrm{ge}}}{t^{(d+1)/2}} \mathsf{d}(y,z).$$

*Proof.* Using (GE) and the fact that the total variation of the measures $r^n$ is $2\sqrt{n}$, we get

$$\begin{aligned}\frac{|r^{n,t}(y) - r^{n,t}(z)|}{\sqrt{n}} &= \left| \int_D \big(p_t(x,y) - p_t(x,z)\big) \frac{\mathrm{d}r^n(x)}{\sqrt{n}} \right| \\ &\leq \mathsf{d}(y,z) \int_D \mathrm{Lip}\big(p_t(x,\,\cdot\,)\big) \frac{\mathrm{d}|r^n|(x)}{\sqrt{n}} \leq \frac{2C_{\mathrm{ge}}}{t^{(d+1)/2}} \mathsf{d}(y,z).\end{aligned}$$ □

We shall need another geometric function related to $D$.

**Definition 2.3.9** (Minimal $\delta$-cover)**.** In the sequel, for $\delta > 0$ we denote by $N_D(\delta)$ be smallest cardinality of a $\delta$-net of $D$, namely a set whose closed $\delta$-neighbourhood contains $D$.

**Proposition 2.3.10** (Uniform bound, $d = 1$)**.** *Assume that ultracontractivity holds with $d = 1$ and that $N_D(\delta) \le \max\{1, C_D\delta^{-1}\}$ for all $\delta > 0$. Then there exists a constant $C = C(C_{\mathrm{ge}}, C_D)$ with the following property: for all $\eta \in (0,1)$, $q \in (0,1)$ and $\eta^{-1}n^{-2q} \le t \le 4C_{\mathrm{ge}}C_D$, we have*

$$\mathbb{P}\left(\sup_{y\in D}\frac{|r^{n,t}(y)|}{\sqrt{n}} > \eta\right) \le C\exp\left(-\gamma n^{1-q}\right)$$

*with $\gamma = \gamma(\eta, C_{\mathrm{uc}})$ and $n \ge n(\eta, q, C_{\mathrm{uc}})$.*

*Proof.* We pick $\delta = \frac{\eta}{4C_{\mathrm{ge}}}t$, so that, by Lemma 2.3.8, with probability 1 we have

$$\frac{|r^{n,t}(y) - r^{n,t}(z)|}{\sqrt{n}} \le \frac{\eta}{2} \qquad \text{for any } y, z \in D \text{ with } \mathsf{d}(y,z) \le \delta. \tag{2.3.21}$$

Let $T$ be a minimal $\delta$-net. Then the condition $t \le 4C_{\mathrm{ge}}C_D$ implies $C_D\delta^{-1} \ge 1$, hence

$$|T| \le C_D\delta^{-1} = \frac{4C_{\mathrm{ge}}C_D}{\eta}t^{-1} \le 4C_{\mathrm{ge}}C_Dn^{2q}.$$

From an application of Lemma 2.3.7 with $\eta/2$ instead of $\eta$ we get

$$\begin{aligned}
\mathbb{P}\left(\sup_{y\in T}\frac{|r^{n,t}(y)|}{\sqrt{n}} > \frac{\eta}{2}\right) &\le 2|T|\exp\left(-\frac{nt^{1/2}}{2C_{\mathrm{uc}}}F(1,\eta/2)\right)\\
&\le 8C_{\mathrm{ge}}C_D\exp\left(2q\log n - \frac{n^{1-q}}{2\eta^{1/2}C_{\mathrm{uc}}}F(1,\eta/2)\right)\\
&\le 8C_{\mathrm{ge}}C_D\exp\left(-\gamma n^{1-q}\right),
\end{aligned}$$

where the last inequality holds with $\gamma = F(1,\eta/2)/(4\eta^{1/2}C_{\mathrm{uc}})$ and $n \ge n(\eta, q, C_{\mathrm{uc}})$, absorbing the logarithm $\log n$ into the power $n^{1-q}$. We conclude since

$$\mathbb{P}\left(\sup_{y\in D}\frac{|r^{n,t}(y)|}{\sqrt{n}} > \eta\right) \le \mathbb{P}\left(\sup_{y\in T}\frac{|r^{n,t}(y)|}{\sqrt{n}} > \frac{\eta}{2}\right). \qquad \square$$

**Proposition 2.3.11** (Uniform bound, $d = 2$)**.** *Assume that ultracontractivity holds with $d = 2$ and that $N_D(\delta) \le \max\{1, C_D\delta^{-2}\}$ for every $\delta > 0$. Then there exists a constant $C = C(C_{\mathrm{ge}}, C_D)$ with the following property: for all $\eta > 0$ there exists $\gamma = \gamma(\eta, C_{\mathrm{uc}})$ such that*

$$\mathbb{P}\left(\sup_{y\in D}\frac{|r^{n,t}(y)|}{\sqrt{n}} > \eta\right) \le \frac{C}{n}$$

*holds for $(16C_DC_{\mathrm{ge}}^2)^{1/3} \ge t \ge \gamma n^{-1}\log n$ and $n \ge n(\eta, C_{\mathrm{uc}})$.*

*Proof.* Given $\eta > 0$, we choose $\gamma$ in such a way that $\gamma F(1,\eta/2)/(2C_{\mathrm{uc}}) = 4$. Then, we define $n(\eta, C_{\mathrm{uc}})$ in such a way that $\gamma\log n \ge \eta^{-2/3}$ for $n \ge n(\eta, C_{\mathrm{uc}})$.

We pick $\delta = \frac{\eta}{4C_{\mathrm{ge}}} t^{3/2}$, so that, by Lemma 2.3.8, with probability 1 we have (2.3.21). Let $T$ be a minimal $\delta$-net. Then the condition $t^3 \leq 16 C_D C_{\mathrm{ge}}^2$ implies $C_D \delta^{-2} \geq 1$,

$$|T| \leq C_D \delta^{-2} = \frac{16 C_D C_{\mathrm{ge}}^2}{\eta^2} t^{-3} \leq 16 C_D C_{\mathrm{ge}}^2 n^3,$$

where we used also the inequality $t \geq \gamma n^{-1} \log n \geq \eta^{-2/3}/n$. From an application of Lemma 2.3.7 with $\eta/2$ instead of $\eta$ we get

$$\begin{aligned}\mathbb{P}\left(\sup_{y\in T} \frac{|r^{n,t}(y)|}{\sqrt{n}} > \frac{\eta}{2}\right) &\leq 2|T| \exp\left(-\frac{nt}{2C_{\mathrm{uc}}} F(1,\eta/2)\right)\\ &\leq 32 C_D C_{\mathrm{ge}}^2 \exp\left(3\log n - \gamma \frac{F(1,\eta/2)}{2C_{\mathrm{uc}}} \log n\right).\end{aligned}$$

Our choice of $\gamma$ then gives

$$\mathbb{P}\left(\sup_{y\in T} \frac{|r^{n,t}(y)|}{\sqrt{n}} > \frac{\eta}{2}\right) \leq \frac{32 C_D C_{\mathrm{ge}}^2}{n}.$$ □

We now report some estimates on the logarithmic mean.

**Lemma 2.3.12.** *For $a, b \geq 0$ and $q > 0$ we have*

$$q(ab)^{q/2} \frac{a-b}{a^q - b^q} \leq M(a,b) \leq q \frac{a^q + b^q}{2} \cdot \frac{a-b}{a^q - b^q}.$$

*Proof.* It is known that

$$\sqrt{ab} \leq M(a,b) \leq \frac{a+b}{2}. \tag{2.3.22}$$

The thesis follows by applying these inequalities to $a^q$ and $b^q$. □

In the following lemma we estimate the logarithmic mean of the densities of $\mu^{n,t,c}$ obtained by a further regularization, i.e. by adding to $\mu^{n,t}$ a small multiple of $\mathfrak{m}$.

**Lemma 2.3.13** (Integral bound)**.** *Define $\mu^{n,t,c} = (1-c)\mu^{n,t} + c\mathfrak{m}$ and let $u^{n,t,c} = (1-c)u^{n,t} + c$ be its probability density, with $c = c(n) \in (0,1]$. If $t^{d/2} = t^{d/2}(n) \geq \gamma n^{-1} \log n$ and $nc(n) \to \infty$ as $n \to \infty$, then*

$$\lim_{n\to\infty} \mathbb{E}\left[\int_D \left(M(u^{n,t,c},1)^{-1} - 1\right)^2 d\mathfrak{m}\right] = 0.$$

*Proof.* Fix $x \in D$ and $\eta \in (0,1)$. By Lemma 2.3.7 we have

$$\mathbb{P}\left(|u^{n,t}(x) - 1| > \eta\right) \leq 2n^{-q},$$

where $q \in (0,1)$ depends only on $d$, $C_{\mathrm{uc}}$, $\gamma$ and $\eta$. In the event $\{|u^{n,t}(x)-1| > \eta\}$, using the first inequality in Lemma 2.3.12 we can estimate the squared difference with the sum of squares to get

$$\left(M(u^{n,t,c}(x),1)^{-1}-1\right)^2 \leq \frac{2}{q^2}\cdot\frac{1}{u^{n,t,c}(x)^q}\left(\frac{u^{n,t,c}(x)^q-1}{u^{n,t,c}(x)-1}\right)^2+2 \leq \frac{2}{q^2c^q}+2.$$

In the complementary event $\{|u^{n,t}(x)-1| \leq \eta\}$, we have $|u^{n,t,c}(x)-1| \leq (1-c)\eta \leq \eta$ and, expanding the squares and using both inequalities in (2.3.22), we get

$$\left(M(u^{n,t,c}(x),1)^{-1}-1\right)^2 \leq \frac{1}{u^{n,t,c}(x)}-\frac{4}{u^{n,t,c}(x)+1}+1 \leq \frac{1}{1-\eta}-\frac{4}{2+\eta}+1.$$

Therefore

$$\mathbb{E}\left[\int_D \left(M(\mu^{n,t,c},1)^{-1}-1\right)^2 \mathrm{d}\mathfrak{m}\right] \leq 2n^{-q}\left(\frac{2}{q^2c(n)^q}+2\right)+\frac{1}{1-\eta}-\frac{4}{2+\eta}+1,$$

hence the growth condition on $c$ gives

$$\limsup_{n\to\infty}\mathbb{E}\left[\int_D \left(M(u^{n,t,c},1)^{-1}-1\right)^2 \mathrm{d}\mathfrak{m}\right] \leq \frac{1}{1-\eta}-\frac{4}{2+\eta}+1.$$

Letting $\eta \to 0$ we obtain the result. □

### 2.3.2 Energy estimates

Retaining Definition 2.3.6 of $r^{n,t}$ from the previous subsection, here we derive energy bounds for the solutions to the following random PDE:

$$\begin{cases} \Delta f^{n,t} = r^{n,t} & \text{in } D, \\ \nabla f^{n,t}\cdot n_D = 0 & \text{on } \partial D \end{cases} \tag{2.3.23}$$

which are uniquely determined up to a (random) additive constant. As we will see (particularly in Section 2.6), these estimates involve either the trace of $\Delta$ or sums indexed by the spectrum $\sigma(\Delta)$ (which contains $\{0\}$ and, by the spectral gap assumption, satisfies $\sigma(\Delta) \subset (-\infty, -C_{\mathrm{sg}}^2] \cup \{0\}$); it is understood that the eigenvalues in these sums are counted with multiplicity.

We recall the so-called trace formula

$$\int_D p_s(x,x)\,\mathrm{d}\mathfrak{m}(x) = \sum_{\lambda\in\sigma(\Delta)} e^{s\lambda} \tag{2.3.24}$$

which follows easily by integration of the representation formula

$$p_s(x,y) = \sum_{\lambda\in\sigma(\Delta)} e^{s\lambda}u_\lambda(x)u_\lambda(y),$$

where $\{u_\lambda\}_{\lambda\in\sigma(\Delta)}$ is an $L^2(\mathfrak{m})$ orthonormal basis of eigenvalues of $\Delta$.

The following expansion (2.3.25) of the trace formula as $s \to 0$ will be useful. In this paper we will only use the leading term in (2.3.25).

**Proposition 2.3.14** (Expansion of the trace formula)**.** *Let $D$ be a bounded Lipschitz domain in $\mathbb{R}^d$ with unit volume. Then*

$$\int_D p_s(x,x)\,\mathrm{d}\mathfrak{m}(x) = (4\pi s)^{-d/2}\left(1+\frac{\sqrt{\pi s}}{2}\mathscr{H}^{d-1}(\partial D)+o(\sqrt{s})\right) \quad \text{as } s\to 0. \tag{2.3.25}$$

*The same holds if $D$ is a smooth, compact $d$-dimensional Riemannian manifold with a smooth boundary (possibly empty).*

*Proof.* The first statement is proved in [Bro93]. The second one, also with additional terms in the expansion, in [MS67]. □

**Lemma 2.3.15** (Representation formula)**.** *Let $f^{n,t}$ be the solution to (2.3.23). For all $t>0$ one has*

$$\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2\,\mathrm{d}\mathfrak{m}\right] = 2\int_t^\infty \left(\int_D p_{2s}(x,x)\,\mathrm{d}\mathfrak{m}(x)-1\right)\mathrm{d}s = -\sum_{\lambda\in\sigma(\Delta)\setminus\{0\}}\frac{e^{2t\lambda}}{\lambda}. \tag{2.3.26}$$

*Proof.* Using the representation formula $g=-\int_0^\infty P_s\Delta g\,\mathrm{d}s$ with $g=f^{n,t}$ we get $f^{n,t}=-\int_0^\infty P_s r^{n,t}\,\mathrm{d}s$, so that

$$\begin{aligned}\int_D |\nabla f^{n,t}|^2\,\mathrm{d}\mathfrak{m} &= -\int_D f^{n,t}\Delta f^{n,t}\,\mathrm{d}\mathfrak{m} = \int_D\left(\int_0^\infty P_s r^{n,t}\,\mathrm{d}s\right) r^{n,t}\,\mathrm{d}\mathfrak{m}\\ &= \int_0^\infty\int_D P_s r^{n,t} r^{n,t}\,\mathrm{d}\mathfrak{m}\,\mathrm{d}s = \int_0^\infty\int_D P_{s/2}r^{n,t}P_{s/2}r^{n,t}\,\mathrm{d}\mathfrak{m}\,\mathrm{d}s\\ &= 2\int_t^\infty\int_D (P_s^* r^n)^2\,\mathrm{d}\mathfrak{m}\,\mathrm{d}s.\end{aligned} \tag{2.3.27}$$

Now, notice that the symmetry and semigroup properties of the transition probabilities give

$$\begin{aligned}\int_D\int_D p_s(x,y)^2\,\mathrm{d}\mathfrak{m}(x)\,\mathrm{d}\mathfrak{m}(y) &= \int_D\int_D p_s(x,y)p_s(y,x)\,\mathrm{d}\mathfrak{m}(y)\,\mathrm{d}\mathfrak{m}(x)\\ &= \int_D p_{2s}(x,x)\,\mathrm{d}\mathfrak{m}(x).\end{aligned}$$

Hence, by Lemma 2.2.6 with $f=p_s(\,\cdot\,,y)$ we can compute

$$\begin{aligned}\mathbb{E}\left[\int_D (P_s^* r^n)^2\,\mathrm{d}\mathfrak{m}\right] &= \int_D \mathbb{E}\left[\big(P_s^* r^n(y)\big)^2\right]\mathrm{d}\mathfrak{m}(y)\\ &= \int_D \mathbb{E}\left[\left(\int_D p_s(x,y)\,\mathrm{d}r^n(x)\right)^2\right]\mathrm{d}\mathfrak{m}(y)\\ &= \int_D [\![p_s(\,\cdot\,,y)]\!]_2^2\,\mathrm{d}\mathfrak{m}(y) = \int_D\int_D\big(p_s(x,y)-1\big)^2\,\mathrm{d}\mathfrak{m}(x)\,\mathrm{d}\mathfrak{m}(y)\\ &= \int_D\int_D p_s(x,y)^2\,\mathrm{d}\mathfrak{m}(x)\,\mathrm{d}\mathfrak{m}(y)-1 = \int_D p_{2s}(x,x)\,\mathrm{d}\mathfrak{m}(x)-1.\end{aligned}$$

By the trace formula (2.3.24), (2.3.26) follows. □

The following lemma basically applies only to 1-dimensional domains, in view of the ultracontractivity assumption with $d = 1$.

**Lemma 2.3.16** (Energy estimate and convergence, $d = 1$). *Let $f^{n,t}$ be the solution to (2.3.23). If $t = t(n) \to 0$ as $n \to \infty$, then*

$$\lim_{n\to\infty} \mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}\right] = \int_0^\infty \left(\int_D p_s(x,x)\, \mathrm{d}\mathfrak{m}(x) - 1\right) \mathrm{d}s = -\sum_{\lambda\in\sigma(\Delta)\setminus\{0\}} \frac{1}{\lambda}. \tag{2.3.28}$$

*If ultracontractivity holds with $d = 1$ we have also*

$$\limsup_{n\to\infty} \mathbb{E}\left[\left(\int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}\right)^2\right] < \infty \tag{2.3.29}$$

*and, in particular, the limit in (2.3.28) is finite.*

*Proof.* The identities (2.3.28) follow by (2.3.26) by taking the limit as $n \to \infty$. If ultracontractivity holds with $d = 1$, we show that the lim sup in (2.3.28) is finite by splitting the integration in $(t, 1)$ and $(1, \infty)$ in the identity

$$\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}\right] = 2\int_t^\infty \int_D \int_D \left(p_s(x,y) - 1\right)^2 \mathrm{d}\mathfrak{m}(x)\, \mathrm{d}\mathfrak{m}(y)\, \mathrm{d}s, \tag{2.3.30}$$

which is a by-product of the intermediate computations made in the proof of Lemma 2.3.15. For $s \in (t, 1)$ we estimate

$$\begin{aligned}\int_D \int_D \left(p_s(x,y) - 1\right)^2 \mathrm{d}\mathfrak{m}(x)\, \mathrm{d}\mathfrak{m}(y) &\le C_{\mathrm{uc}} s^{-1/2} \int_D \int_D |p_s(x,y) - 1| \, \mathrm{d}\mathfrak{m}(x)\, \mathrm{d}\mathfrak{m}(y) \\ &\le 2C_{\mathrm{uc}} s^{-1/2}.\end{aligned}$$

For $s \in (1, \infty)$ instead

$$\begin{aligned}\int_D \int_D \left(p_s(x,y) - 1\right)^2 \mathrm{d}\mathfrak{m}(x)\, \mathrm{d}\mathfrak{m}(y) &= \int_D \|P_{s-1} P_1^*(\delta_y - \mathfrak{m})\|_2^2 \, \mathrm{d}\mathfrak{m}(y) \\ &\le e^{-2C_{\mathrm{sg}}(s-1)} \int_D \|P_1^*(\delta_y - \mathfrak{m})\|_2^2 \, \mathrm{d}\mathfrak{m}(y) \\ &\le 4\|P_1^*\|_{\mathcal{M}\to L^2}^2 e^{-2C_{\mathrm{sg}}(s-1)}.\end{aligned}$$

In conclusion, for some geometric constant $C$, one has

$$\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}\right] \le C\left(\int_t^1 s^{-1/2}\, \mathrm{d}s + \int_1^\infty e^{-2C_{\mathrm{sg}} s}\, \mathrm{d}s\right),$$

from which the finiteness of (2.3.28) readily follows.

To show (2.3.29), we start from (2.3.27) and, with the aid of Lemma 2.2.6, we can estimate

$$\begin{aligned}\mathbb{E}\left[\left(\int_D |\nabla f^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right)^2\right] &= \mathbb{E}\left[\left(2\int_t^\infty \int_D (P_s^* r^n)^2 \,\mathrm{d}\mathfrak{m}\,\mathrm{d}s\right)^2\right] \\ &= 4\int_t^\infty \int_t^\infty \int_D \int_D \mathbb{E}\left[\left(P_s^* r^n(y)\right)^2 \left(P_{s'}^* r^n(z)\right)^2\right] \mathrm{d}\mathfrak{m}(y)\,\mathrm{d}\mathfrak{m}(z)\,\mathrm{d}s\,\mathrm{d}s' \\ &\le 4\int_t^\infty \int_t^\infty \int_D \int_D \Big(3[\![p_s(\,\cdot\,,y)]\!]_2^2 [\![p_{s'}(\,\cdot\,,z)]\!]_2^2 \\ &\qquad + \frac{1}{n}[\![p_s(\,\cdot\,,y)]\!]_4^2 [\![p_{s'}(\,\cdot\,,z)]\!]_4^2\Big)\,\mathrm{d}\mathfrak{m}(y)\,\mathrm{d}\mathfrak{m}(z)\,\mathrm{d}s\,\mathrm{d}s' \\ &= 3\left(2\int_t^\infty \int_D [\![p_s(\,\cdot\,,y)]\!]_2^2 \,\mathrm{d}\mathfrak{m}(y)\,\mathrm{d}s\right)^2 \\ &\qquad + \frac{1}{n}\left(2\int_t^\infty \int_D [\![p_s(\,\cdot\,,y)]\!]_4^2 \,\mathrm{d}\mathfrak{m}(y)\,\mathrm{d}s\right)^2 \\ &= 3\left(\sum_{\lambda\in\sigma(\Delta)\setminus\{0\}} \frac{e^{2t\lambda}}{\lambda}\right)^2 + \frac{1}{n}\left(2\int_t^\infty \int_D [\![p_s(\,\cdot\,,y)]\!]_4^2 \,\mathrm{d}\mathfrak{m}(y)\,\mathrm{d}s\right)^2.\end{aligned}$$

In order to show that the lim sup of last integral is finite we split the integration in $(t,1)$ and $(1,\infty)$. For $s\in(t,1)$ we use

$$\begin{aligned}[\![p_s(\,\cdot\,,y)]\!]_4^4 &\le \int_D \left(p_s(x,y)-1\right)^4 \mathrm{d}\mathfrak{m}(x) \\ &\le C_{\mathrm{uc}}^3 s^{-3/2}\int_D |p_s(x,y)-1|\,\mathrm{d}\mathfrak{m}(x) \le 2C_{\mathrm{uc}}^3 s^{-3/2}.\end{aligned}$$

For $s\in(1,\infty)$ instead

$$\begin{aligned}[\![p_s(\,\cdot\,,y)]\!]_4^4 &\le C_{\mathrm{uc}}^2 s^{-1}[\![p_s(\,\cdot\,,y)]\!]_2^2 \\ &\le C_{\mathrm{uc}}^2 s^{-1}\|P_s^*(\delta_y-\mathfrak{m})\|_2^2 \le C_{\mathrm{uc}}^2 e^{-2C_{\mathrm{sg}}(s-1)}\|P_1^*(\delta_y-\mathfrak{m})\|_2^2.\end{aligned}$$

Putting these estimates together,

$$\int_t^\infty [\![p_s(\,\cdot\,,y)]\!]_4^2 \,\mathrm{d}s \le \sqrt{2}C_{\mathrm{uc}}^{3/2}\int_t^1 s^{-3/4}\,\mathrm{d}s + C_{\mathrm{uc}}\|P_1^*(\delta_y-\mathfrak{m})\|_2 \int_1^\infty e^{-C_{\mathrm{sg}}(s-1)}\,\mathrm{d}s,$$

which is bounded, uniformly in $y$ and $t$, because $\|P_1^*(\delta_y-\mathfrak{m})\|_2 \le 2\|P_1^*\|_{\mathcal{M}\to L^2}$. □

**Lemma 2.3.17** (Renormalized energy estimate and convergence, $d=2$)**.** *Assume that ultracontractivity holds with $d=2$. Let $f^{n,t}$ be the solution to (2.3.23). If $t=t(n)\to 0$ as $n\to\infty$ and $t\ge C/n$ for some $C>0$, then*

$$\limsup_{n\to\infty} \frac{1}{(\log t)^2}\,\mathbb{E}\left[\int_D |\nabla f^{n,t}|^4 \,\mathrm{d}\mathfrak{m}\right] < \infty. \tag{2.3.31}$$

*In particular*

$$\limsup_{n\to\infty} \frac{1}{|\log t|} \mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right] < \infty. \tag{2.3.32}$$

*Moreover, under the assumptions on $D$ of Proposition 2.3.14, one has*

$$\lim_{n\to\infty} \frac{1}{|\log t|} \mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right] = \frac{1}{4\pi}. \tag{2.3.33}$$

*Proof.* As in the proof of Lemma 2.3.16, we start from the representation formula (2.3.30), and we consider the cases $s \in (t,1)$, where we use ultracontractivity with $d = 2$ and $s \in (1,\infty)$. We obtain, for some geometric constant $C$,

$$\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right] \le C\left(\int_t^1 s^{-1}\,\mathrm{d}s + \int_1^\infty e^{-2C_{\mathrm{sg}} s}\,\mathrm{d}s\right) \le C(|\log t| + 1),$$

from which (2.3.32) readily follows. To prove (2.3.33), we notice that the same argument actually gives that

$$\frac{1}{|\log t|}\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right] - \frac{2}{|\log t|}\int_t^1 \left(\int_D p_{2s}(x,x)\,\mathrm{d}\mathfrak{m}(x) - 1\right)\mathrm{d}s$$

is infinitesimal as $n \to \infty$. Combining this information with (2.3.25) of Proposition 2.3.14, we obtain (2.3.33).

To deal with (2.3.31), we introduce the Paley-Littlewood function

$$S(g) = \left(\int_0^\infty (s\partial_s P_s g)^2 \frac{\mathrm{d}s}{s}\right)^{1/2}.$$

Using the Riesz transform bound and the fundamental theorem [Ste70] $\|g\|_p^p \le c_p \|S(g)\|_p^p$ for any $p \in (1,\infty)$ and $g$ with $\int_D g\,\mathrm{d}\mathfrak{m} = 0$, we obtain

$$\begin{aligned}\int_D |\nabla f^{n,t}|^4 \,\mathrm{d}\mathfrak{m} &\le C_{\mathrm{rt}} \int_D \left|(-\Delta)^{1/2} f^{n,t}\right|^4 \mathrm{d}\mathfrak{m} \le C_{\mathrm{rt}} c_4 \int_D S\left((-\Delta)^{1/2} f^{n,t}\right)^4 \mathrm{d}\mathfrak{m} \\ &= C_{\mathrm{rt}} c_4 \int_0^\infty\int_0^\infty\int_D s\left(\partial_s P_s (-\Delta)^{1/2} f^{n,t}\right)^2 s'\left(\partial_{s'} P_{s'}(-\Delta)^{1/2} f^{n,t}\right)^2 \mathrm{d}\mathfrak{m}\,\mathrm{d}s\,\mathrm{d}s'.\end{aligned}$$

Using the fact that $\partial_t P_t = \Delta P_t$ and that the operators $\Delta$, $P_t$ and $(-\Delta)^{1/2}$ commute we have

$$\partial_\tau P_\tau (-\Delta)^{1/2} f^{n,t} = (-\Delta)^{1/2} P^*_{\tau+t} r^n,$$

so that

$$\int_D |\nabla f^{n,t}|^4 \,\mathrm{d}\mathfrak{m} \le C_{\mathrm{rt}} c_4 \int_0^\infty\int_0^\infty\int_D \left((-s\Delta)^{1/2} P^*_{s+t} r^n\right)^2 \left((-s'\Delta)^{1/2} P^*_{s'+t} r^n\right)^2 \mathrm{d}\mathfrak{m}\,\mathrm{d}s\,\mathrm{d}s'.$$

Consider the operator $T_s^t : L^2(\mathfrak{m}) \to L^2(\mathfrak{m})$, represented by the kernel $K_s^t$,

$$(T_s^t \mu)(y) = \left((-s\Delta)^{1/2} P^*_{s+t}\mu\right)(y) = \int_D K_s^t(x,y)\,\mathrm{d}\mu(x)$$

and notice that

$$\int_D K_s^t(x,y)\,\mathrm{d}\mathfrak{m}(x) = T_s^t\mathfrak{m}(y) = 0.$$

In addition, since $T_s^t$ is self-adjoint, the kernel $K_s^t$ is symmetric and

$$T_s^t\delta_x(y) = K_s^t(x,y) = K_s^t(y,x). \tag{2.3.34}$$

Taking the expectation of the integrand,

$$\begin{aligned}
\mathbb{E}\Big[\big((-s\Delta)^{1/2}P^*_{s+t}r^n\big)^2(y)\big((-s'\Delta)^{1/2}P^*_{s'+t}r^n\big)^2(y)\Big] &= \mathbb{E}\left[(T_s^t r^n)^2(y)(T_{s'}^t r^n)^2(y)\right] \\
&= \mathbb{E}\left[\left(\int_D K_s^t(x,y)\,\mathrm{d}r^n(x)\right)^2\left(\int_D K_{s'}^t(x',y)\,\mathrm{d}r^n(x')\right)^2\right] \\
&\leq 3\frac{n-1}{n}[\![K_s^t(\,\cdot\,,y)]\!]_2^2[\![K_{s'}^t(\,\cdot\,,y)]\!]_2^2 + \frac{1}{n}[\![K_s^t(\,\cdot\,,y)]\!]_4^2[\![K_{s'}^t(\,\cdot\,,y)]\!]_4^2.
\end{aligned}$$

Integrating in $s$ and $s'$ we obtain

$$\begin{aligned}
&\int_0^\infty\int_0^\infty \mathbb{E}\Big[\big((-s\Delta)^{1/2}P^*_{s+t}r^n\big)^2(y)\,\big((-s'\Delta)^{1/2}P^*_{s'+t}r^n\big)^2(y)\Big]\,\mathrm{d}s\,\mathrm{d}s' \\
&\qquad\leq 3\frac{n-1}{n}\left(\int_0^\infty [\![K_s^t(\,\cdot\,,y)]\!]_2^2\,\mathrm{d}s\right)^2 + \frac{1}{n}\left(\int_0^\infty [\![K_{s'}^t(\,\cdot\,,y)]\!]_4^2\,\mathrm{d}s'\right)^2.
\end{aligned}$$

Since $(P_t)_{t\geq 0}$ is a bounded analytic semigroup, complex interpolation yields that, for $p\in(1,\infty)$, $(-\tau\Delta)^{1/2}P_{\tau/2} : L^p \to L^p$ is continuous with norms uniformly bounded for $\tau \geq 0$ [Yos80, Sections X.10–11], hence we have the estimate

$$\begin{aligned}
[\![K_s^t(\,\cdot\,,y)]\!]_p = [\![T_s^t\delta_y]\!]_p = \|T_s^t\delta_y\|_p &= \|T_s^t(\delta_y - \mathfrak{m})\|_p \\
&= \left\|(-s\Delta)^{1/2}P_{s/2}P^*_{s/2+t}(\delta_y-\mathfrak{m})\right\|_p \\
&\leq C_p\|P^*_{s/2+t}(\delta_y-\mathfrak{m})\|_p,
\end{aligned}$$

where in the first equality we used (2.3.34). We consider

$$\int_0^\infty [\![K_s^t(\,\cdot\,,y)]\!]_p^2\,\mathrm{d}s \leq C_p^2\int_0^\infty \|P^*_{s/2+t}(\delta_y-\mathfrak{m})\|_p^2\,\mathrm{d}s = 2C_p^2\int_t^\infty \|P^*_s(\delta_y-\mathfrak{m})\|_p^2\,\mathrm{d}s.$$

Now we split the integrals for $s\in(t,2)$ and $s\in(2,\infty)$. In the former interval we use the estimate

$$\begin{aligned}
\|P^*_s(\delta_y-\mathfrak{m})\|_p &= \left(\int_D |p_s(x,y)-1|^p\,\mathrm{d}\mathfrak{m}(x)\right)^{1/p} \\
&\leq \left(\int_D \big(C_{\mathrm{uc}}s^{-1}\big)^{p-1}|p_s(x,y)-1|\,\mathrm{d}\mathfrak{m}(x)\right)^{1/p} \\
&\leq 2^{1/p}C_{\mathrm{uc}}^{(p-1)/p}s^{-(p-1)/p}.
\end{aligned}$$

In the latter interval we use the estimate

$$\begin{aligned}\|P_s^*(\delta_y - \mathfrak{m})\|_p &= \|P_1 P_{(s-2)} P_1^*(\delta_y - \mathfrak{m})\|_p \\ &\le \|P_1\|_{L^2\to L^p} e^{-C_{\rm sg}(s-2)} \|P_1^*(\delta_y - \mathfrak{m})\|_2 \\ &\le \|P_1\|_{L^2\to L^p} \|P_1^*\|_{\mathcal{M}\to L^2} e^{-C_{\rm sg}(s-2)} \|\delta_y - \mathfrak{m}\|_{\mathcal{M}} \\ &\le 2e^{2C_{\rm sg}} \|P_1\|_{L^2\to L^p} \|P_1^*\|_{\mathcal{M}\to L^2} e^{-C_{\rm sg} s}.\end{aligned}$$

Putting these estimates together, in the case $p = 2$ we have

$$\int_t^\infty \|P_s^*(\delta_y - \mathfrak{m})\|_2^2 \,\mathrm{d}s \le C\left(\int_t^2 s^{-1}\,\mathrm{d}s + \int_2^\infty e^{-2C_{\rm sg}s}\,\mathrm{d}s\right) \le C(|\log t| + 1)$$

for some geometric constant $C$. In the case $p = 4$ we have also

$$\int_t^\infty \|P_s^*(\delta_y - \mathfrak{m})\|_4^2 \,\mathrm{d}s \le C\left(\int_t^2 s^{-3/2}\,\mathrm{d}s + \int_2^\infty e^{-2C_{\rm sg}s}\,\mathrm{d}s\right) \le C\left(\frac{1}{\sqrt{t}} + 1\right).$$

This yields

$$\begin{aligned}3\frac{n-1}{n}\left(\int_0^\infty [\![K_s^t(\,\cdot\,,y)]\!]_2^2 \,\mathrm{d}s\right)^2 + \frac{1}{n}\left(\int_0^\infty [\![K_s^t(\,\cdot\,,y)]\!]_4^2 \,\mathrm{d}s\right)^2 \\ \le C\frac{n-1}{n}(\log t)^2 + \frac{C}{n}\left(\frac{1}{t} + 1\right).\end{aligned}$$

In conclusion

$$\begin{aligned}\mathbb{E}\left[\int_D |\nabla f^{n,t}|^4 \,\mathrm{d}\mathfrak{m}\right] \frac{1}{(\log t)^2} &\le \frac{C}{(\log t)^2}\int_D \left(\frac{n-1}{n}(\log t)^2 + \frac{1}{nt} + \frac{1}{n}\right)\mathrm{d}\mathfrak{m}(y) \\ &\le C\left[1 + \frac{1}{(\log t)^2 nt} + \frac{1}{(\log t)^2 n}\right]\end{aligned}$$

is uniformly bounded as $n \to \infty$ by the assumptions on $t = t(n)$. □

## 2.4 Proof of the main result

In this section we prove Theorem 2.1.1. In the proof of the upper bound we need only to assume the regularizing properties of $P_t$ listed in Section 2.3; in particular this inequality covers also the case $D = [0,1]^2$ and compact 2-dimensional Riemannian manifolds with smooth boundary. In the proof of the lower bound we need also to assume that $D$ has no boundary; by a comparison argument, since the distance in $\mathbb{T}^2$ is smaller than the distance in $[0,1]^2$, we recover also the lower bound for $D = [0,1]^2$.

We include also the 1-dimensional case (whose proofs are a bit simpler), which covers the case of the interval and the case of the circle. For brevity we state the result only in the Riemannian case, but the strength of this method relies in the fact that it can be extended to more general 1-dimensional spaces (see also Section 2.6).

**Theorem 2.4.1.** *Assume that either $D = [0,1]$ or $D = \mathbb{T}^1$ and let $\mathfrak{m}$ be the length measure. Then*

$$\lim_{n\to\infty} n\,\mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] = -\sum_{\lambda\in\sigma(\Delta)\setminus\{0\}} \frac{1}{\lambda}.$$

*In particular, from Euler's formula $\pi^2 = 6\sum_{k\geq 1} k^{-2}$, the limit equals $1/6$ for $D = [0,1]$ and $1/12$ for $D = \mathbb{T}^1$.*

*Remark* 2.4.2. In the case $D = [0,1]$ and $\mathfrak{m} = \mathscr{L}^1 \llcorner D$ we can explicitly compute $n\,\mathbb{E}[W_2^2(\mu^n, \mathfrak{m})]$ and $n\,\mathbb{E}[W_2^2(\mu^n, \nu^n)]$ as follows (and in particular, the former is identically equal to $1/6$). For any fixed $n \in \mathbb{N}$, let $X_{(k)}$ and $Y_{(k)}$ denote the order statistics of the random variables $(X_i)_{i=1}^n$ and $(Y_i)_{i=1}^n$. It is well known that $X_{(k)}$ and $Y_{(k)}$ are distributed according to the beta distribution $X_{(k)} \sim Y_{(k)} \sim B(k, n+1-k)$.

The optimal map is given by the monotone rearrangement of the mass, therefore

$$\begin{aligned}
\mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] &= \mathbb{E}\left[\sum_{k=1}^n \int_{(k-1)/n}^{k/n} (X_{(k)} - t)^2\,\mathrm{d}t\right] = \sum_{k=1}^n \int_{(k-1)/n}^{k/n} \mathbb{E}[(X_{(k)} - t)^2]\,\mathrm{d}t \\
&= \sum_{k=1}^n \int_{(k-1)/n}^{k/n} \left(\mathrm{Var}(X_{(k)}) + (\mathbb{E}[X_{(k)}] - t)^2\right)\mathrm{d}t \\
&= \sum_{k=1}^n \int_{(k-1)/n}^{k/n} \left[\frac{(k+1)k}{(n+2)(n+1)} - 2t\frac{k}{n+1} + t^2\right]\mathrm{d}t \\
&= \sum_{k=1}^n \left[\frac{(k+1)k}{(n+2)(n+1)n} - \frac{(2k-1)k}{(n+1)n^2} + \frac{3k^2-3k+1}{3n^3}\right] = \frac{1}{6n}.
\end{aligned}$$

Similarly, in the bipartite case we have

$$\begin{aligned}
\mathbb{E}\left[W_2^2(\mu^n, \nu^n)\right] &= \mathbb{E}\left[\frac{1}{n}\sum_{k=1}^n (X_{(k)} - Y_{(k)})^2\right] = \frac{2}{n}\sum_{k=1}^n \left(\mathbb{E}[X_{(k)}^2] - \mathbb{E}[X_{(k)}]^2\right) \\
&= \frac{2}{n}\sum_{k=1}^n \mathrm{Var}(X_{(k)}) = \frac{2}{n}\sum_{k=1}^n \frac{k(n+1-k)}{(n+1)^2(n+2)} = \frac{1}{3(n+1)}.
\end{aligned}$$

## 2.4.1 Upper bound

**Theorem 2.4.3** (Upper bound, $d = 1$)**.** *Assume that ultracontractivity holds with $d = 1$. Then*

$$\limsup_{n\to\infty} n\,\mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] \leq -\sum_{\lambda\in\sigma(\Delta)\setminus\{0\}} \frac{1}{\lambda}.$$

*Proof.* Fix $q \in (1/2, 1)$, $\eta \in (0,1)$ and let $t = t(n) = \eta^{-1} n^{-2q}$. Consider the event

$$A_\eta = A_{\eta,n} = \left\{\sup_{y\in D} \frac{|r^{n,t}(y)|}{\sqrt{n}} \leq \eta\right\}.$$

By Proposition 2.3.10, since $W_2^2(\mu^n, \mathfrak{m}) \le (\operatorname{diam} D)^2$, for $n$ large enough we have

$$\begin{aligned} n\,\mathbb{E}\left[W_2^2(\mu^n,\mathfrak{m})\right] &= n\,\mathbb{E}\left[W_2^2(\mu^n,\mathfrak{m})\chi_{A_\eta}\right] + n\,\mathbb{E}\left[W_2^2(\mu^n,\mathfrak{m})\chi_{A_\eta^c}\right] \\ &\le n\,\mathbb{E}\left[W_2^2(\mu^n,\mathfrak{m})\chi_{A_\eta}\right] + C(\operatorname{diam} D)^2 n \exp\left(-\gamma n^{1-q}\right) \end{aligned}$$

with $C = C(C_D, C_{\mathrm{ge}})$ and $\gamma = \gamma(\eta, C_{\mathrm{uc}}) > 0$.

Using the Young inequality for products with $\alpha > 0$ and $W_2^2(\mu^n, \mu^{n,t}) \le C_{\mathrm{dr}} t$ we have

$$\begin{aligned} W_2^2(\mu^n,\mathfrak{m}) &\le \left(W_2(\mu^{n,t},\mathfrak{m}) + W_2(\mu^n,\mu^{n,t})\right)^2 \\ &\le (1+\alpha)W_2^2(\mu^{n,t},\mathfrak{m}) + (1+\alpha^{-1})W_2^2(\mu^n,\mu^{n,t}) \\ &\le (1+\alpha)W_2^2(\mu^{n,t},\mathfrak{m}) + (1+\alpha^{-1})C_{\mathrm{dr}} t. \end{aligned}$$

Therefore, since $nt \to 0$, it is sufficient to estimate

$$\limsup_{n\to\infty} n\,\mathbb{E}\left[W_2^2(\mu^{n,t},\mathfrak{m})\chi_{A_\eta}\right].$$

To this end, we apply Proposition 2.2.3 with $u_0 = u^{n,t}$ and $u_1 = 1$. Since $f^{n,t}$ solves (2.3.23) from Proposition 2.2.3 we get

$$W_2^2(\mu^{n,t},\mathfrak{m}) \le \frac{1}{n}\int_D \frac{|\nabla f^{n,t}|^2}{M(u^{n,t},1)}\,\mathrm{d}\mathfrak{m}.$$

In the event $A_\eta$ we have $u^{n,t} \ge 1-\eta$ in $D$, hence the first inequality in (2.3.22) gives

$$\frac{1}{M(u^{n,t},1)} \le \frac{1}{\sqrt{u^{n,t}}} \le \frac{1}{\sqrt{1-\eta}}.$$

The previous two inequalities and Lemma 2.3.16 give

$$\begin{aligned} \limsup_{n\to\infty} n\,\mathbb{E}\left[W_2^2(\mu^{n,t},\mathfrak{m})\chi_{A_\eta}\right] &\le \lim_{n\to\infty} \frac{1}{\sqrt{1-\eta}}\,\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2\,\mathrm{d}\mathfrak{m}\right] \\ &= -\frac{1}{\sqrt{1-\eta}} \sum_{\lambda\in\sigma(\Delta)\setminus\{0\}} \frac{1}{\lambda}. \end{aligned}$$

In conclusion we have

$$\limsup_{n\to\infty} n\,\mathbb{E}\left[W_2^2(\mu^n,\mathfrak{m})\right] \le -\frac{1+\alpha}{\sqrt{1-\eta}} \sum_{\lambda\in\sigma(\Delta)\setminus\{0\}} \frac{1}{\lambda}$$

and we obtain the thesis by letting first $\alpha \to 0$ and then $\eta \to 0$. □

**Theorem 2.4.4** (Upper bound, $d = 2$)**.** *Assume that $D$ is as in Proposition 2.3.14 and that ultracontractivity holds with $d = 2$. Then*

$$\limsup_{n\to\infty} \frac{n}{\log n}\,\mathbb{E}\left[W_2^2(\mu^n,\mathfrak{m})\right] \le \frac{1}{4\pi}.$$

*Proof.* Fix $\gamma > 0$ and let $t(n) = c(n) = \gamma n^{-1} \log n$. Let us set

$$\mu^{n,t,c} = (1-c)\mu^{n,t} + c\mathfrak{m}, \qquad u^{n,t,c} = (1-c)u^{n,t} + c$$

as in Lemma 2.3.13. From the joint convexity of $W_2^2$ (see (2.2.4)) we immediately get

$$W_2^2(\mu^{n,t}, \mu^{n,t,c}) \le (\operatorname{diam} D)^2 c$$

Using the Young inequality for products with $\alpha > 0$ and $W_2^2(\mu^n, \mu^{n,t}) \le C_{\mathrm{dr}} t$, we have

$$\begin{aligned} W_2^2(\mu^n, \mathfrak{m}) &\le \big(W_2(\mu^{n,t,c}, \mathfrak{m}) + W_2(\mu^n, \mu^{n,t}) + W_2(\mu^{n,t}, \mu^{n,t,c})\big)^2 \\ &\le (1+\alpha) W_2^2(\mu^{n,t,c}, \mathfrak{m}) + 2(1+\alpha^{-1})\big[W_2^2(\mu^n, \mu^{n,t}) + W_2^2(\mu^{n,t}, \mu^{n,t,c})\big] \\ &\le (1+\alpha) W_2^2(\mu^{n,t,c}, \mathfrak{m}) + 2(1+\alpha^{-1})[C_{\mathrm{dr}} t + (\operatorname{diam} D)^2 c]. \end{aligned}$$

We start by estimating the contribution of the first term.

To this end we apply Proposition 2.2.3 with $u_0 = u^{n,t,c}$ and $u_1 = 1$. Recalling that $f^{n,t}$ solves the PDE $\Delta f^{n,t} = \sqrt{n}(u^{n,t} - 1)$ with homogeneous Neumann boundary conditions, we get

$$\Delta\left(\frac{1-c}{\sqrt{n}} f^{n,t}\right) = u^{n,t,c} - 1,$$

hence Proposition 2.2.3 gives

$$W_2^2(\mu^{n,t,c}, \mathfrak{m}) \le \frac{(1-c)^2}{n} \int_D \frac{|\nabla f^{n,t}|^2}{M(u^{n,t,c}, 1)} \, d\mathfrak{m} \le \frac{1}{n} \int_D \frac{|\nabla f^{n,t}|^2}{M(u^{n,t,c}, 1)} \, d\mathfrak{m}. \tag{2.4.1}$$

Adding and subtracting $|\nabla f^{n,t}|^2$ to the integrand we obtain

$$\begin{aligned} &\mathbb{E}\left[\int_D \frac{|\nabla f^{n,t}|^2}{M(u^{n,t,c}, 1)} \, d\mathfrak{m}\right] \\ &\qquad = \mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \, d\mathfrak{m}\right] + \mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \left(M(u^{n,t,c}, 1)^{-1} - 1\right) d\mathfrak{m}\right]. \end{aligned}$$

We deal with the two addends separately. For the former, since the function $f^{n,t}$ solves (2.3.23), $t \ge C/n$ and $|\log t| / \log n \to 1$ as $n \to \infty$, Lemma 2.3.17 gives

$$\lim_{n\to\infty} \frac{1}{\log n} \mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \, d\mathfrak{m}\right] = \frac{1}{4\pi}.$$

For the latter, by Cauchy-Schwarz inequality we have

$$\begin{aligned} &\limsup_{n\to\infty} \frac{1}{\log n} \mathbb{E}\Big[\int_D |\nabla f^{n,t}|^2 \big(M(u^{n,t,c}, 1)^{-1} - 1\big) \, d\mathfrak{m}\Big] \\ &\qquad \le \left(\limsup_{n\to\infty} \frac{1}{\log n} \mathbb{E}\left[\int_D |\nabla f^{n,t}|^4 \, d\mathfrak{m}\right]^{1/2}\right) \\ &\qquad\qquad \cdot \left(\lim_{n\to\infty} \mathbb{E}\left[\int_D \left(M(u^{n,t,c}, 1)^{-1} - 1\right)^2 d\mathfrak{m}\right]^{1/2}\right) \end{aligned}$$

which converges to 0 by Lemma 2.3.17 and Lemma 2.3.13.

Recalling (2.4.1), we deduce

$$\limsup_{n\to\infty} \frac{n}{\log n} \mathbb{E}[W_2^2(\mu^{n,t,c}, \mathfrak{m})] \le \frac{1}{4\pi}.$$

In conclusion

$$\limsup_{n\to\infty} \frac{n}{\log n} \mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] \le \frac{(1+\alpha)}{4\pi} + 2(1+\alpha^{-1})[C_{\mathrm{dr}} + (\operatorname{diam} D)^2]\gamma$$

and the thesis follows letting first $\gamma \to 0$ and then $\alpha \to 0$. □

## 2.4.2 Lower bound

**Theorem 2.4.5** (Lower bound, $d = 1$)**.** *Assume that ultracontractivity holds with $d = 1$ and that $N_D(\delta) \le \max\{1, C_D\delta^{-1}\}$ for every $\delta > 0$. Then*

$$\liminf_{n\to\infty} n\,\mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] \ge - \sum_{\lambda\in\sigma(\Delta)\setminus\{0\}} \frac{1}{\lambda}.$$

*Proof.* Fix $q \in (0,1)$, $\eta \in (0,1)$ and let $t = t(n) = \eta^{-1}n^{-2q}$. By Proposition 2.3.10 the complement of the event

$$A_\eta = A_{\eta,n} = \left\{\sup_{y\in D} \frac{|r^{n,t}(y)|}{\sqrt{n}} \le \eta\right\} \tag{2.4.2}$$

has infinitesimal probability as $n \to \infty$. By the contractivity assumption we have

$$W_2^2(\mu^n, \mathfrak{m}) \ge e^{2Kt} W_2^2(\mu^{n,t}, \mathfrak{m}).$$

Therefore it is sufficient to estimate $\liminf_{n\to\infty} n\,\mathbb{E}[W_2^2(\mu^{n,t}, \mathfrak{m})\chi_{A_\eta}]$ from below. By duality,

$$\begin{aligned}\frac{1}{2}W_2^2(\mu^{n,t}, \mathfrak{m}) &\ge \sup\left\{\int_D f\,\mathrm{d}\mu^{n,t} + \int_D g\,\mathrm{d}\mathfrak{m} \;\middle|\; f(x) + g(y) \le \frac{\mathsf{d}(x,y)^2}{2}\right\}\\ &= \sup\left\{\int_D f\frac{\mathrm{d}r^{n,t}}{\sqrt{n}} + \int_D (f+g)\,\mathrm{d}\mathfrak{m} \;\middle|\; f(x) + g(y) \le \frac{\mathsf{d}(x,y)^2}{2}\right\}.\end{aligned} \tag{2.4.3}$$

Let $f^{n,t}$ be the solution to (2.3.23) and define $f = -f^{n,t}/\sqrt{n}$, so that $\|\Delta f\|_\infty \le \eta$ in the event $A_\eta$, and we can estimate thanks to (2.3.3)

$$\|(\Delta f)^+\|_\infty + \frac{e^{2K^+t} - 1}{2}\|\nabla f\|_\infty^2 \le \omega(\eta) \tag{2.4.4}$$

with $\omega(\eta) \to 0$ as $\eta \to 0$. To this function $f$ we associate the potential $g$ given by Corollary 2.3.3, hence we get (still in the event $A_\eta$)

$$\begin{aligned}\frac{1}{2} W_2^2(\mu^{n,t}, \mathfrak{m}) &\geq \int_D (f+g) \, \mathrm{d}\mathfrak{m} + \int_D f \frac{\mathrm{d}r^{n,t}}{\sqrt{n}} \\ &\geq -e^{\omega(\eta)} \int_D \frac{|\nabla f|^2}{2} \, \mathrm{d}\mathfrak{m} - \int_D f \Delta f \, \mathrm{d}\mathfrak{m} \\ &= \left(1 - \frac{e^{\omega(\eta)}}{2}\right) \frac{1}{n} \int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}.\end{aligned}$$

Thus, by Lemma 2.3.16,

$$\begin{aligned}\frac{1}{2 - e^{\omega(\eta)}} \liminf_{n\to\infty} n \, \mathbb{E}\left[W_2^2(\mu^{n,t}, \mathfrak{m}) \chi_{A_\eta}\right] &\geq \liminf_{n\to\infty} \mathbb{E}\left[\chi_{A_\eta} \int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}\right] \\ &\geq \lim_{n\to\infty} \mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}\right] - \limsup_{n\to\infty} \mathbb{E}\left[\chi_{A_\eta^c} \int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}\right] \\ &= - \sum_{\lambda \in \sigma(\Delta)\setminus\{0\}} \frac{1}{\lambda}\end{aligned}$$

because

$$\begin{aligned}&\limsup_{n\to\infty} \mathbb{E}\left[\chi_{A_\eta^c} \int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}\right] \\ &\qquad \leq \limsup_{n\to\infty} \mathbb{P}(A_{\eta,n}^c)^{1/2} \left(\mathbb{E}\left[\left(\int_D |\nabla f^{n,t}|^2 \, \mathrm{d}\mathfrak{m}\right)^2\right]\right)^{1/2} = 0\end{aligned}$$

by Hölder inequality and (2.3.29). The thesis follows letting $\eta \to 0$. □

**Theorem 2.4.6** (Lower bound, $d=2$)**.** *Assume that ultracontractivity holds with $d = 2$ and that $N_D(\delta) \leq C\delta^{-2}$ for every $\delta > 0$. Then*

$$\liminf_{n\to\infty} \mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] \frac{n}{\log n} \geq \frac{1}{4\pi}.$$

*Proof.* By Proposition 2.3.11, for any $\eta \in (0,1)$ there is $\gamma > 0$ such that, if we let $t = t(n) = \gamma n^{-1} \log n$, the event $A_\eta$ in (2.4.2) satisfies $\mathbb{P}(A_\eta^c) \leq C/n$, for $n$ large enough and some $C > 0$ independent of $n$. As in the previous proof, thanks to contractivity it is sufficient to estimate from below

$$\liminf_{n\to\infty} \frac{n}{\log n} \mathbb{E}\left[W_2^2(\mu^{n,t}, \mathfrak{m}) \chi_{A_\eta}\right].$$

Let $f^{n,t}$ be the solution to (2.3.23) and define $f = -f^{n,t}/\sqrt{n}$, so that $\|\Delta f\|_\infty \leq \eta$ in the event $A_\eta$. To this function $f$ we associate the potential $g$ given by

Corollary 2.3.3, hence thanks to the duality formula (2.4.3) we can estimate, in the event $A_\eta$,

$$\begin{aligned}\frac{1}{2}W_2^2(\mu^{n,t},\mathfrak{m}) &\geq \int_D (f+g)\,\mathrm{d}\mathfrak{m} + \int_D f\frac{\mathrm{d}r^{n,t}}{\sqrt{n}} \\ &\geq -e^{\omega(\eta)}\int_D \frac{|\nabla f|^2}{2}\,\mathrm{d}\mathfrak{m} - \int_D f\Delta f\,\mathrm{d}\mathfrak{m} \\ &= \left(1-\frac{e^{\omega(\eta)}}{2}\right)\frac{1}{n}\int_D |\nabla f^{n,t}|^2\,\mathrm{d}\mathfrak{m}\end{aligned}$$

with $\omega(\eta)$ as in (2.4.4). Since $t \geq C/n$ for some positive constant $C$ and $|\log t|/\log n \to 1$, from Lemma 2.3.17 we get

$$\begin{aligned}\frac{1}{2-e^{\omega(\eta)}}\liminf_{n\to\infty}\frac{n}{\log n}\,\mathbb{E}\left[W_2^2(\mu^{n,t},\mathfrak{m})\chi_{A_\eta}\right] &\geq \liminf_{n\to\infty}\mathbb{E}\left[\chi_{A_\eta}\int_D |\nabla f^{n,t}|^2\,\mathrm{d}\mathfrak{m}\right]\frac{1}{\log n} \\ \geq \lim_{n\to\infty}\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2\,\mathrm{d}\mathfrak{m}\right]\frac{1}{\log n} &- \limsup_{n\to\infty}\mathbb{E}\left[\chi_{A_\eta^c}\int_D |\nabla f^{n,t}|^2\,\mathrm{d}\mathfrak{m}\right]\frac{1}{\log n} \\ = \frac{1}{4\pi}&\end{aligned}$$

because

$$\begin{aligned}\limsup_{n\to\infty}\mathbb{E}\left[\chi_{A_\eta^c}\int_D |\nabla f^{n,t}|^2\,\mathrm{d}\mathfrak{m}\right]\frac{1}{\log n} &\leq \\ \leq \limsup_{n\to\infty}\mathbb{P}(A_\eta^c)^{1/2}&\left(\mathbb{E}\left[\int_D |\nabla f^{n,t}|^4\,\mathrm{d}\mathfrak{m}\right]\frac{1}{(\log n)^2}\right)^{1/2} = 0\end{aligned}$$

by Hölder inequality and (2.3.31). In conclusion we have

$$\liminf_{n\to\infty}\frac{n}{\log n}\,\mathbb{E}\left[W_2^2(\mu^n,\mathfrak{m})\right] \geq \frac{1}{4\pi}$$

and the thesis follows letting $\eta \to 0$. □

*Remark* 2.4.7. In this remark we sketch the proof of the concentration property (2.1.5); see also [Led01; BL16] for more details and references. Notice also that the concentration property, when written in terms of deviation from the expectation, holds independently of the convergence of the renormalized expectations as $n \to \infty$.

It is well-known since the seminal paper [GM83] that the spectral gap assumption is stable under tensorization and implies exponential concentration, more precisely

$$\alpha_{\mathfrak{m}^n}(r) \leq Ce^{-2\sqrt{C_{\mathrm{sg}}}r},$$

with $C$ numerical constant. Here $\alpha_{\mathfrak{m}^n}$ is the supremum of $1-\mathfrak{m}^n(A^r)$ among all Borel sets $A$ with $\mathfrak{m}^n(A) \geq 1/2$, where $A^r$ is the open $r$ neighbourhood of $A$. Now, the basic observation is that the mapping $L_n$ associating to $(x_1, \ldots, x_n) \in D^n$ the empirical measure is $n^{-1/2}$-Lipschitz, if in the target space $\mathscr{P}(D)$ we use the distance $W_2$. By looking at the inclusion $L_n^{-1}(A^r) \supset \big(L_n^{-1}(A)\big)^{rn^{1/2}}$ between enlargements, this gives that the concentration function $\alpha_{Q^n}$ of $(L_n)_\# \mathfrak{m}^n$ satisfies

$$\alpha_{Q^n}(r) \le Ce^{-2\sqrt{C_{\mathrm{sg}}nr}}.$$

By standard arguments (passing through the deviation from the median), this exponential concentration leads to the inequality

$$Q^n\big(\{\nu : |G(\nu) - \mathbb{E}[G]| > r\}\big) \le C' e^{-2\sqrt{C_{\mathrm{sg}}nr}}.$$

for some new numerical constant $C'$, for any 1-Lipschitz function $G : \mathscr{P}(D) \to \mathbb{R}$. Using $G(\nu) = W_2(\nu, \mathfrak{m})$ and Cavalieri's formula we then get that $Z_n = W_2(\mu^n, \mathfrak{m})$ satisfy

$$\mathbb{E}\big[|Z_n - \mathbb{E}[Z_n]|^2\big] \le \frac{C'}{2C_{\mathrm{sg}}n} \int_0^\infty se^{-s}\,\mathrm{d}s,$$

so that

$$\mathbb{E}\left[\left|\sqrt{\frac{n}{\log n}}Z_n - \sqrt{\frac{n}{\log n}}\,\mathbb{E}[Z_n]\right|^2\right] \le \frac{C'}{2C_{\mathrm{sg}}\log n} \int_0^\infty se^{-s}\,\mathrm{d}s \tag{2.4.5}$$

and, in particular $n(\log n)^{-1}(\mathbb{E}[Z_n^2] - \mathbb{E}[Z_n]^2) \to 0$. Since $n(\log n)^{-1}\,\mathbb{E}[Z_n^2] \to (4\pi)^{-1}$ we obtain that $n(\log n)^{-1}\,\mathbb{E}[Z_n]^2 \to (4\pi)^{-1}$, hence (2.4.5) gives

$$\lim_{n\to\infty} \mathbb{E}\left[\left|\sqrt{\frac{n}{\log n}}Z_n - \frac{1}{\sqrt{4\pi}}\right|^2\right] = 0,$$

which immediately gives (2.1.5).

Under the stronger assumption that $\mathfrak{m}$ satisfies the dimension-free Gaussian concentration property, namely

$$\alpha_{\mathfrak{m}^n}(r) \le Ce^{-cr^2}$$

with $c$, $C > 0$, the concentration estimate (2.4.5) can be improved to $O((\log n)^{-2})$. The dimension-free Gaussian concentration property is implied by the logarithmic Sobolev inequality, and the latter holds for compact Riemannian manifolds without boundary and with a positive lower bound on Ricci curvature (see for instance [Led01]), as the 2-dimensional sphere.

### 2.4.3 The bipartite case

We prove now the bipartite part of Theorem 2.1.1. It will be convenient to introduce a notation $(\Omega, \mathbb{P})$ for the underlying probability space.

**Lemma 2.4.8.** *Let $D \subset \mathbb{R}^d$ be a compact set and assume that $\mathfrak{m} \in \mathscr{P}(D)$ is absolutely continuous w.r.t. the Lebesgue measure. The $L^2(D, \mathfrak{m}; D)$-valued maps*

$$\Omega \ni \omega \mapsto T^{\mu^n(\omega)}, \quad \Omega \ni \omega \mapsto T^{\nu^n(\omega)}$$

*providing the optimal maps from $\mathfrak{m}$ to $\mu^n(\omega)$ and $\nu^n(\omega)$ are measurable and independent.*

*Proof.* The independence of $(X_i, Y_i)$ easily implies that the two measure-valued random variables $\mu^n(\omega)$, $\nu^n(\omega)$ are measurable and independent, where in $\mathscr{P}(D)$ we consider the Borel $\sigma$-algebra induced by the topology of weak convergence in duality with $C(D)$. Now, recalling Proposition 2.2.1, since independence is stable under composition with continuous functions the statement follows. □

**Proposition 2.4.9.** *Let $D \subset \mathbb{R}^d$ be a bounded domain. For all $n \geq 1$ one has*

$$\mathbb{E}\left[W_2^2(\mu^n, \nu^n)\right] \leq 2\,\mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] - 2\int_D \left|\mathbb{E}\left[T^{\mu^n}(x) - x\right]\right|^2 \mathrm{d}\mathfrak{m}(x). \tag{2.4.6}$$

*Proof.* If $S, T : \Omega \to L^2(D, \mathfrak{m}; \mathbb{R}^d)$ are independent, one has the identity

$$\mathbb{E}\left[\int_D \langle S^\omega(x), T^\omega(x)\rangle \,\mathrm{d}\mathfrak{m}(x)\right] = \int_D \langle \mathbb{E}\left[S^\omega(x)\right], \mathbb{E}\left[T^\omega(x)\right]\rangle \,\mathrm{d}\mathfrak{m}(x). \tag{2.4.7}$$

We sketch the argument of the proof: if $S = \lambda e$, $T = \lambda' e'$, with $\lambda, \lambda' : \Omega \to \mathbb{R}^d$ and $e, e'$ orthogonal unit vectors of $L^2(D, \mathfrak{m})$, then $\lambda$ and $\lambda'$ are independent and (2.4.7) reduces to $\mathbb{E}[\langle\lambda, \lambda'\rangle] = \langle \mathbb{E}[\lambda], \mathbb{E}[\lambda']\rangle$. By bilinearity, (2.4.7) still holds if $S$ and $T$ take their values in the vector space generated on $\mathbb{R}^d$ by a finite orthonormal set $\{e_1, \ldots, e_k\}$ of $L^2(D, \mathfrak{m})$. By a standard projection argument, and by approximation, we recover the general result.

For all $\omega \in \Omega$ the plan $(T^{\mu^n(\omega)}, T^{\nu^n(\omega)})_\# \mathfrak{m}$ is a coupling between $\mu^n(\omega)$ and $\nu^n(\omega)$. Hence (omitting for simplicity the dependence on $\omega$) and using (2.4.7) with $S = T^{\mu_n}$, $T = T^{\nu^n}$ one has

$$\begin{aligned}
\mathbb{E}\left[W_2^2(\mu^n, \nu^n)\right] &\leq \mathbb{E}\left[\int_D \left|T^{\mu^n} - T^{\nu^n}\right|^2 \mathrm{d}\mathfrak{m}\right] \\
&= \mathbb{E}\left[\int_D \left(\left|T^{\mu^n}(x) - x\right|^2 + \left|T^{\nu^n}(x) - x\right|^2 - 2\langle T^{\mu^n}(x) - x, T^{\nu^n}(x) - x\rangle\right) \mathrm{d}\mathfrak{m}(x)\right] \\
&= 2\,\mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] - 2\,\mathbb{E}\left[\int_D \langle T^{\mu^n}(x) - x, T^{\nu^n}(x) - x\rangle \,\mathrm{d}\mathfrak{m}(x)\right] \\
&= 2\,\mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] - 2\int_D \left|\mathbb{E}\left[T^{\mu^n}(x) - x\right]\right|^2 \mathrm{d}\mathfrak{m}(x),
\end{aligned}$$

where we used that $\mathbb{E}\left[W_2^2(\mu^n, \mathfrak{m})\right] = \mathbb{E}\left[W_2^2(\nu^n, \mathfrak{m})\right]$ since $\mu^n$ and $\nu^n$ have the same law. □

In particular, combining the inequality in (2.4.6) (neglecting for a moment the negative term in the right hand side) with the first part of Theorem 2.1.1, we obtain

$$\limsup_{n\to\infty} \frac{n}{\log n}\,\mathbb{E}\left[W^2_{2,\mathbb{T}^2}(\mu^n,\nu^n)\right] \le \limsup_{n\to\infty} \frac{n}{\log n}\,\mathbb{E}\left[W^2_{2,[0,1]^2}(\mu^n,\nu^n)\right] \le \frac{1}{2\pi}. \tag{2.4.8}$$

Next, we deal with lower bounds. It will be sufficient, by a comparison argument, to provide the lower bound only in the flat torus.

**Proposition 2.4.10.** *Let* $\mathrm{D} = \mathbb{T}^2$*. Then*

$$\liminf_{n\to\infty} \frac{n}{\log n}\,\mathbb{E}\left[W^2_2(\mu^n,\nu^n)\right] \ge \frac{1}{2\pi}. \tag{2.4.9}$$

*Proof.* Similarly to the proof of Theorem 2.4.6, for $\eta \in (0,1)$ we introduce the event

$$A_\eta = A_{\eta,n} = \left\{ \sup_{y\in D} \frac{|r^{n,t}(y)|}{\sqrt{n}} \le \frac{\eta}{2},\ \sup_{y\in D} \frac{|s^{n,t}(y)|}{\sqrt{n}} \le \frac{\eta}{2} \right\},$$

(with $s^{n,t}$ equal to the density of $\sqrt{n}(\mu^{n,t} - \nu^{n,t})$ w.r.t. $\mathfrak{m}$) whose probability tends to 1 as $n \to \infty$. By the contractivity assumption in $W_2$ we have $W_2^2(\mu^n,\nu^n) \ge e^{2Kt} W_2^2(\mu^{n,t},\nu^{n,t})$, therefore it is sufficient to study the asymptotic behaviour of

$$\mathbb{E}\left[W^2_2(\mu^{n,t},\nu^{n,t})\chi_{A_\eta}\right].$$

To this end, we let $f^{n,t}$ be the solution to (2.3.23), $g^{n,t}$ the solution to the same equation with $s^{n,t}$ in place of $r^{n,t}$ and $h^{n,t} = f^{n,t} - g^{n,t}$. Define $h = -h^{n,t}/\sqrt{n}$, so that $\Delta h = -(r^{n,t} - s^{n,t})/\sqrt{n}$ and $\|\Delta h\|_\infty \le \eta$ in the event $A_\eta$. To this function $h$ we associate the potential $k$ given by Corollary 2.3.3, hence we can estimate, in the event $A_\eta$ (with $\omega(\eta)$ defined as in (2.4.4) with $f$ replaced by $h$),

$$\begin{aligned}
\frac{1}{2} W_2^2(\mu^{n,t},\nu^{n,t}) &\ge \int_D h\,\mathrm{d}\mu^{n,t} + \int_D k\,\mathrm{d}\nu^{n,t} \\
&= \int_D (h+k)\,\mathrm{d}\mathfrak{m} + \int_D h \frac{\mathrm{d}(r^{n,t} - s^{n,t})}{\sqrt{n}} + \int_D (h+k)\frac{\mathrm{d}s^{n,t}}{\sqrt{n}} \\
&\ge -e^{\omega(\eta)} \int_D \frac{|\nabla h|^2}{2}\,\mathrm{d}\mathfrak{m} + \int_D |\nabla h|^2\,\mathrm{d}\mathfrak{m} + \int_D (h+k)\frac{\mathrm{d}s^{n,t}}{\sqrt{n}} \\
&\ge \left(1 - \frac{e^{\omega(\eta)}}{2}\right)\frac{1}{n}\int_D |\nabla h^{n,t}|^2\,\mathrm{d}\mathfrak{m} - \left|\int_D (h+k)\frac{\mathrm{d}s^{n,t}}{\sqrt{n}}\right|.
\end{aligned}$$

Since $h + k \le 0$, we have

$$\left|\int_D (h+k)\frac{\mathrm{d}s^{n,t}}{\sqrt{n}}\right| \le -\eta \int_D (h+k)\,\mathrm{d}\mathfrak{m} \le \eta e^{\omega(\eta)} \int_D \frac{|\nabla h|^2}{2}\,\mathrm{d}\mathfrak{m},$$

therefore, still in the event $A_\eta$,

$$\frac{1}{2} W_2^2(\mu^{n,t}, \nu^{n,t}) \geq \left(1 - (1+\eta)\frac{e^{\omega(\eta)}}{2}\right) \frac{1}{n} \int_D |\nabla h^{n,t}|^2 \,\mathrm{d}\mathfrak{m}.$$

The proof now concludes as before, noticing that, by independence of $\mu^n$ and $\nu^n$,

$$\begin{aligned}
&\mathbb{E}\left[\int_D |\nabla h^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right] \\
&= \mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right] + \mathbb{E}\left[\int_D |\nabla g^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right] - 2\,\mathbb{E}\left[\int_D \langle \nabla f^{n,t}, \nabla g^{n,t}\rangle \,\mathrm{d}\mathfrak{m}\right] \\
&= 2\,\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right] + 2\,\mathbb{E}\left[\int_D f^{n,t} \Delta g^{n,t} \,\mathrm{d}\mathfrak{m}\right] \\
&= 2\,\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right] + 2\int_D \mathbb{E}[f^{n,t}]\,\mathbb{E}[s^{n,t}] \,\mathrm{d}\mathfrak{m} = 2\,\mathbb{E}\left[\int_D |\nabla f^{n,t}|^2 \,\mathrm{d}\mathfrak{m}\right]
\end{aligned}$$

and

$$\mathbb{E}\left[\int_D |\nabla h^{n,t}|^4 \,\mathrm{d}\mathfrak{m}\right] \leq 16\,\mathbb{E}\left[\int_D |\nabla f^{n,t}|^4 \,\mathrm{d}\mathfrak{m}\right]. \qquad \square$$

From the previous result we get

$$\liminf_{n\to\infty} \frac{n}{\log n}\,\mathbb{E}\left[W^2_{2,[0,1]^2}(\mu^n, \nu^n)\right] \geq \liminf_{n\to\infty} \frac{n}{\log n}\,\mathbb{E}\left[W^2_{2,\mathbb{T}^2}(\mu^n, \nu^n)\right] \geq \frac{1}{2\pi}$$

which, combined with (2.4.8), concludes the proof (2.1.3). By looking at (2.4.6) we see also that (2.1.4) holds, and this concludes the proof of Theorem 2.1.1.

## 2.5 A new proof of the AKT lower bound

In this section we see how a minor modification of the ansatz of [Car+14] provides a new proof of the lower bound in [AKT84], written in terms of expectations; the upper bound follows immediately from Theorem 2.1.1 and Hölder inequality.

The following real analysis lemma is well known, we state it for the case of the flat torus. Its proof (see for instance [AF84]) can be obtained by considering the sublevel sets of the maximal function of $|\nabla h|$.

**Lemma 2.5.1** (Lusin approximation of Sobolev functions)**.** *For all $p > 1$, $h \in H^{1,p}(\mathbb{T}^d)$ and all $\lambda > 0$ there exists a $\lambda$-Lipschitz function $\varphi : \mathbb{T}^d \to \mathbb{R}$ with*

$$\mathfrak{m}(\{h \neq \varphi\}) \leq \frac{C(d,p)}{\lambda^p} \int_{\mathbb{T}^d} |\nabla h|^p \,\mathrm{d}\mathfrak{m}. \tag{2.5.1}$$

**Theorem 2.5.2.** *If $D = \mathbb{T}^2$ one has*

$$\liminf_{n\to\infty} \sqrt{\frac{n}{\log n}}\, \mathbb{E}\left[W_1(\mu^n, \nu^n)\right] > 0.$$

*By the triangle inequality, the same holds for the matching to the reference measure.*

*Proof.* As in the proof of the lower bound for $p = 2$ we can use contractivity, reducing ourselves to estimating from below the Wasserstein distance between the regularized measures $\mu^{n,t} = u^{n,t}\mathfrak{m}$, $\nu^{n,t} = v^{n,t}\mathfrak{m}$. Let $M > 0$ be fixed and set $c(n) = M\sqrt{n^{-1}\log n}$. Let $t = t(n) = \gamma n^{-1}\log n$ with $\gamma$ sufficiently large and let $h^{n,t}$ be as in the proof of the lower bound in the case $p = 2$, so that $h = h^{n,t}/\sqrt{n}$ satisfies

$$\lim_{n\to\infty} \frac{n}{\log n}\, \mathbb{E}\left[\int_D |\nabla h|^2 \,\mathrm{d}\mathfrak{m}\right] = \frac{1}{2\pi}. \tag{2.5.2}$$

Denote by $\varphi$ the $c(n)$-Lipschitz function provided by Lemma 2.5.1. We denote by $E_n$ the set $\{h \neq \varphi\}$ and from (2.5.1) and (2.5.2) we obtain the estimates

$$\mathbb{E}\left[\mathfrak{m}(E_n)\right] \leq \frac{C(2,2)}{c(n)^2}\, \mathbb{E}\left[\int_D |\nabla h|^2 \,\mathrm{d}\mathfrak{m}\right] \leq \frac{2C(2,2)}{2\pi M^2}$$

for $n$ large enough, so that we can use Hölder inequality and (2.3.31) to get, for some positive constant $C > 0$,

$$\mathbb{E}\left[\int_{E_n} |\nabla h|^2 \,\mathrm{d}\mathfrak{m}\right] \leq \frac{C}{M}\frac{\log n}{n} \tag{2.5.3}$$

for $n$ large enough. Another application of Hölder's inequality yields

$$\mathbb{E}\left[\int_{E_n} |\nabla h| \,\mathrm{d}\mathfrak{m}\right] \leq \mathbb{E}\left[\int_{E_n} |\nabla h|^2 \,\mathrm{d}\mathfrak{m}\right]^{1/2} \mathbb{E}\left[\mathfrak{m}(E_n)\right]^{1/2} \leq \frac{C}{M^{3/2}}\sqrt{\frac{\log n}{n}} \tag{2.5.4}$$

again for some positive constant $C > 0$ (possibly larger than the one in (2.5.3)).

From Kantorovich's duality formula we get

$$c(n)W_1(\mu^{n,t}, \nu^{n,t}) \geq \left|\int_D \varphi(u^{n,t} - v^{n,t}) \,\mathrm{d}\mathfrak{m}\right| = \left|\int_D \langle \nabla h, \nabla\varphi\rangle \,\mathrm{d}\mathfrak{m}\right|,$$

where we used the PDE $\Delta h = u^{n,t} - v^{n,t}$ solved by $h$. Therefore

$$W_1(\mu^{n,t}, \nu^{n,t}) \geq \frac{1}{c(n)}\int_D |\nabla h|^2 \,\mathrm{d}\mathfrak{m} - \frac{1}{c(n)}\left|\int_{E_n} \langle \nabla h, \nabla h - \nabla\varphi\rangle \,\mathrm{d}\mathfrak{m}\right|.$$

By (2.5.2), the first term is asymptotic to $(2\pi M)^{-1}\sqrt{n^{-1}\log n}$. We will see that, for $M$ sufficiently large, the first term dominates the second one. Indeed, we have

$$\frac{1}{c(n)}\left|\int_{E_n} \langle \nabla h, \nabla h - \nabla\varphi\rangle \,\mathrm{d}\mathfrak{m}\right| \leq \frac{1}{c(n)}\left[\int_{E_n} |\nabla h|^2 + |\nabla h| c(n) \,\mathrm{d}\mathfrak{m}\right]$$

Taking expectation, using (2.5.3) and (2.5.4) we have the inequality, for $n$ sufficiently large,

$$\frac{1}{c(n)}\, \mathbb{E}\left[\int_{E_n} |\nabla h|^2 + |\nabla h| c(n) \,\mathrm{d}\mathfrak{m}\right] \leq C\left(\frac{1}{M^2} + \frac{1}{M^{3/2}}\right)\sqrt{\frac{\log n}{n}}. \qquad \square$$

## 2.6 Open problems and extensions

In this section we discuss open problems, the present limitations of our technique, and some potential generalizations.

**Improvements in the case $p = d = 2$.** In this case the more demanding prediction of [Car+14], currently still open, is

$$\lim_{n\to\infty}\left(\frac{n}{\log n}\,\mathbb{E}\left[W_2^2(\mu^n,\nu^n)\right]-\frac{1}{2\pi}\right)\log n\in\mathbb{R}.$$

In this connection notice also that our technique for the lower bound requires $t = \gamma n^{-1}\log n$ with $\gamma$ sufficiently large, while necessarily in the upper bound one is forced to take $t = \gamma n^{-1}\log n$ with $\gamma$ small. Other open problems regard the distribution of the random variables $\frac{n}{\log n}W_2^2(\mu^n,\nu^n)$ and the matching problem involving more general reference measures $\mathfrak{m}$ (the Gaussian case is particularly interesting, where the role of the heat semigroup is played by the Ornstein-Uhlenbeck semigroup, see [Led] for very recent results in this direction, in any number of dimensions).

**Different powers and dimensions.** Our proof in the case $d = 2$ exploits the extra room given by the logarithmic correction to the "natural" scale $n^{-1/d}$. Let us discuss the difficulties coming from $p \neq 2$ and $d > 2$ separately, of course the problem is even more challenging if both things happen.

If $d = 2$ and $p = 1$, we have already seen in Section 2.5 that the proof can be adapted to obtain the tight lower bound of [AKT84]. Via Hölder's inequality, one obtains the tight upper and lower bounds also for $1 < p < 2$, and we believe that also the case $p > 2$ could be covered, by estimating $\mathbb{E}\left[|\nabla f^{n,t}|^k\right]$ with $k$ large integer (we did this for $k = 2, 4$). On the other hand, proving convergence of the renormalized expectations seems to require a more precise scheme, since the gradients of solutions to the Monge-Ampère equation describe the optimal transport map $T$ only when $p = 2$; in this vein, one could consider (see [AGS08, Theorem 6.2.4]) the linearizations of

$$T = \mathrm{Id} - |\nabla\phi|^{\frac{2-p}{p-1}}\nabla\phi, \qquad \rho_1(T)\det(\nabla T) = \rho_0.$$

In the case $p = 1$, an alternative PDE possibility could be given by the construction of the transport density via a $q$-Laplacian approximation in [EG99], $q \to \infty$, which led to the first rigorous proof of the optimal transport map for Monge's problem.

If $p = 2$ and $d > 2$, the prediction of [Car+14] is that

$$n^{2/d}\,\mathbb{E}\left[W_2^2(\mu^n,\nu^n)\right] - c_d = \frac{\xi}{2\pi^2}n^{-1+2/d} + o\big(n^{-1+2/d}\big),$$

where $c_d$ is not conjectured and the coefficient $\xi$ is explicitly given in terms of the Epstein function. However, our regularization technique seems to fail, at least for the purpose of computing $c_d$ (namely proving convergence of the renormalized expectations). For instance, from (2.3.25) we get $\mathbb{E}\left[|\nabla f^{n,t}|^2\right] \sim t^{1-d/2}$, and therefore choosing $t = \gamma n^{-2/d}$ one is led to the estimate (even assuming that the factor due the logarithmic mean can be neglected) from above of $\mathbb{E}[W_2^2(\mu^n, \mathfrak{m})]$ with a term behaving like

$$C_{\mathrm{dr}}\gamma n^{-2/d} + Cn^{-1}\gamma^{1-d/2}n^{-2/d(1-d/2)} = C_{\mathrm{dr}}\gamma n^{-2/d} + C\gamma^{1-d/2}n^{-2/d}.$$

Therefore, while we get the correct rate $n^{-2/d}$, it is not clear how to let $\gamma \to 0$ to eliminate the cost due to the short time regularization.

**A class of abstract metric measure spaces.** We already noticed that in our proof the geometry of the domain enters only through the properties of the heat semigroup $P_t$ with homogeneous Neumann boundary conditions. As a matter of fact, let us briefly indicate how our proof works, still in the case $d = 2$, for the class $RCD^*(K, d)$ of "Riemannian" metric measure spaces $(X, \mathsf{d}, \mathfrak{m})$, extensively studied and characterized in [AGS15; AMS15; EKS15]. This class of possibly nonsmooth metric measure spaces, includes for instance all compact Riemannian manifolds without boundary, or "convex" manifolds with boundary, namely manifolds having the property that geodesics between any two points do not touch the boundary (as it happens for compact convex domains in $\mathbb{R}^d$). The class $RCD^*(K, d)$ can be characterized either in terms of suitable $K$-convexity properties w.r.t. $W_2$-geodesics (of the logarithmic entropy for $d = \infty$ [AGS15], of power entropy [EKS15] or nonlinear diffusion semigroups [AMS15] in the case $d < \infty$), or in terms of Bochner's inequality, very much in the spirit of the Bakry-Émery theory (see [BGL14] for a nice introduction to the subject). In the very recent work [JLZ14], all regularizing properties of $P_t$ needed for our proof to work have been proved in the context of $RCD^*(K, d)$ spaces. The only missing ingredient in this more abstract framework is the asymptotic expansion of the trace formula provided by Proposition 2.3.14, but thanks to (2.3.26) our results can be stated in terms of the limit

$$\lim_{t \to 0^+} \sum_{\lambda \in \sigma(\Delta) \setminus \{0\}} \frac{e^{2\lambda t}}{\lambda \log t}$$

whenever it exists.

# Chapter 3

# Linear extensions through random projection

## 3.1 Introduction

The aim of this chapter is to provide extension theorems $\mathrm{Lip}(X;Z) \to \mathrm{Lip}(Y;Z)$ where $X \subset Y$ is a closed subset of a complete metric space $(Y, \mathsf{d})$ and $Z$ is a Banach space, under hypotheses just on the space $X$ alone and not on the ambient space $Y$. The exposition is based upon the article in preparation [BDS].

In [LN05] the authors provide the following extension theorem for Lipschitz functions in a metric setting.

**Theorem** (Lee and Naor [LN05]). *Let $X \subset (Y, \mathsf{d})$ be a doubling metric space with doubling constant $\lambda_X$. Then there is an extension $T : \mathrm{Lip}(X;Z) \to \mathrm{Lip}(Y;Z)$ such that*

$$\mathrm{Lip}(Tf) \leq C \log(\lambda_X) \,\mathrm{Lip}(f) \qquad \forall f \in \mathrm{Lip}(X;Z),$$

*where $C$ is a universal constant.*

Our goal is to obtain more directly the previous result, through a simpler proof based on ideas appearing in [JLS86]. See also [LN04; Oht09] for related discussions. Moreover, we provide also a $C^1$ extension result in the spirit of Whitney [Whi34].

The main theorems of the chapter are Theorem 3.4.1 for the Lipschitz extension and Theorem 3.4.3 for the $C^1$ extension respectively. The structure is as follows: in Section 3.2 we contruct partitions of unity, both in the Lipschitz and $C^1$ version; in Section 3.3 we use these partitions to build Lipschitz and $C^1$ random projections of a space onto a subspace and finally in Section 3.4 we prove the extension theorems using the previously developed tools.

### 3.1.1 Notation and preliminaries

Let $(X, \mathsf{d})$ be a complete metric space. We will denote with $B(x, r)$ the open ball of radius $r$, centered at $x$ and, for $A \subseteq X$, we define $\mathsf{d}(x, A) = \inf\{\mathsf{d}(x, x') : x' \in A\}$.

We will denote by $\mathrm{Lip}(X;Z)$ the set of Lipschitz functions with values in $Z$; if the second space is dropped it means that $Z=\mathbb{R}$. Moreover, given $f\in\mathrm{Lip}(X;Z)$, we denote by $\mathrm{Lip}(f)$ the least Lipschitz constant for the function $f$. We make use of the notion of slope of a function $f:X\to\mathbb{R}$ defined as

$$|\nabla f|(x)=\limsup_{y\to x}\frac{|f(y)-f(x)|}{\mathsf{d}(y,x)}.$$

We will be dealing with measures supported in metric spaces: we denote by $\mathscr{P}(X)$ the set of Borel probability measures on $X$, with $\mathscr{M}_+(X)$ the set of finite nonnegative Borel measures on $X$ and with $\mathscr{M}(X;Z)$ the set of vector valued measures with finite total variation. As before, if the second spaces is omitted then $Z=\mathbb{R}$ and so it will reduce to the space of signed measures.

Of crucial importance in the sequel will be the $W_1$ Wasserstein distance, already presented in the introduction. We recall here the dual representation because it will be the more relevant for the further development. We define it in an extended way, not restricted to $\mathscr{P}_1(X)$, to allow for more flexibility.

**Definition 3.1.1** (Wasserstein distance)**.** Let $\mu_1,\mu_2\in\mathscr{P}(X)$. Then we define

$$W_1(\mu,\nu)=\sup\left\{\int_X f\,\mathrm{d}\mu-\int_X f\,\mathrm{d}\nu : f\in\mathrm{Lip}(X),\ \mathrm{Lip}(f)\le 1\right\},$$

allowing it to be possibly infinite.

*Remark* 3.1.2. Notice that $W_1(\mu_1,\mu_2)$ does not need to be finite. However it is finite whenever $\int_X \mathsf{d}(x,x_0)\,\mathrm{d}(\mu_1+\mu_2)(x)<\infty$, i.e. $\mu_1,\mu_2\in\mathscr{P}_1(X)$: this is the case for example when $\mu_1$ and $\mu_2$ have both bounded support. A useful inequality in the sequel, that follows directly from the definition, is

$$\left|\int_X f\,\mathrm{d}\mu_1-\int_X f\,\mathrm{d}\mu_2\right|\le\mathrm{Lip}(f)W_1(\mu_1,\mu_2).\tag{3.1.1}$$

Throughout the paper we use the notation $\lesssim$ to omit a universal constant not depending on $X$, $Y$, the doubling constant $\lambda$ or anything of this sort. We will use two notion of dimensionality of a metric space: the *doubling constant* and the *metric capacity*.

**Definition 3.1.3** (Doubling metric space)**.** $(X,\mathsf{d})$ is a doubling metric space if there exists $\lambda\in\mathbb{N}$ such that every ball of radius $2r$ can be covered with at most $\lambda$ balls of radius $r$. The least such constant is $\lambda_X$, the doubling constant of $X$[1].

**Definition 3.1.4** (Metric capacity)**.** Given a metric space $(X,\mathsf{d})$ we define the *metric capacity*[2] $\kappa_X:(0,1]\to\mathbb{N}\cup\{\infty\}$ as

$$\kappa_X(\varepsilon)=\sup\left\{k:\exists x_0,\dots,x_k\in X,\ \exists r>0\text{ s.t. }\bigsqcup_{i=1}^k B(x_i,\varepsilon r)\subset B(x_0,r)\right\}.$$

[1]In the sequel we will drop the dependence on $X$ when there is no room for confusion

[2]For short, just *capacity* in the sequel.

It can be verified that if $\kappa_X(\varepsilon) < \infty$ for some $\varepsilon < 1/3$, then $\kappa_X(t)$ is finite for every $t \in (0,1]$. Even if it is true that $X$ has a finite doubling constant iff $X$ has a finite metric capacity, it is more natural to use the latter in some of the constructions. However since we want the final result to depend only on the doubling constant of $X$, we will make use of the following proposition comparing $\lambda$ and $\kappa$.

**Proposition 3.1.5** (Comparing $\kappa$ and $\lambda$)**.** *Let $X$ be a metric space. Then we have that*

*(i)* $\lambda \leq \kappa_X(1/5)$*;*

*(ii)* $\kappa_X(\varepsilon) \leq \lambda^k$ *whenever* $\frac{1}{2^k} < \varepsilon \leq \frac{1}{2^{k-1}}$*.*

*Proof.* Considering a maximal family $\mathcal{F} = \{B(x_i, \varepsilon r)\}_{i\in I}$ of disjoint balls contained in $B(x_0, r)$ we have $|\mathcal{F}| \leq \kappa(\varepsilon)$ and moreover $B\big(x_0, (1-\varepsilon)r\big) \subseteq \cup_i B(x_i, 2\varepsilon r)$. Choosing $\varepsilon = 1/5$ and thanks to the arbitrariness of $r$ and $x_0$ we get that $\lambda \leq \kappa_X(1/5)$.

In order to prove the second inequality we first observe that for we can cover $B(x_0, 2^k r)$ with less than $\lambda^k$ balls of radius $r$: let us consider $\mathcal{F}' = \{B(y_i, r)\}$ such a family. Let $\frac{1}{2^k} < \varepsilon \leq \frac{1}{2^{k-1}}$ and $\mathcal{F} = \{B(x_i, \varepsilon 2^k r)\}$ be a disjoint family of balls contained in $B(x_0, 2^k r)$. It is now easy to see that $B(y_i, r)$ can contain at most one $x_i$; then we have $|\mathcal{F}| \leq |\mathcal{F}'| \leq \lambda^k$ and so $\kappa_X(\varepsilon) \leq \lambda^k$.

□

## 3.2 Whitney-type partitions

The way to the extension results follows the same path traced by Whitney for his theorem, with the addition of some ideas that we have learnt from [JLS86]. The first step is to construct suitable partitions of unity so that manually built local extensions can be patched together at the global level. Since our goal is to prove Lipschitz and $C^1$ extendability, we are going to need two different kind of partitions, one for each purpose. The underlying ideas are the same in both cases; in particular, the attentive reader will notice that in the $C^1$ construction we try to replicate the proof of the Lipschitz version, with appropriate modifications.

**Proposition 3.2.1** (Relative Lipschitz partition of unity)**.** *Let $(Y, \mathsf{d})$ be a metric space and $X \subset Y$ a closed subset with finite doubling constant $\lambda$. Then there exists a countable family $\{V_i, \varphi_i, x_i\}_i$ such that:*

*(i)* $\{V_i\}_i$ *is a locally finite covering of* $Y \setminus X$ *with covering constant* $3\lambda^4$*;*

*(ii)* $\{\varphi_i\}_i$ *is a partition of unity on* $Y \setminus X$ *such that* $\{\varphi_i > 0\} \subset V_i$ *and*

$$\sum_i |\nabla \varphi_i|(y) \lesssim \frac{\log \lambda}{\mathsf{d}(y, X)};$$

*(iii) the points* $x_i$ *belong to* $X$ *and* $\mathsf{d}(y, x_i) \lesssim \mathsf{d}(y, X)$ *if* $y \in V_i$.

*Proof.* This follows directly from Lemma 3.2.5 below, re-indexing the family $\{V_i^n, \varphi_i^n, x_i^n\}_{i,n}$. □

The idea is that thanks to (iii) we have that $x_i$ is an approximate projection of any $y \in V_i$ on $X$ and in fact this partition of unity will help us define a *random projection*. The estimate (ii) will be instead crucial to prove Lipschitz estimates. The next proposition will be used to prove an extension of Whitney theorem for Banach spaces, requiring the partition of unity to be $C^1$. Unfortunately the dependence of $\lambda$ in the estimates of the slopes is much worse in this case: it will be interesting to have a class of Banach spaces where we can recover the same logarithmic behavior as in the Lipschitz case.

**Proposition 3.2.2** (Relative $C^1$ partition of unity)**.** *Let* $Y$ *be a Banach space whose norm belongs to* $C^1(Y \setminus \{0\})$ *and let* $X \subset Y$ *be a closed subset with doubling constant* $\lambda$. *Then there exists a family* $\{V_i, \varphi_i, x_i\}_i$ *such that:*

*(i)* $\{V_i\}_i$ *is a locally finite covering of* $Y \setminus X$ *with covering constant* $5\lambda^4$*;*

*(ii)* $\{\varphi_i\}_i$ *is a partition of unity on* $Y \setminus X$ *such that* $\{\varphi_i > 0\} \subset V_i$ *and*

$$\sum_i |\nabla \varphi_i|(y) \lesssim \frac{\lambda^4 \log \lambda}{\mathsf{d}(y, X)};$$

*(iii) the points* $x_i$ *belong to* $X$ *and* $\mathsf{d}(y, x_i) \lesssim \mathsf{d}(y, X)$ *if* $y \in V_i$.

*Proof.* This follows directly from Lemma 3.2.6, taking the family $\{A_i^n, \varphi_i^n, x_i^n\}_{i,n}$. □

**Lemma 3.2.3.** *Let* $(X, \mathsf{d})$ *be a metric space. Then for every* $r > 0$ *there exists a family of disjoint balls* $\{(B_i = B(x_i, r)\}_{i \in I}$ *such that* $\{2B_i = B(x_i, 2r)\}_{i \in I}$ *is a covering of* $X$.

*Proof.* Let $\mathcal{F} = \{(B_i)_{i \in I} : B_i \cap B_j = \emptyset\}$ be the collection of all disjoint families of open balls of radius $r$. A simple application of Zorn's lemma shows that there exist a maximal family $(B_i)_{i \in I}$. Suppose by contradiction that $x \notin 2B_i$ for any $i \in I$. Then $B(x, r)$ is disjoint from every $B_i$, contradicting the maximality. □

**Lemma 3.2.4** (Whitney-type covering)**.** *Let* $(Y, \mathsf{d})$ *be a complete metric space and* $X \subset Y$ *a closed subset with finite capacity. For every* $n \in \mathbb{Z}$ *let* $\{B_i^n = B(x_i^n, 2^n)\}_{i \in I_n}$ *be a family given by Lemma 3.2.3. Let*

$$\tilde{V}_i^n = \{y \in Y \setminus X : 2^n \le \mathsf{d}(y, X) < 2^{n+1} \text{ and } \mathsf{d}(y, x_i^n) = \min_{j \in I_n} \mathsf{d}(y, x_j^n)\}.$$

*Then the family of enlarged sets* $\mathcal{F} = \left\{V_i^n = (\tilde{V}_i^n)_{2^{n-1}} : n \in \mathbb{Z}, i \in I_n\right\}$ *has the following properties:*

*(i) $\mathcal{F}$ is a locally finite covering of $Y \setminus X$ with constant $3\kappa_X(1/10)$;*

*(ii) for every $y \in Y \setminus X$ we have $\mathsf{d}(y, X)/4 \leq \max_{V\in\mathcal{F}}\{\mathsf{d}(y, V^c)\} \leq \mathsf{d}(y, X)$.*

*Proof.* First of all, it is obvious that $\mathcal{F}$ is a covering: in fact also $\{\tilde{V}_i^n\}_{i,n}$ is a covering. Let us prove that for $y \in V_i^n$ we have $\mathsf{d}(y, x_i^n) \leq 9 \cdot 2^{n-1}$. By definition, for every $\varepsilon > 0$ there exists $\tilde{y} \in \tilde{V}_i^n$ and $x \in X$ such that

$$\mathsf{d}(y, \tilde{y}) < \mathsf{d}(y, \tilde{V}_i^n) + \varepsilon \leq 2^{n-1} + \varepsilon \qquad \text{and} \qquad \mathsf{d}(\tilde{y}, x) < \mathsf{d}(\tilde{y}, X) + \varepsilon \leq 2^{n+1} + \varepsilon.$$

Then, by the covering property of $\{2B_i^n\}_{i\in I_n}$ we know that there exists $j$ such that $x \in 2B_j^n$ and so $\mathsf{d}(x, x_j^n) \leq 2^{n+1}$. In particular, by definition of $\tilde{V}_i^n$ we obtain

$$\begin{aligned}\mathsf{d}(y, x_i^n) &\leq \mathsf{d}(\tilde{y}, x_i^n) + \mathsf{d}(\tilde{y}, y) \leq \mathsf{d}(\tilde{y}, x_j^n) + \mathsf{d}(\tilde{y}, y) \\ &\leq \mathsf{d}(\tilde{y}, x) + \mathsf{d}(x, x_j^n) + \mathsf{d}(\tilde{y}, y) \leq 9 \cdot 2^{n-1} + 2\varepsilon.\end{aligned}$$

In order to get the local finiteness in (i) we use the fact that if $y \in V_i^n \cap V_j^n$ then we have $\mathsf{d}(y, x_i^n) \leq 9 \cdot 2^{n-1}$ and $\mathsf{d}(y, x_j^n) \leq 9 \cdot 2^{n-1}$. In particular we have $x_j^n \in B(x_i^n, 9 \cdot 2^n)$ and so $B(x_j^n, 2^n) \subseteq B(x_i^n, 10 \cdot 2^n)$. In particular we get that $\sharp\{j : y \in V_j^n\} \leq \kappa_X(1/10)$. Now, knowing that $y \in V_i^n$ implies $2^{n-1} < \mathsf{d}(y, X) < 2^{n+2}$ we have at most three possible choices for $n$ and at most $\kappa_X(1/10)$ sets for every $n$, so the conclusion.

For (ii) the inequality $\max_{V\in\mathcal{F}}\{\mathsf{d}(y, V^c)\} \leq \mathsf{d}(y, X)$ is trivial since $X \subset V^c$ for all $V$. For the other inequality we know that $y \in \tilde{V}_i^n$ for some $i, n$ and in particular we have $\mathsf{d}(y, (V_i^n)^c) \geq 2^{n-1}$ by the definition of $V_i^n$. But then we have

$$\frac{\mathsf{d}(y, X)}{4} < 2^{n-1} \leq \mathsf{d}(y, (V_i^n)^c) \leq \max_{V\in\mathcal{F}}\{\mathsf{d}(y, V^c)\}. \qquad \square$$

**Lemma 3.2.5** (Lipschitz partition of unity)**.** *Let $\{V_i^n\}_{i,n}$ be the sets given by Lemma 3.2.4. For $m > 0$ define the functions*

$$\tilde{\varphi}_i^n(y) = \mathsf{d}^m\big(y, (V_i^n)^c\big) \quad \textit{and} \quad \varphi_i^n(y) = \frac{\tilde{\varphi}_i^n(y)}{\sum\limits_{k,j} \tilde{\varphi}_j^k(y)}.$$

*Then the family $\{\varphi_i^n\}_i^n$ is a partition of unity with the property that*

$$\sum_{n,i} |\nabla \varphi_i^n|(y) \lesssim \frac{\log \lambda}{\mathsf{d}(y, X)}.$$

*Proof.* Thanks to the sublinearity of the slope, the chain rule, and the fact that $|\nabla \mathsf{d}(y, A)| \leq 1$ for every $A$, we obtain

$$|\nabla \varphi_i^n|(y) \leq m\frac{\mathsf{d}^{m-1}\big(y, (V_i^n)^c\big)}{\sum_{k,j} \mathsf{d}^m\big(y, (V_j^k)^c\big)} + m\frac{\mathsf{d}^m\big(y, (V_i^n)^c\big) \cdot \sum_{k,j} \mathsf{d}^{m-1}\big(y, (V_j^k)^c\big)}{\Big(\sum_{k,j} \mathsf{d}^m\big(y, (V_j^k)^c\big)\Big)^2}.$$

In order to have a clearer exposition, we fix $\{\mathsf{d}_l\}_{l\in\{1,\dots,N\}} = \{\mathsf{d}^{m-1}\big(y,(V_j^k)^c\big)\}_{j,k}$ where we included all couples $j,k$ such that $y \in V_j^k$; in particular we have $N \le 2\kappa_X(1/10)$. Then summing up on the indices $i,n$ and simplifying we get

$$\sum_{i,n} |\nabla\varphi_i^n|(y) \le m\frac{\sum_l \mathsf{d}_l^{m-1}}{\sum_l \mathsf{d}_l^m} + m\frac{\sum_l \mathsf{d}_l^m \cdot \sum_l \mathsf{d}_l^{m-1}}{(\sum_l \mathsf{d}_l^m)^2} = 2m\frac{\sum_l \mathsf{d}_l^{m-1}}{\sum_l \mathsf{d}_l^m}.$$

Now we use the inequality between the means $\left(\frac{\sum_l \mathsf{d}_l^{m-1}}{N}\right)^{1/(m-1)} \le \left(\frac{\sum_l \mathsf{d}_l^m}{N}\right)^{1/m}$, obtaining

$$\sum_{i,n} |\nabla\varphi_i^n|(y) \le 2m\frac{N^{1/m}}{(\sum_l \mathsf{d}_l^m)^{1/m}}.$$

By Lemma 3.2.4 (ii), we have $\max_l\{\mathsf{d}_l\} \ge \mathsf{d}(y,X)/4$ and so, using Proposition 3.1.5 (ii) and then setting $m = \log_2\lambda$ we find

$$|\nabla\varphi_i^n|(y) \le 2m\frac{N^{1/m}}{\max_l\{\mathsf{d}_l\}} \le \frac{8m\big(2\kappa(1/10)\big)^{1/m}}{\mathsf{d}(y,X)} \le 256\frac{\log_2(\lambda)}{\mathsf{d}(y,X)}.$$

□

**Lemma 3.2.6** ($C^1$ partition of unity)**.** *Let $X$ and $Y$ be as in Proposition 3.2.2 and for every $n\in\mathbb{Z}$ let $\{B_i^n = B(x_i^n, 2^n)\}_{i\in I_n}$ be the family given by Lemma 3.2.3. Then there exists a partition of unity $\{\varphi_i^n\}_{i,n}$ of $Y\setminus X$ such that, denoting $A_i^n = \{\varphi_i^n > 0\}$, we have that*

*(i)* $\{A_i^n\}_{i,n}$ *is a covering of $Y\setminus X$ with covering constant less than $C\lambda^6$;*

*(ii)* *if $y\in A_i^n$ then $\mathsf{d}(y,x_i^n) \lesssim \mathsf{d}(y,X)$;*

*(iii)* $\sum_{i,n}|\nabla\varphi_i^n|(y) \lesssim \frac{\lambda^5\log\lambda}{\mathsf{d}(y,X)}$.

*Proof.* The idea is to take

$$\varphi_i^n(y) = \frac{\tilde\varphi_i^n(y)}{\sum\limits_{k,j}\tilde\varphi_j^k(y)},$$

where

$$\tilde\varphi_i^n(y) = \xi\left(8\ell - \frac{|x_i^n - y|}{2^n}\right)\cdot\xi\left(\frac{|x_i^n - y|}{2^n} - \ell\right)\cdot\prod_{x_j^n\sim x_i^n}\xi\left(\frac{|x_j^n - y|}{2^n} - \frac{|x_i^n - y|}{2^n} + \delta\right)$$

and

- $\delta \ll 1 \ll \ell$;
- $\xi : \mathbb{R}\to[0,1]$ is a suitably chosen increasing $C^1$ function satysfying $\xi(t) = 0$ for $t\le 0$ and $\xi(t) = 1$ for $t\ge\delta$,

- $\xi' \leq f(\xi)$ for a positive concave function $f : [0,\infty) \to [0,\infty)$ with $f(0) = 0$ to be specified later,
- the notation $x_j^n \sim x_i^n$ means that $|x_j^n - x_i^n| \leq 2^n(9\ell - \delta)$.

Fix $N = \kappa_X\big(1/(9\ell - \delta + 1)\big)$. We will prove the lemma through the following steps.

(a) $\tilde{\varphi}_i^n(y) > 0$ implies $(\ell - 2 - \delta)2^n \leq \mathsf{d}(y, X) \leq 8\ell \cdot 2^n$.

(b) Let $I_n(y) = \{i \in I_n : \tilde{\varphi}_i^n(y) > 0\}$, then $|I_n(y)| \leq \kappa_X\big(1/(16\ell + 1)\big)$. Moreover $|\{n : I_n(y) \neq \emptyset\}| \leq \big\lfloor \log_2\big(8\ell/(\ell - 2 - \delta)\big)\big\rfloor$.

(c) $|\nabla \tilde{\varphi}_i^n|(y) \leq 2(N + 1)2^{-n} f\big(\tilde{\varphi}_i^n(y)\big)$.

(d) If $2\ell \leq \mathsf{d}(y, X)2^{-n} \leq 4\ell$ then there exists $i \in I_n$ such that

$$\tilde{\varphi}_i^n(y) \geq \xi(4\ell - 2)\xi(\ell)\xi(\delta)^N = 1,$$

so that in particular $\sum_{i,n} \tilde{\varphi}_i^n(y) \geq 1$ for every $y \in Y \setminus X$.

We start by proving (a). It is obvious that $\mathsf{d}(y, X) \leq |y - x_i^n| \leq 8\ell \cdot 2^n$. For the other inequality suppose by contradiction that there exists $x \in X$ such that $|y - x| < 2^n(\ell - 2 - \delta)$; then there exists $j$ such that $|x - x_j^n| \leq 2^{n+1}$ and so, by triangle inequality we have $|x_j^n - x_i^n| \leq 2^n(9\ell - \delta)$ and in particular $x_j^n \sim x_i^n$. Then, using $\varphi_i^n(y) > 0$ we get

$$|y - x_j^n| \geq |y - x_i^n| - \delta 2^n \geq (\ell - \delta)2^n,$$

which is in contradiction with

$$|y - x_j^n| \leq |y - x| + |x - x_j^n| < (\ell - \delta)2^n.$$

In order to prove (b) we fix $i \in I_n(y)$ and observe that for all $j \in I_n(y)$ we have $|x_j^n - y| \leq 8\ell \cdot 2^n$, and in particular $|x_j^n - x_i^n| \leq 8\ell \cdot 2^{n+1}$, so that $B(x_j^n, 2^n) \subseteq B\big(x_i^n, (16\ell + 1)2^n\big)$ and thus the conclusion follows using the definition of $\kappa_X$. For the second cardinality computation, assume that $y \in A_i^{n_1} \cap A_j^{n_2}$; then from (a) we deduce $|n_1 - n_2| \leq \log_2\big(8\ell/(\ell - 2 - \delta)\big)$.

For (c) it is sufficient to use the chain rule, the fact that the distance to a fixed point is 1-Lipschitz and that $f(a)b \leq f(ab)$ for $a, b \leq 1$ because of the concavity.

The last point follows from taking $i \in I_n$ that minimizes $|y - x_i^n|$. In this way we have that all the factors in the last product are always bigger than $\xi(\delta)$. As for the first two factor, for sure we have $|y - x_i^n| \geq 2\ell \cdot 2^n$ and, calling $\bar{y}$ a projection of $y$ on $X$, there exists $j$ such that $|x_j^n - \bar{y}| \leq 2^{n+1}$. By the minimality of $i$ we get

$$|y - x_i^n| \leq |y - x_j^n| \leq |y - \bar{y}| + |x_j^n - \bar{y}| \leq 2^n(4\ell + 2).$$

These two inequalities let us conclude.

We now compute $|\nabla\varphi_i^n|$. Setting $K(y) = |\{(j,n) : \varphi_j^n(y) > 0\}|$, from (b) we deduce that

$$K(y) \leq \kappa_X\big(1/(16\ell+1)\big)\left\lfloor \log_2\big(8\ell/(\ell-2-\delta)\big)\right\rfloor, \tag{3.2.1}$$

which implies ($i$). Now, using (c) we get

$$|\nabla\varphi_i^n|(y) \leq \frac{2(N+1)}{2^n}\cdot\left(\frac{f\big(\tilde\varphi_i^n(y)\big)}{\sum_{j,k}\tilde\varphi_j^k(y)} + \frac{\tilde\varphi_i^n(y)}{\sum_{j,k}\tilde\varphi_j^k(y)}\cdot\frac{\sum_{j,k} f\big(\tilde\varphi_j^k(y)\big)}{\sum_{j,k}\tilde\varphi_j^k(y)}\right)$$

$$\begin{aligned}
\sum_{i,n}|\nabla\varphi_i^n|(y) &\leq \frac{2(N+1)}{2^n}\cdot\left(\frac{\sum_{j,k} f\big(\tilde\varphi_j^k(y)\big)}{\sum_{j,k}\tilde\varphi_j^k(y)} + \frac{\sum_{j,k}\tilde\varphi_j^k(y)}{\sum_{j,k}\tilde\varphi_j^k(y)}\cdot\frac{\sum_{j,k} f\big(\tilde\varphi_j^k(y)\big)}{\sum_{j,k}\tilde\varphi_j^k(y)}\right)\\
&= \frac{4(N+1)}{2^n}\cdot\frac{\frac{1}{K(y)}\sum_{j,k} f\big(\tilde\varphi_j^k(y)\big)}{\frac{1}{K(y)}\sum_{j,k}\tilde\varphi_j^k(y)} \leq \frac{4(N+1)}{2^n}\cdot\frac{f\Big(\frac{1}{K(y)}\sum_{j,k}\tilde\varphi_j^k(y)\Big)}{\frac{1}{K(y)}\sum_{j,k}\tilde\varphi_j^k(y)}\\
&\leq \frac{4(N+1)}{2^n}\cdot K(y) f\left(\frac{1}{K(y)}\right)\\
&\leq \frac{1}{\mathsf{d}(y,X)}\cdot[32\ell(N+1)]K(y) f\left(\frac{1}{K(y)}\right),
\end{aligned}$$

where we used the concavity of $f$, the fact that $f(t)/t$ is decreasing (it follows from $f(0)=0$ and the concavity), and that $\sum_{j,k}\tilde\varphi_j^k(y)\geq 1$ by (d).

Now we choose $\ell=3$, $\delta=1/2$, and

$$f(t) = \frac{2m}{\delta}t^{1-1/m}$$

which allows the existence of the function $\xi$ as required before by a simple cutoff argument applied to $\tilde\xi(t) = \chi_{[0,\infty)}(t)\left(\frac{2t}{\delta}\right)^m$. From (3.2.1) we deduce that

$$K(y) \leq 4\kappa_X(1/49) \leq 4\lambda_X^6,$$

we obtain also $N = \kappa_X(2/55) \leq \lambda^5$ and we take $m = \log(4\lambda_X^6)$.

We can now finish the proof by estimating

$$\begin{aligned}
\sum_{i,n}|\nabla\varphi_i^n|(y) &\leq \frac{1}{\mathsf{d}(y,X)}\cdot 4[96(N+1)]mK(y)^{1/m}\\
&\lesssim \frac{1}{\mathsf{d}(y,X)}\cdot\lambda^5 m e^{m/m} = \frac{1}{\mathsf{d}(y,X)}\lambda^5\log(\lambda).
\end{aligned}$$

□

## 3.3 Random projections

The following concept has been introduced by Ohta [Oht09] and by Ambrosio and Puglisi [AP16]. In these articles the authors identify a generalization of a deterministic projection onto a subset, an idea that underlies several extension results.

**Definition 3.3.1** (Random projection)**.** Let $X$ be a closed subspace of a metric space $(Y, \mathsf{d})$. We say that a map $\mu : Y \to \mathscr{P}(X) : y \mapsto \mu_y$ is a *random projection* if $\mu_x = \delta_x$ whenever $x \in X$. We say that it is a *Lipschitz random projection* if $\mu \in \mathrm{Lip}\big(Y; W_1(X)\big)$.

**Theorem 3.3.2.** *Let $X \subset (Y, \mathsf{d})$ be a closed subset with doubling constant $\lambda$. Then there exists a Lipschitz random projection $\mu \in \mathrm{Lip}\big(Y; W_1(X)\big)$ with*

$$\mathrm{Lip}(\mu) \lesssim \log \lambda.$$

*Remark* 3.3.3. Notice that any Lipschitz random projection $\mu$ gives automatically a bounded linear extension operator $T : \mathrm{Lip}(X, Z) \to \mathrm{Lip}(Y, Z)$ for every Banach space $Z$ in the following way:

$$(Tf)(y) = \int_X f(x)\, \mathrm{d}\mu_y(x).$$

In fact, thanks to (3.1.1) we have

$$|(Tf)(y) - (Tf)(y')| = \left| \int_X f(x)\, \mathrm{d}(\mu_y - \mu_{y'}) \right| \leq \mathrm{Lip}(f)\, \mathrm{Lip}(\mu) \mathsf{d}(y, y').$$

Therefore the proof of Theorem 3.3.2 can be seen as a proof of the existence of a bounded linear extension operator (see Theorem 3.4.1).

*Proof.* Without loss of generality we can assume that $Y$ is a Banach space, by possibly embedding $Y \subset C_b(Y)$ thanks to the isometric immersion

$$y \mapsto \mathsf{d}(\,\cdot\,, y) - \mathsf{d}(\,\cdot\,, y_0),$$

where $y_0 \in Y$ is a generic fixed point: this is useful because in order to prove that some function $F : Y \in Z$ is $L$-Lipschitz we need only to prove that its slope is bounded by $L$.

Let $\{V_i, \varphi_i, x_i\}_i$ be given by Proposition 3.2.1. Let us then define the random projection

$$\mu_y = \sum_i \varphi_i(y) \delta_{x_i} \quad \text{for } y \in Y \setminus X, \qquad \mu_y = \delta_y \quad \text{for } y \in X.$$

Given a function $f \in \mathrm{Lip}_1(X)$, for $y \in Y \setminus X$ we can compute the slope

$$\begin{aligned}
\left| \nabla_y \int_X f(x)\, \mathrm{d}\mu_y(x) \right| &= \left| \nabla_y \sum_i \varphi_i(y) f(x_i) \right| \\
&= \left| \nabla_y \sum_i \varphi_i(y) [f(x_i) - f(x_{i_0})] \right| \\
&\leq \sum_i |\nabla_y \varphi_i(y)| \cdot |f(x_i) - f(x_{i_0})| \\
&\leq \sum_i |\nabla_y \varphi_i(y)| \cdot \mathsf{d}(x_i, x_{i_0}),
\end{aligned}$$

where $i_0$ is any fixed index for which $y \in V_{i_0}$. In order for $|\nabla_y \varphi_i(y)|$ to be non-zero, one must have $y \in V_i$, therefore from the properties of the points $x_i$'s we infer that $\mathsf{d}(x_i, x_{i_0}) \lesssim \mathsf{d}(y, X)$. With this observation we can continue the previous estimate and obtain

$$\left|\nabla_y \int_X f(x)\,\mathrm{d}\mu_y(x)\right| \lesssim \sum_i |\nabla_y \varphi_i(y)| \cdot \mathsf{d}(y, X) \lesssim \frac{\log\lambda}{\mathsf{d}(y, X)}\mathsf{d}(y, X) = \log\lambda.$$

For points $x \in X$ and $y \in Y \setminus X$ instead we have the estimate

$$\begin{aligned}\left|\int_X f(z)\,\mathrm{d}\mu_y(z) - \int_X f(z)\,\mathrm{d}\mu_x(z)\right| &= \left|\sum_i \varphi_i(y)[f(x_i) - f(x)]\right| \\ &\le \sum_i \varphi_i(y)\big(|f(x_i) - f(x_{i_0})| + |f(x_{i_0}) - f(x)|\big) \\ &\le \sum_i \varphi_i(y)[\mathsf{d}(x_i, x_{i_0}) + \mathsf{d}(x_{i_0}, x)] \\ &\lesssim \mathsf{d}(y, X) + \mathsf{d}(x_{i_0}, x) \\ &\le \mathsf{d}(y, X) + \mathsf{d}(x_{i_0}, y) + \mathsf{d}(y, x) \\ &\lesssim \mathsf{d}(y, x),\end{aligned}$$

so that we have a (better) bound on the slope also at the points in $X$. This fact shows that the map $y \mapsto \int_X f\,\mathrm{d}\mu_y$ has Lipschitz constant less than $\log\lambda$, up to a universal multiplicative constant.

Finally, Definition 3.1.1 of $W_1$ implies that $\mathrm{Lip}(\mu) \lesssim \log\lambda$, indeed. □

We now move on to the corresponding $C^1$ concept of random projection.

**Definition 3.3.4.** Let $X$ be a subset of a Banach space $Y$. We say that a map $\mu : Y \to \mathscr{P}(X)$ is a *regular random projection* if the following conditions hold:

(i) for every $y \in Y$ the measure $\mu_y$ is concentrated on $B\big(y, \eta\mathsf{d}(y, X)\big)$ for some $\eta > 0$;

(ii) for all $f \in C(X)$ the map $F(y) = \int_X f(x)\,\mathrm{d}\mu_y(x)$ is well defined, belongs to $C(Y) \cap C^1(Y \setminus X)$, and there exists $\nu : Y \setminus X \to \mathscr{M}(X; Y^*)$ such that

$$\mathrm{d}F_y = \int_X f(x)\,\mathrm{d}\nu_y(x) \qquad \text{for all } y \in Y \setminus X; \tag{3.3.1}$$

(iii) for all $y \in Y \setminus X$ the measure $\nu_y$ is concentrated on $B\big(y, \eta\mathsf{d}(y, X)\big)$ and its total variation can be estimated with

$$\|\nu_y\|_{\mathrm{TV}} \le \frac{C_X}{\mathsf{d}(y, X)}.$$

*Remark* 3.3.5. With the definition above we have that $\nu_x(X) = 0$ for all $x \in Y \setminus X$, since

$$\nu_y(X) = \int_X 1 \, \mathrm{d}\nu_y = \mathrm{d}\left(\int_X 1 \, \mathrm{d}\mu_x\right)_y = \mathrm{d}1_y = 0.$$

**Theorem 3.3.6** (Regular random projection). *Let $Y$ be a Banach space whose norm belongs to $C^1(Y \setminus \{0\})$ and let $X \subset Y$ be a closed subset with doubling constant $\lambda$. Then there exists a regular random projection $\mu_y$ whose associated $\nu_y$ has total variation*

$$\|\nu_y\|_{\mathrm{TV}} \lesssim \frac{\lambda^4 \log \lambda}{\mathsf{d}(y, X)}.$$

*Proof.* Let $\{V_i, \varphi_i, x_i\}_i$ be given by Proposition 3.2.2. Let us then define the random projection

$$\mu_y = \sum_i \varphi_i(y)\delta_{x_i} \quad \text{for } y \in Y \setminus X, \qquad \mu_y = \delta_y \quad \text{for } y \in X.$$

Property (i) of Definition 3.3.4 follows immediately from (iii) of Proposition 3.2.2. Let us fix $f \in C(X)$. The function $F(y) = \int_X f(x) \, \mathrm{d}\mu_y(x)$ is clearly well defined since the measure $\mu_y$ is supported on a finite number of points. Moreover, it is also $C^1(Y \setminus X)$ because the coefficients $\varphi_i(y)$ are $C^1$ themselves. Given a point $y \in Y \setminus X$, it is immediate to check that the differential of $F$ at the point $y$ is represented through (3.3.1) by the vector measure

$$\nu_y = \sum_i \mathrm{d}(\varphi_i)_y \delta_{x_i}.$$

Finallly, (iii) of Definition 3.3.4 follows from (ii) of Proposition 3.2.2. □

## 3.4 Linear extension operators

### 3.4.1 Lipschitz

In this section we state and prove the main result about the extendability of Lipschitz functions. The theorem has already appeared in [LN05], but we provide two independent and shorter proofs.

**Theorem 3.4.1.** *Let $(Y, \mathsf{d})$ be a metric space and $X \subset Y$ a closed subset with finite doubling constant $\lambda$; let moreover $Z$ be a Banach space. Then there exists a linear extension operator $T : \mathrm{Lip}(X; Z) \to \mathrm{Lip}(Y; Z)$ such that*

$$\mathrm{Lip}(Tf) \lesssim \log \lambda \, \mathrm{Lip}(f) \qquad \forall f \in \mathrm{Lip}(X; Z).$$

As already observed in Remark 3.3.3, this result can be obtained already as a direct consequence of Theorem 3.3.2, but we wanted also to provide a self-contained proof that does not require the construction of a partition of unity, but instead exploits the existence of a doubling measure $\mathfrak{m}$ supported on the whole $X$.

*Direct proof.* Without loss of generality we can assume that $Y$ is a Banach space, by embedding $Y \subset C_b(Y)$ thanks to the isometric immersion

$$y \mapsto \mathsf{d}(\,\cdot\,, y) - \mathsf{d}(\,\cdot\,, y_0),$$

where $y_0 \in Y$ is a fixed point. In particular we can assume that also $X$ is complete by considering its new closure. Let $\mathfrak{m}$ be a doubling measure on $X$, provided for instance by [VK88]. We consider the random projection $\mu : Y \to \mathscr{P}(X)$ absolutely continuous with respect to $\mathfrak{m}$ given by

$$\mu_y = u_y(x)\mathfrak{m} = \frac{\varphi^m\left(\frac{\mathsf{d}(y,x)}{\mathsf{d}(y,X)}\right)}{\int_X \varphi^m\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right) \mathrm{d}\mathfrak{m}(z)}\mathfrak{m},$$

where $\varphi \in C^1\big([0,\infty); [0,1]\big)$ is such that $\varphi(t) = 1$ for $t \leq 2$, $\varphi(t) = 0$ for $t \geq 3$ and $m > 0$ is a parameter to be optimized later. Notice that the denominator is non-zero because $\mathfrak{m}$ is doubling. Roughly speaking, this $\mu$ has to be intended as a suitably smoothed version of

$$\tilde{\mu}_y = \frac{\mathfrak{m} \llcorner B\big(y, 3\mathsf{d}(y,X)\big)}{\mathfrak{m}(B\big(y, 3\mathsf{d}(y,X)\big))}.$$

Given a function $f \in \mathrm{Lip}(X; Z)$, we define its extension $Tf$ by

$$Tf(y) = \int_X f(x)\, \mathrm{d}\mu_y(x).$$

In order to compute $\mathrm{Lip}(Tf)$, we now proceed by estimating the slope of the density $u_y$.

By Leibniz and Fatou[3] we have

$$|\nabla_y u_y(x)| \leq \frac{\left|\nabla_y \varphi^m\left(\frac{\mathsf{d}(y,x)}{\mathsf{d}(y,X)}\right)\right|}{\int_X \varphi^m\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right) \mathrm{d}\mathfrak{m}(z)} + \frac{\varphi^m\left(\frac{\mathsf{d}(y,x)}{\mathsf{d}(y,X)}\right) \int_X \left|\nabla_y \varphi^m\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\right| \mathrm{d}\mathfrak{m}(z)}{\left[\int_X \varphi^m\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right) \mathrm{d}\mathfrak{m}(z)\right]^2}$$

Integrating in $x$ and simplifying we obtain

$$\int_X |\nabla_y u_y(x)|\, \mathrm{d}\mathfrak{m}(x) = 2\frac{\int_X \left|\nabla_y \varphi^m\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\right| \mathrm{d}\mathfrak{m}(z)}{\int_X \varphi^m\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right) \mathrm{d}\mathfrak{m}(z)}.$$

[3] To apply the latter in order to the pass the slope inside the integral, we need also that

$$\sup_{\substack{z \in X \\ \mathsf{d}(y,y') < \frac{1}{2}\mathsf{d}(y,X)}} \frac{1}{\mathsf{d}(y,y')} \left|\varphi^m\left(\frac{\mathsf{d}(y',z)}{\mathsf{d}(y',X)}\right) - \varphi^m\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\right| < \infty.$$

One can then compute

$$\begin{aligned}\left|\nabla_y\varphi^m\!\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\right| &\le m\varphi^{m-1}\!\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\left|\varphi'\!\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\right|\cdot\left|\nabla_y\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\right|\\ &\le m\varphi^{m-1}\!\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\left|\varphi'\!\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\right|\frac{1}{\mathsf{d}(y,X)}\left(1+\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right).\end{aligned}$$

Plugging this into the previous equation, observing that the ratio $\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}<3$ where $\varphi$ is not vanishing and using Hölder inequality in the second step[4] we get

$$\begin{aligned}\int_X|\nabla_y u_y(x)|\,\mathrm{d}\mathfrak{m}(x) &\le \frac{8m}{\mathsf{d}(y,X)}\cdot\frac{\int_X\varphi^{m-1}\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\left|\varphi'\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\right|\mathrm{d}\mathfrak{m}(z)}{\int_X\varphi^m\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\mathrm{d}\mathfrak{m}(z)}\\ &\le \frac{8m}{\mathsf{d}(y,X)}\left(\frac{\int_X\left|\varphi'\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\right|^m\mathrm{d}\mathfrak{m}(x)}{\int_X\varphi^m\left(\frac{\mathsf{d}(y,z)}{\mathsf{d}(y,X)}\right)\mathrm{d}\mathfrak{m}(x)}\right)^{1/m}\\ &\le \frac{8m}{\mathsf{d}(y,X)}\left(\frac{\mathfrak{m}\big(B\big(y,3\mathsf{d}(y,X)\big)\big)}{\mathfrak{m}\big(B\big(y,2\mathsf{d}(y,X)\big)\big)}\right)^{1/m}.\end{aligned}$$

The ratio appearing in the last formula is related to the doubling constant $\lambda$, however one has to be a bit careful because the point $y$ does not belong to $X$. By fixing a point $\tilde{y}\in X$ such that $\mathsf{d}(y,\tilde{y})\le(1+\varepsilon)\mathsf{d}(y,X)$ we get

$$\frac{\mathfrak{m}\big(B\big(y,3\mathsf{d}(y,X)\big)\big)}{\mathfrak{m}\big(B\big(y,2\mathsf{d}(y,X)\big)\big)}\le\frac{\mathfrak{m}\big(B\big(\tilde{y},(4+\varepsilon)\mathsf{d}(y,X)\big)\big)}{\mathfrak{m}\big(B\big(\tilde{y},(1-\varepsilon)\mathsf{d}(y,X)\big)\big)}\le\lambda^3.$$

Hence

$$\int_X|\nabla_y u_y(x)|\,\mathrm{d}\mathfrak{m}(x)\lesssim\frac{m\lambda^{3/m}}{\mathsf{d}(y,X)}\lesssim\frac{\log\lambda}{\mathsf{d}(y,X)}$$

by choosing $m=\frac{1}{3}\log\lambda$.

We can finally estimate the Lipschitz constant of $Tf$. We start with its slope at $y\in Y\setminus X$. Fixing a point $\tilde{y}\in X$ such that $\mathsf{d}(y,\tilde{y})\lesssim\mathsf{d}(y,X)$, we have

$$\begin{aligned}|\nabla Tf|(y) &\le \left|\nabla_y\int_X[f(x)-f(\tilde{y})]\,\mathrm{d}\mu_y(x)\right|\\ &\le \int_{B\left(y,3\mathsf{d}(y,X)\right)}|f(x)-f(\tilde{y})|\cdot|\nabla_y u_y(x)|\,\mathrm{d}\mathfrak{m}(x)\\ &\lesssim \int_{B\left(y,3\mathsf{d}(y,X)\right)}\mathrm{Lip}(f)[\mathsf{d}(x,y)+\mathsf{d}(y,\tilde{y})]\frac{\log\lambda}{\mathsf{d}(y,X)}\,\mathrm{d}\mu_y(x)\\ &\lesssim \mathrm{Lip}(f)\mathsf{d}(y,X)\frac{\log\lambda}{\mathsf{d}(y,X)}\\ &\lesssim \log\lambda\,\mathrm{Lip}(f),\end{aligned}$$

[4]With exponents $m/(m-1)$ and $m$.

where we were able to bring the slope inside the integral because the difference ratios near $y$ are uniformly bounded in $x$. Similarly, for $x \in X$ and $y \in Y \setminus X$ one can compute

$$\begin{aligned}|Tf(y) - Tf(x)| &\leq \int_X |f(z) - f(x)| \,\mathrm{d}\mu_y(z) \\ &\leq \mathrm{Lip}(f) \int_{B\left(y, 3\mathsf{d}(y,X)\right)} \mathsf{d}(z,x) \,\mathrm{d}\mu_y(z) \\ &\leq \mathrm{Lip}(f) \int_{B\left(y, 3\mathsf{d}(y,X)\right)} [\mathsf{d}(z,y) + \mathsf{d}(y,x)] \,\mathrm{d}\mu_y(z) \\ &\lesssim \mathrm{Lip}(f)[\mathsf{d}(y,X) + \mathsf{d}(y,x)] \\ &\lesssim \mathrm{Lip}(f)\mathsf{d}(x,y)\end{aligned}$$

These two computations prove the Lipschitzianity of the map $Tf$, whith constant $\mathrm{Lip}(Tf) \lesssim \log\lambda \,\mathrm{Lip}(f)$, since the space $Y$ is Banach. □

*Remark* 3.4.2. Actually, the previous proof is an alternative self-contained construction of a Lipschitz random projection $\mu$ that does not use a Lipschitz partition of unity.

### 3.4.2 Whitney

The goal of this section is to generalize Whitney's extension theorem [Whi34] to Banach spaces.

Let $Y$ be a Banach space and let $X \subset Y$ be a closed subset of $X$, we assume that $f : X \to \mathbb{R}$ and $L : X \to Y^*$ are given functions. We define

$$R(x,y) = f(y) - f(x) - L_x(y-x) \qquad x, y \in X.$$

Our aim is to find conditions on $R$ and $X$ in order to have a $C^1$ extension of $f$ at the whole $Y$ and we want that its differential coincides with $L$ in $X$. The classical Whitney's extension theorem ensures that when $Y = \mathbb{R}^n$ and $R(x,y) = o(|x-y|)$ in a suitable sense then the $C^1$ extension there exists. Our result is the following:

**Theorem 3.4.3.** *Let $Y$ be a Banach space whose norm belongs to $C^1(Y \setminus \{0\})$ and let $X \subset Y$ be a closed subset with doubling constant $\lambda$. Given two continuous functions $f : X \to \mathbb{R}$ and $L : X \to Y^*$, define the remainder*

$$R(x,y) = f(y) - f(x) - L_x(y-x) \qquad \text{for } x, y \in X,\ x \neq y$$

*and assume that the function*

$$(x,y) \mapsto \frac{R(x,y)}{|y-x|}$$

*can be extended to a continuous function on* $X \times X$ *that takes the value* $0$ *where* $y = x$*. Then there exists an extension* $\tilde{f} \in C^1(Y)$ *such that* $d\tilde{f}_x = L_x$ *for all* $x \in X$*.*

*Moreover, the extension operator* $(f, L) \mapsto \tilde{f}$ *is linear.*

First we prove a key lemma, that is an integral version of $R(x, y) = o(|x - y|)$, given our hypotesis on $R$.

**Lemma 3.4.4.** *Let* $\bar{\mu} : Y \to \mathscr{M}_+(X)$ *be a weakly measurable map such that* $|\bar{\mu}_y|(X) \leq 1$ *and there exists* $C > 0$ *such that* $\operatorname{supp} \bar{\mu}_y \in B\big(y, C\mathsf{d}(y, X)\big)$ *for all* $y \in Y$*. Assuming the hypothesis of the Theorem 3.4.3, for all* $x \in X$ *we have*

$$\int_X |R(z, x)| \, \mathrm{d}\bar{\mu}_y(z) = o(|x - y|) \qquad \text{as } y \to x.$$

*Proof.* Let $\tilde{y} \in X$ be a point such that $|y - \tilde{y}| \leq 2\mathsf{d}(y, X)$. We can estimate

$$\begin{aligned} |R(z, x)| &\leq |R(z, x) - R(z, \tilde{y})| + |R(z, \tilde{y})| \\ &= |f(\tilde{y}) - f(x) - L_z(\tilde{y} - x)| + |R(z, \tilde{y})| \\ &\leq |f(\tilde{y}) - f(x) - L_x(\tilde{y} - x)| + |(L_z - L_x)(\tilde{y} - x)| + |R(z, \tilde{y})| \\ &\leq |R(x, \tilde{y})| + \|L_z - L_x\| |\tilde{y} - x| + |R(z, \tilde{y})|. \end{aligned}$$

We observe that

$$|\tilde{y} - x| \leq |\tilde{y} - y| + |y - x| \leq 2\mathsf{d}(y, X) + |y - x| \leq 3|y - x|, \tag{3.4.1}$$

therefore we have

$$\int_X |R(z, x)| \, \mathrm{d}\bar{\mu}_y(z) \leq \underbrace{|R(x, \tilde{y})|}_{A} + \underbrace{3|y - x| \int_X |L_z - L_x| \, \mathrm{d}\bar{\mu}_y(z)}_{B} + \underbrace{\int_X |R(z, \tilde{y})| \, \mathrm{d}\bar{\mu}_y(z)}_{C}.$$

We analize each contribution separately.

($A$) Using (3.4.1) and the continuity of $(x, y) \mapsto R(x, y)/|x - y|$ we have

$$\frac{|R(x, \tilde{y})|}{|x - y|} \leq 3 \frac{|R(x, \tilde{y})|}{|x - \tilde{y}|} \to 0.$$

($B$) The term $\int_X |L_z - L_x| \, \mathrm{d}\bar{\mu}_y(z)$ is infinitesimal as $y$ goes to $x$ because the map $z \mapsto |L_z - L_x|$ is continuous and $\operatorname{supp} \bar{\mu}_y \in B\big(y, C\mathsf{d}(y, X)\big)$.

$(C)$ We can estimate

$$\begin{aligned}
\int_X |R(z,\tilde{y})| \,\mathrm{d}\bar{\mu}_y(z) &= \int_{X\cap B\left(y,C\mathsf{d}(y,X)\right)} |R(z,\tilde{y})| \,\mathrm{d}\bar{\mu}_y(z) \\
&= \int_{X\cap B\left(y,C\mathsf{d}(y,X)\right)} |z-\tilde{y}| \frac{|R(z,\tilde{y})|}{|z-\tilde{y}|} \,\mathrm{d}\bar{\mu}_y(z) \\
&\leq \int_X |\tilde{y}-y| \frac{|R(z,\tilde{y})|}{|z-\tilde{y}|} \,\mathrm{d}\bar{\mu}_y(z) \\
&\qquad + \int_{X\cap B\left(y,C\mathsf{d}(y,X)\right)} |y-z| \frac{|R(z,\tilde{y})|}{|z-\tilde{y}|} \,\mathrm{d}\bar{\mu}_y(z) \\
&\leq |\tilde{y}-y| \int_X \frac{|R(z,\tilde{y})|}{|z-\tilde{y}|} \,\mathrm{d}\bar{\mu}_y(z) \\
&\qquad + C\mathsf{d}(y,X) \int_X \frac{|R(z,\tilde{y})|}{|z-\tilde{y}|} \,\mathrm{d}\bar{\mu}_y(z) \\
&\leq (2+C)|y-x| \int_X \frac{|R(z,\tilde{y})|}{|z-\tilde{y}|} \,\mathrm{d}\bar{\mu}_y(z).
\end{aligned}$$

Finally we observe that again using (3.4.1) we have $\tilde{y} \to x$ and thanks to the continuity of $(x,y) \mapsto R(x,y)/|x-y|$ we have

$$\int_X \frac{|R(z,\tilde{y})|}{|z-\tilde{y}|} \,\mathrm{d}\bar{\mu}_y(z) \leq \sup_{z\in B\left(y,C\mathsf{d}(y,X)\right)\cap X} \frac{|R(z,\tilde{y})|}{|z-\tilde{y}|} \to 0. \qquad \square$$

*Proof of Theorem 3.4.3.* Let $\mu$ be a regular random projection as provided by Theorem 3.3.6. We define the extension of $f$ as

$$\tilde{f}(y) = \int_X [f(z) + L_z(y-z)] \,\mathrm{d}\mu_y(z). \tag{3.4.2}$$

We first prove that the function $\tilde{f}$ is differentiable at any point $x \in X$ and that $\mathrm{d}f_x = L_x$. Indeed, we have

$$\begin{aligned}
|\tilde{f}(y) - \tilde{f}(x) - L_x(y-x)| &= \left| \int_X [f(z) + L_z(y-z)] \,\mathrm{d}\mu_y(z) - f(x) - L_x(y-x) \right| \\
&\leq \left| \int_X [f(x) - f(z) - L_z(x-z)] \,\mathrm{d}\mu_y(z) \right| \\
&\qquad + \left| \int_X (L_z - L_x)(y-x) \,\mathrm{d}\mu_y(z) \right| \\
&\leq \int_X |R(z,x)| \,\mathrm{d}\mu_y(z) + |y-x| \int_X |L_z - L_x| \,\mathrm{d}\mu_y(z),
\end{aligned}$$

the last term is $o(|y-x|)$ thanks to Lemma 3.4.4 and the continuity of $L$.

Now we observe that $\tilde{f} \in C^1(Y \setminus X)$ and

$$\mathrm{d}\tilde{f}_y = \int_X L_z \, \mathrm{d}\mu_y(z) + \int_X [f(z) + L_z(y-z)] \, \mathrm{d}\nu_y(z) \qquad \forall y \in Y \setminus X$$

by a simple differentiation of (3.4.2) and using (ii) of Definition 3.3.4.

In order to conclude the proof we have to check that $y \mapsto \mathrm{d}\tilde{f}_y$ is a continuous map from $Y$ to $Y^*$. We already know that the differential of $\tilde{f}$ is continuous on the open set $Y \setminus X$ and when it is restricted to $X$, therefore it is enough to estimate $|\mathrm{d}\tilde{f}_y - \mathrm{d}\tilde{f}_x|$ with $y \in Y \setminus X$ and $x \in X$. Fixing a point $\tilde{y} \in X$ such that $|y - \tilde{y}| \leq 2\mathsf{d}(y, X)$, we have

$$\begin{aligned} |\mathrm{d}\tilde{f}_y - \mathrm{d}\tilde{f}_x| &\leq |\mathrm{d}\tilde{f}_y - \mathrm{d}\tilde{f}_{\tilde{y}}| + |\mathrm{d}\tilde{f}_{\tilde{y}} - \mathrm{d}\tilde{f}_x| \\ &= |\mathrm{d}\tilde{f}_y - \mathrm{d}\tilde{f}_{\tilde{y}}| + |L_{\tilde{y}} - L_x|. \end{aligned}$$

Now we estimate the first term as

$$\begin{aligned} |\mathrm{d}\tilde{f}_y - \mathrm{d}\tilde{f}_{\tilde{y}}| &= \left| \left( \int_X L_z \, \mathrm{d}\mu_y(z) + \int_X [f(z) + L_z(y-z)] \, \mathrm{d}\nu_y(z) \right) - L_{\tilde{y}} \right| \\ &\leq \left| \int_X f(z) + L_z(y-z) \, \mathrm{d}\nu_y(z) \right| + \left| \int_X L_z \; d\mu_y(z) - L_{\tilde{y}} \right| \\ &\leq \left| \int_X f(z) + L_z(y-z) \, \mathrm{d}\nu_y(z) \right| + \int_X |L_z - L_{\tilde{y}}| \, \mathrm{d}\mu_y(z). \end{aligned}$$

Recalling Remark 3.3.5 we have

$$\begin{aligned} \left| \int_X f(z) + L_z(y-z) \, \mathrm{d}\nu_y(z) \right| &= \left| \int_X f(z) - f(\tilde{y}) - L_z(z-\tilde{y}) \, \mathrm{d}\nu_y(z) \right| \\ &\quad + \left| \int_X L_z(y-\tilde{y}) \, \mathrm{d}\nu_y(z) \right| \\ &\leq \int_X |R(z,\tilde{y})| \, \mathrm{d}|\nu_y|(z) + |y-\tilde{y}| \int_X |L_z - L_{\tilde{y}}| \, \mathrm{d}|\nu_y|(z). \end{aligned}$$

Using the property (iii) in Definition 3.3.4 we can write $|\nu_y| = \frac{C}{\mathsf{d}(y,X)} \bar{\mu}_y$ and we notice that $\bar{\mu}_y$ satisfies the hypotesis in Lemma 3.4.4. Moreover recalling the assumption $|y - \tilde{y}| \leq 2\mathsf{d}(y, X)$ we have

$$\begin{aligned} &\left| \int_X f(z) + L_z(y-z) \, \mathrm{d}\nu_y(z) \right| \\ &\qquad \leq \frac{C}{\mathsf{d}(y,X)} \int_X |R(z,\tilde{y})| \, \mathrm{d}\bar{\mu}_y(z) + \frac{C|y-\tilde{y}|}{\mathsf{d}(y,X)} \int_X |L_z - L_{\tilde{y}}| \, \mathrm{d}\bar{\mu}_y(z) \\ &\qquad\qquad \leq \frac{2C}{|\tilde{y} - y|} \int_X |R(z,\tilde{y})| \, \mathrm{d}\bar{\mu}_y(z) + 2C \int_X |L_z - L_{\tilde{y}}| \, \mathrm{d}\bar{\mu}_y(z). \end{aligned}$$

Finally putting all together

$$|\mathrm{d}\tilde{f}_y - \mathrm{d}\tilde{f}_x| \leq |L_{\tilde{y}} - L_x| + (2C+1)\int_X |L_z - L_{\tilde{y}}|\,\mathrm{d}\mu_y(z) + \frac{2C}{|\tilde{y}-y|}\int_X |R(z,\tilde{y})|\,\mathrm{d}\bar{\mu}_y(z).$$

Recalling $|x - \tilde{y}| \leq 3|x - y|$ and Lemma 3.4.4 we conclude that $|\mathrm{d}\tilde{f}_y - \mathrm{d}\tilde{f}_x| \to 0$ when $y$ goes to $x$. This shows that $\mathrm{d}\tilde{f}$ is continuous also in every point of $X$ and concludes the proof. □

# Part II

# Multi-marginal optimal transport

# Chapter 4

# Introduction to the multi-marginal optimal transport

A natural problem in Quantum Physics consists in studying the behavior of $N$ electrons subject to the interaction with some nuclei, their mutual interaction and the effect of an external potential. In this setting, a relevant quantity is the ground state energy of the system, which can be found by solving the Schrödinger equation. However, this procedure is computationally very costly even for a small number of electrons; Density Functional Theory proposes an alternative method to compute the ground state energy and was first introduced by Hohenberg and Kohn [HK64] and then by Kohn and Sham [KS65]. Because of its low computational cost and of its accuracy, it is considered the most popular method for electronic structure calculations in condensed matter physics and quantum chemistry.

In [BPG12; CFK13] the authors present a mathematical model for the strong interaction limit of Density Functional Theory; they study the minimal interaction of $N$ electrons and the semiclassical limit of DFT. They want to determine the ground state energy

$$E_0 = \min_{\psi} \big\{ T[\psi] + V_{ee}[\psi] + V_{\text{ext}}[\psi] \big\}$$

of a system of $N$ electrons in an external potential (orbiting the nucleus of an atom, for instance), where $\psi \in H^1\big(\mathbb{R}^{3N}; \mathbb{C}\big)$, $\|\psi\|_{L^2} = 1$, is the wave function of the system and the three terms appearing on the right are respectively the kinetic energy

$$T[\psi] = \frac{1}{2} \int_{\mathbb{R}^{3N}} |\nabla \psi(x_1, \dots, x_N)|^2 \, dx_1 \cdots dx_N,$$

the electron-electron interaction energy

$$V_{ee}[\psi] = \sum_{1 \le i < j \le N} \int_{\mathbb{R}^{3N}} \frac{1}{|x_i - x_j|} |\psi(x_1, \dots, x_N)|^2 \, dx_1 \cdots dx_N,$$

and the external energy

$$V_{\text{ext}}[\psi] = \sum_{i=1}^{N} \int_{\mathbb{R}^{3N}} v(x_i) |\psi(x_1, \dots, x_N)|^2 \, dx_1 \cdots dx_N$$

induced by a given potential $v : \mathbb{R}^3 \to \mathbb{R} \cup \{\infty\}$. The idea is then to express everything in terms of the single electron density induced by $\psi$ (denoted by $\psi \downarrow \rho$)

$$\rho(x) = \int_{\mathbb{R}^{3(N-1)}} |\psi(x, x_2, \dots, x_N)|^2 \, dx_2 \cdots dx_N.$$

The external energy is easily rewritten as $V_{\text{ext}}[\psi] = N \int_{\mathbb{R}^3} v(x) \, d\rho(x)$. Hohenberg and Kohn then write

$$E_0 = \min_{\rho} \left\{ F_{HK}(\rho) + N \int_{\mathbb{R}^3} v(x) \, d\rho(x) \right\}$$

where

$$F_{HK}(\rho) = \min_{\psi \downarrow \rho} \big\{ T[\psi] + V_{ee}[\psi] \big\}$$

is the *universal Hohenberg-Kohn functional*. From the physical point of view, the difficulty lies in approximating this functional. The simplification introduced by Kohn and Sham consists in writing $F_{HK}(\rho) = F_{KS}(\rho) + F_{xc}(\rho)$ where

$$F_{KS}(\rho) = \min_{\psi \downarrow \rho} T[\psi]$$

is the *Kohn-Sham functional* and $F_{xc}(\rho)$ is the so called *exchange-correlation energy*, which takes into account the electron-electron interaction and needs to be accurately estimated. Clearly $F_{xc}(\rho) \geq \min_{\psi \downarrow \rho} V_{ee}[\psi]$ and there are situations in which this estimate provides a suitable approximation, that is we can assume

$$F_{HK}(\rho) \simeq F_{KS}(\rho) + \min_{\psi \downarrow \rho} V_{ee}[\psi],$$

for example when the electron-electron interaction is preponderant, the so called *strictly correlated electrons* regime.

It's at this point that the optimal transport theory comes into play: the minimization $\min_{\psi \downarrow \rho} V_{ee}[\psi]$ can be seen as an instance of the Monge multimarginal optimal transport problem.

This problem (for which we refer the reader to the recent survey [DGN17], where the state of the art about it is described) consists in the minimization

$$(M) = \inf \left\{ \int_{\mathbb{R}^n} C\big(x, T_2(x), \dots, T_N(x)\big) \, d\rho(x) : T_2, \dots, T_N \in \mathcal{T}(\rho) \right\}, \quad (4.0.1)$$

where $\rho \in \mathscr{P}(\mathbb{R}^n)$ is a given probability measure, $C : (\mathbb{R}^n)^N \to [0, \infty]$ is the Coulomb interaction

$$C(x_1, \dots, x_N) = \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} \qquad \forall (x_1, \dots, x_N) \in (\mathbb{R}^n)^N, \quad (4.0.2)$$

and $\mathcal{T}(\rho)$ is the set of admissible transport maps

$$\mathcal{T}(\rho) = \{ T : \mathbb{R}^n \to \mathbb{R}^n \text{ Borel} : T_\sharp \rho = \rho \} .$$

Since the cost is symmetric, a natural variant of the Monge problem allows only cyclical maps

$$(M_{\text{cycl}}) = \inf \left\{ \int_{\mathbb{R}^n} C\big(x, T(x), \ldots, T^{(N-1)}(x)\big)\, d\rho(x) : T \in \mathcal{T}(\rho),\, T^{(N)} = \text{Id} \right\}$$

where with $T^{(k)}$ we denote the composition of $T$ with itself for $k$ times. Following the standard theory of optimal transport as presented in Chapter 1, we also introduce the Kantorovich problem

$$(K) = \min \left\{ \int_{(\mathbb{R}^n)^N} c(x_1, \ldots, x_N)\, d\gamma(x_1, \ldots, x_N) : \gamma \in \Pi(\rho) \right\},$$

where $\Pi(\rho)$ is the set of transport plans

$$\Pi(\rho) = \left\{ \gamma \in \mathscr{P}(\mathbb{R}^{nN}) : \pi^i_\sharp \gamma = \rho,\, i = 1, \ldots, N \right\}$$

and $\pi^i : (\mathbb{R}^n)^N \to \mathbb{R}^n$ are the projections on the $i$-th component for $i = 1, \ldots, N$. To every $(N-1)$-uple of transport maps $T_2, \ldots, T_N \in \mathcal{T}(\rho)$ we canonically associate the transport plan $\gamma = (Id, T_2, \ldots, T_N)_\sharp \rho \in \Pi(\rho)$. As proved in [CD15], if $\rho$ is non-atomic the values of the minimum problems coincide

$$(K) = (M) = (M_{\text{cycl}}).$$

Existence of optimal transport plans in $(K)$ follows from a standard compactness and lower semicontinuity argument. In turn, existence of optimal maps in $(M)$ is largely open; it is understood only with $N = 2$ marginals in any dimension $n$ and in dimension $n = 1$ with any number $N$ of marginals (see [CFK13] and [CDD15] respectively). In a different context, optimal cyclical maps as in $(M_{\text{cycl}})$ appear in [GM14] for some particular costs generated by vector fields. Regarding the special case of spherically symmetric densities in dimension more than 1 and with any number of marginals, in [Sei99; SGS07] the authors have conjectured the validity of the same structure as the one-dimensional case. This conjecture however turns out to be false and Chapter 5 is dedicated to the discussion of this problem.

As regards uniqueness of optimal symmetric plans with Coulomb cost, it holds in dimension 1, but, as shown in [Pas13], it fails in the same class already when we consider spherically symmetric densities in $\mathbb{R}^2$, for any $N$. On the other hand, the Kantorovich duality works also for this cost (see [RR98]) and the dual problem admits maximizers (namely, Kantorovich's potentials), as shown by De Pascale [De 15]; moreover, in [CFP15] the limit of symmetric optimal plans as $N \to \infty$ is shown to be the infinite product measure of $\rho$ with itself.

Finally, there is the important question of the finiteness of the problem (K). In [BCP16] the authors provide a positive result under the assumption that the marginal $\rho$ does not have atoms of size $\frac{1}{N(N-1)^2}$. As we will see, the correct threshold for the finiteness is $1/N$ and will be obtained in Chapter 6. The question is linked also to the regularity properties of the dual potentials, as shown in the same article [BCP16], so we obtain the same results under the more general assumption. As a byproduct of the construction one obtains also the continuity of the cost with respect to the marginal $\rho$. This again is taken from [BCP16], with the improvements on the estimates.

# Chapter 5

# Counterexamples in multi-marginal optimal transport with Coulomb cost and spherically symmetric data

## 5.1 Introduction

Beyond the 1-dimensional case, which is well understood, a physically relevant case is given by spherically symmetric densities $\rho$ in $\mathbb{R}^n$, with any number of marginals. In the physics literature, they appear in [Sei99; SGS07] to study simple atoms like Helium ($N = 2$), Litium ($N = 3$), and Berillium ($N = 4$). In this case the problem reduces, thanks to the spherical symmetry, to a problem in 1-dimension, with a more complicated cost function (see [Pas13], where this reduction is rigorously described). In the class of admissible transport maps for problem ($M_{\text{cycl}}$), Seidl, Gori Giorgi and Savin identified some particularly simple maps: roughly speaking, they divide $\mathbb{R}^n$ in $N$ spherical shells, each containing one electron in average, and consider the transport maps which send each shell onto the next one by a monotonically increasing or decreasing map. They conjecture the optimality of one of these maps in ($M_{\text{cycl}}$).

In the following, we provide counterexamples to the conjecture showing that there are cases in which none of these maps are optimal in problem ($M_{\text{cycl}}$). On the other hand, we also point out situations where some of these maps satisfy optimality conditions, namely $c$-monotonicity. We deal for simplicity with radial measures in $\mathbb{R}^2$ with 3 marginals, although similar examples and computations can be carried out in any dimension and with any number of marginals. The result applies in the to the physically relevant cases described above and shows that the optimal maps for radially symmetric data exibit a richer structure than the one depicted in [Sei99; SGS07]. In [DNG], currently in preparation, further numerical examples and considerations will be provided on the same topic.

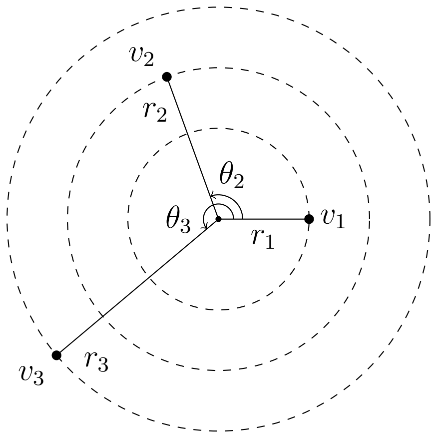



Figure 5.1: A configuration of three charges at distances $r_1$, $r_2$ and $r_3$ with angles $\theta_2$ and $\theta_3$.

The plan of the paper is the following. In Section 5.2 we present the problem with spherically symmetric data, we recall the notion of $c$-monotonicity and a few properties of optimal transport maps, and we give some examples and counterexamples. In Sections 5.3 and 5.4 we study the properties of the cost for close radii and for spread apart radii, respectively. In Section 5.5 we apply these properties to give rigorous proofs of the examples and counterexamples.

## 5.2 Examples and counterexamples

### 5.2.1 Monge and Kantorovich problems with radial densities

As we mentioned above, the transport problem (4.0.1) reduces to a 1-dimensional one (i.e., by proving that spheres get mapped to spheres), as rigorously done in [Pas13]. Assuming from now on $N = 3$ and denoting $(0,\infty)$ by $\mathbb{R}_+$, given three radii $r_1, r_2, r_3 \in \mathbb{R}_+$, we consider the associated *exact cost* (see Figure 5.1)

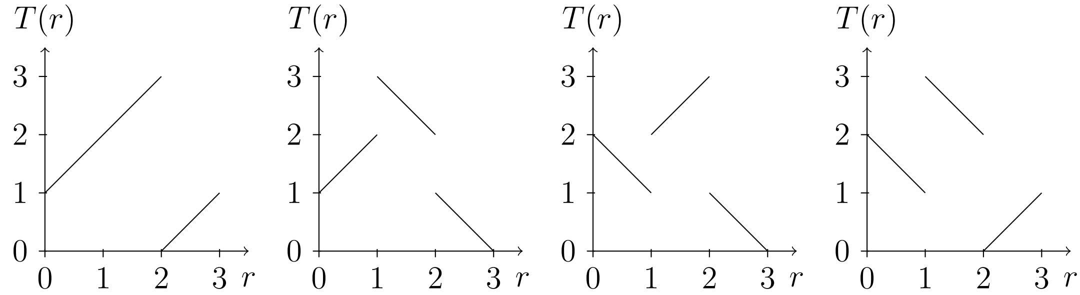
$$c(r_1, r_2, r_3) = \min\left\{ \frac{1}{|v_2 - v_1|} + \frac{1}{|v_3 - v_2|} + \frac{1}{|v_1 - v_3|} : |v_i| = r_i,\ i = 1, 2, 3 \right\}, \tag{5.2.1}$$

which is a positive, symmetric, continuous function. Given a non-atomic probability measure $\rho \in \mathscr{P}(\mathbb{R}_+)$, the set of transport maps reads as

$$\mathcal{T}(\rho) = \{\, T : \mathbb{R}_+ \to \mathbb{R}_+ \text{ Borel} : T_\sharp\rho = \rho \,\},$$

and the cyclical Monge problem corresponding to (4.0.1) can be written as

$$(M_{\text{cycl}}) = \inf\left\{ \int_{\mathbb{R}_+} c\big(x, T(x), T^{(2)}(x)\big)\, d\rho(x) : T \in \mathcal{T}(\rho),\ T^{(3)} = \text{Id} \right\}. \tag{5.2.2}$$




(a) $III$ map. (b) $IDD$ map. (c) $DID$ map. (d) $DDI$-map.

Figure 5.2: The four types of maps considered in the conjecture in the case of a uniform density on $[0, 3]$.

We also introduce the set of transport plans

$$\Pi(\rho) = \left\{ \gamma \in \mathscr{P}(\mathbb{R}^3_+) : \pi^i_\sharp \gamma = \rho,\ i = 1, 2, 3 \right\},$$

where $\pi^i : (\mathbb{R}_+)^3 \to \mathbb{R}_+$ are the projections on the $i$-th component for $i = 1, 2, 3$, and the Kantorovich multimarginal problem

$$(K) = \min \left\{ \int_{(\mathbb{R}_+)^3} c(r_1, r_2, r_3)\, d\gamma(r_1, r_2, r_3) : \gamma \in \Pi(\rho) \right\}. \tag{5.2.3}$$

### 5.2.2 Some special maps

In the following definition, we introduce some special transport maps, which were conjectured in [SGS07] to be good candidates for optimality in problem (5.2.2).

**Definition 5.2.1.** Let $\rho \in \mathscr{M}(\mathbb{R}_+)$ be a non-atomic probability measure and let $d_1, d_2 \in \mathbb{R}_+$ such that $\rho([0, d_1]) = \rho([d_1, d_2]) = \rho([d_2, \infty]) = 1/3$. The $DDI$-map $T : \mathbb{R}_+ \to \mathbb{R}_+$ associated to $\rho$ is the unique (up to $\rho$-negligible sets) map such that $T_\sharp \rho = \rho$ and

- $T$ maps $(0, d_1)$ onto $(d_1, d_2)$ decreasingly,
- $T$ maps $(d_1, d_2)$ onto $(d_2, \infty)$ decreasingly,
- $T$ maps $(d_2, \infty)$ onto $(0, d_1)$ increasingly.

Similarly, we define, for instance, the $DID$-map mapping $(0, d_1)$ onto $(d_1, d_2)$ decreasingly, $(d_1, d_2)$ onto $(d_2, \infty)$ increasingly and $(d_2, \infty)$ onto $(0, d_1)$ decreasingly.

The $\{D, I\}^3$-class associated to $\rho$ is composed by the maps with all the possible monotonicities, under the condition that $T^{(3)} = \mathrm{Id}$: therefore we have $III$, $IDD$, $DID$ and $DDI$, (see Figure 5.2).

In the rest of the paper we answer the following question:

**Question 5.2.2.** Is the $DDI$-map associated to $\rho$ optimal in problem (5.2.2) for every measure $\rho \in \mathscr{P}(\mathbb{R}_+)$? Is one of the maps in $\{D, I\}^3$-class associated to $\rho$ optimal in problem (5.2.2) for every non-atomic probability measure $\rho \in \mathscr{P}(\mathbb{R}_+)$?

### 5.2.3 A necessary condition for optimality: $c$-monotonicity

Before presenting the examples and counterexamples, we recall a well-known optimality condition in optimal transport.

**Definition 5.2.3.** Let $c : (\mathbb{R}_+)^N \to [0, \infty]$ be a cost function. We say that a set $\Gamma \subset (\mathbb{R}_+)^N$ is $c$-monotone with respect to $p \subseteq \{1, \dots, N\}$ if

$$c(x) + c(y) \leq c(X(x, y, p)) + c(Y(x, y, p)) \qquad \forall x, y \in \Gamma, \tag{5.2.4}$$

where $X(x, y, p), Y(x, y, p) \in (\mathbb{R}_+)^N$ are obtained from $x$ and $y$ by exchanging their coordinates on the complement of $p$, namely

$$X_i(x, y, p) = \begin{cases} x_i & \text{if } i \in p \\ y_i & \text{if } i \notin p \end{cases} \qquad Y_i(x, y, p) = \begin{cases} y_i & \text{if } i \in p \\ x_i & \text{if } i \notin p \end{cases} \qquad \forall i \in \{1, ..., N\}. \tag{5.2.5}$$

We say that $\Gamma \subset (\mathbb{R}_+)^N$ is $c$-monotone if (5.2.4) holds true for every $p \subseteq \{1, \dots, N\}$.

Let $\gamma \in \Pi(\rho)$ be a transport plan. The following Proposition ([Pas12, Lemma 2], see also [CDD15, Proposition 2.2], where the result is used to describe optimal maps with Coulomb cost in 1 dimension) presents a necessary condition for optimality of $\gamma$.

**Proposition 5.2.4.** *Let $c : (\mathbb{R}_+)^3 \to [0, \infty]$ be a continuous cost and let $\rho$ be a probability measure on $(\mathbb{R}_+)$. Let $\gamma \in \Pi(\rho)$ be an optimal transport plan for problem (5.2.3) and assume $(K) < \infty$ (therefore $\gamma$ has finite cost). Then* $\operatorname{supp} \gamma$ *is c-monotone.*

*Remark* 5.2.5. Given an optimal plan $\gamma$, the support of $\gamma$ is $c$-monotone even in a stronger sense than the one in Definition 5.2.3. More precisely, given two points $x$ and $y$ (for simplicity, assume that all their coordinates are distinct to avoid multiplicity issues), we have that

$$c(x) + c(y) \leq c(X) + c(Y) \tag{5.2.6}$$

for every choice of $X, Y \in (\mathbb{R}_+)^N$ such that the union of the coordinates of $X$ and $Y$ is the same as the union of the coordinates of $x$ and $y$. Indeed, given any permutation $\sigma$ of the coordinates of $(\mathbb{R}_+)^N$, we have that $\sigma(y)$ is in the support of the symmetrization of $\gamma$, which is still optimal because of the symmetry of the optimal plan. Hence, applying Proposition 5.2.4 to $x$ and $\sigma(y)$, we obtain (5.2.6) for any $X$ and $Y$.

### 5.2.4 Counterexamples

The first example shows that the $DDI$-map is not always optimal in problem (5.2.2), by taking as marginal a measure which is concentrated in a small neighborhood of the unit sphere.

**Counterexample 5.2.6.** *There exists $\varepsilon > 0$ such that, setting*

$$\rho_\varepsilon = \frac{1}{12\varepsilon} 1_{[1,1+12\varepsilon]}\, dr \in \mathscr{M}(\mathbb{R}_+),$$

*the $DDI$-map associated to $\rho_\varepsilon$ is not $c$-monotone and, therefore, not optimal in problem (5.2.2).*

The proof is based on the analysis of $c$-monotonicity for similar radii, obtained by Taylor expanding the cost around the point $(1, 1, 1)$.

The next example modifies the previous one by sending $1/6$ of the total mass far away; in this way, the cost of the orbits of these points (which have two coordinates close to 1 and one large coordinate) can be easily computed. Thanks to this property, we can show that none of the maps in the $\{D, I\}^3$-class can be optimal, since their support is not $c$-monotone.

**Counterexample 5.2.7.** *There exist $M, \varepsilon > 0$ such that, setting*

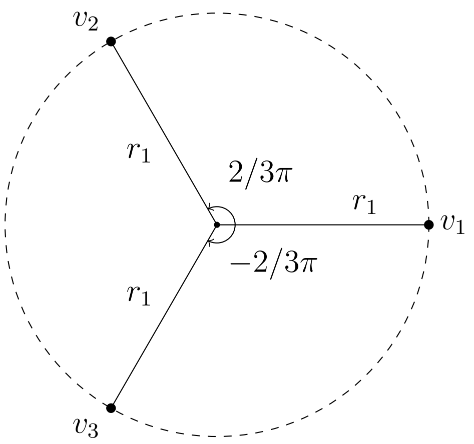
$$\rho_{M,\varepsilon} = \left(\frac{1}{6\varepsilon} 1_{[1,1+5\varepsilon]} + \frac{1}{6} 1_{[M,M+1]}\right) dr \in \mathscr{M}(\mathbb{R}_+),$$

*none of the maps in the $\{D, I\}^3$-class associated to $\rho_{M,\varepsilon}$ is optimal in problem (5.2.2).*

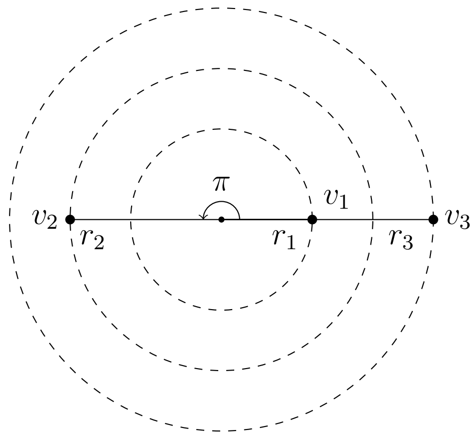
*Remark* 5.2.8. In Remark 5.5.2 we will see a similar result for the problem with 4 marginals. However, we preferred to restrict the presentation to the case with 3 marginals since the ideas involved are the same, but the computations are easier.

There are particular measures $\rho$ for which the $DDI$-map is $c$-monotone (whereas this property fails in Counterexample 5.2.6 and 5.2.7). For this reason one may expect that this map is also optimal in problem (5.2.2), but, to show this, sufficient conditions for optimality (stronger than $c$-monotonicity) would have to be identified.

**Proposition 5.2.9** (Examples of $c$-monotone $DDI$-maps)**.** *There exists $M > 0$ such that for any probability measure $\rho$ such that $\rho([1, 2]) = \rho([3, 4]) = \rho([M, \infty)) = 1/3$ the $DDI$-map is $c$-monotone (according to Definition 5.2.3).*




(a) A configuration of three charges at the same distance $r_1$ from the origin with angles $\theta_2 = 2/3\pi$ and $\theta_3 = -2/3\pi$.




(b) A configuration of three charges at distances $r_1$, $r_2$ and $r_3$ with angles $\theta_2 = \pi$ and $\theta_3 = 0$.

## 5.3 Taylor expansion of the cost at $r_1 = r_2 = r_3 = 1$

In this section we want to address the following problem: given three radii $r_1(t)$, $r_2(t)$ and $r_3(t)$ parametrized by $t \in \mathbb{R}$ and starting from the value 1 at $t = 0$, what is the expansion of $c\big(r_1(t), r_2(t), r_2(t)\big)$ in powers of $t$ at $t = 0$?

First, we notice that at $t = 0$ the optimal angles are $\pm 2/3\pi$ and $c(1,1,1) = \sqrt{3}$. Indeed, given three unitary vectors $v_1, v_2, v_3$, calling $\alpha_1$ the angle between $v_2$ and $v_3$ (and cyclical), we have that $|v_1 - v_2| = 2\sin(\alpha_3/2)$ (and cyclical), therefore, by Jensen's inequality and by the convexity of $\alpha \mapsto \big[2\sin(\alpha/2)\big]^{-1}$ in $[0, 2\pi]$,

$$\begin{aligned}\frac{1}{|v_2 - v_1|} + \frac{1}{|v_3 - v_2|} + \frac{1}{|v_1 - v_3|} &= \sum_{i=1}^{3} \frac{1}{2\sin(\alpha_i/2)} \\ &\geq \frac{3}{2\sin\big((\alpha_1 + \alpha_2 + \alpha_3)/6\big)} = \sqrt{3},\end{aligned}$$

with equality if and only if the triangle is equilateral.

Taking the angles to be exactly $\pm 2/3\pi$ leads to the following cost

$$\begin{aligned}c_\triangle(r_1, r_2, r_3) &:= \frac{1}{\sqrt{r_1^2 + r_1 r_2 + r_2^2}} + \frac{1}{\sqrt{r_2^2 + r_2 r_3 + r_3^2}} + \frac{1}{\sqrt{r_1^2 + r_1 r_3 + r_3^2}} \\ &\geq c(r_1, r_2, r_3).\end{aligned} \tag{5.3.1}$$

However the inequality is strict as soon as the three radii are different and the approximation of $c$ with $c_\triangle$ is too rough to deduce that they enjoy the same $c$-monotonicity structures. Therefore, we perform a finer analysis.

We want to take into account only the first order variation of the radii as functions of $t$, so it is natural to consider three linearly varying radii

$$r_1(t) = 1 + a_1 t, \qquad r_2(t) = 1 + a_2 t, \qquad r_3(t) = 1 + a_3 t$$

where $a_1, a_2, a_3 \in \mathbb{R}$ are some constants. To these radii we associate the exact cost

$$g(a_1, a_2, a_3, t) = c(1 + a_1 t, 1 + a_2 t, 1 + a_3 t), \tag{5.3.2}$$

and we study the expansion of this function near $t = 0$.

**Lemma 5.3.1.** *Let $a_1, a_2, a_3 \in \mathbb{R}$ and let $g$ be as in (5.3.2). Then we have that*

$$g(a, b, c, 0) = \sqrt{3}.$$

$$\frac{\partial g}{\partial t}(a_1, a_2, a_3, 0) = -\frac{a_1 + a_2 + a_3}{\sqrt{3}},$$

$$\frac{\partial^2 g}{\partial t^2}(a_1, a_2, a_3, 0) = \frac{4(a_1^2 + a_2^2 + a_3^2) + 6(a_1 a_2 + a_2 a_3 + a_3 a_1)}{5\sqrt{3}},$$

$$\begin{aligned}\frac{\partial^3 g}{\partial t^3}(a_1, a_2, a_3, 0) = &- \frac{308(a_1^3 + a_2^3 + a_3^3)}{375\sqrt{3}} \\ &- \frac{888(a_1^2 a_2 + a_1 a_2^2 + a_2^2 a_3 + a_2 a_3^2 + a_3^2 a_1 + a_3 a_1^2) + 498 a_1 a_2 a_3}{375\sqrt{3}}.\end{aligned} \tag{5.3.3}$$

In the proof, we will write the Coulomb potential of three charges in terms of the distances from the origin and the angles between the charges. Given three radii $r_1$, $r_2$, $r_3$ and two angles $\theta_2$ and $\theta_3$, we define the *Coulomb potential* of the configuration of charges depicted in Figure 5.1:

$$C(r_1, r_2, r_3, \theta_2, \theta_3) = \frac{1}{|v_2 - v_1|} + \frac{1}{|v_3 - v_2|} + \frac{1}{|v_1 - v_3|} \tag{5.3.4}$$

where

$$v_1 = (r_1, 0), \qquad v_2 = r_2(\cos\theta_2, \sin\theta_2), \qquad v_3 = r_3(\cos\theta_3, \sin\theta_3).$$

By definition of $c$, we notice that

$$c(r_1, r_2, r_3) = \min_{\theta_2, \theta_3 \in \mathbb{R}} C(r_1, r_2, r_3, \theta_2, \theta_3). \tag{5.3.5}$$

*Proof of Lemma 5.3.1.* For $t \in \mathbb{R}$ and $\theta = (\theta_2, \theta_3) \in \mathbb{R}^2$ we define also the function

$$G(t, \theta) = C(1 + a_1 t, 1 + a_2 t, 1 + a_3 t, \theta_2, \theta_3).$$

Then $g(t) = G\big(t, \theta_0(t)\big)$ where $\theta_0(t)$ is the pair of angles which minimizes (5.3.5). From this optimality condition we know that

$$G_\theta\big(t, \theta_0(t)\big) = 0.$$

We want to apply the implicit function theorem to find the behavior of $\theta_0(t)$. It's easy to check that $\theta_0(0) = (2/3\pi, -2/3\pi)$ and a direct computation shows that

$$G_{\theta\theta}\big(0, \theta_0(0)\big) = \frac{5}{6\sqrt{3}} \begin{pmatrix} 1 & -1/2 \\ -1/2 & 1 \end{pmatrix} \in \mathrm{Inv}(\mathbb{R}^2; \mathbb{R}^2).$$

Therefore $\theta_0 \in C^\infty\big((-\varepsilon, \varepsilon)\big)$ for some $\varepsilon > 0$ and we can compute its derivatives in 0. In particular, we have that

$$\theta_0'(0) = G_{\theta\theta}^{-1} \cdot G_{t\theta}\Big|_{(0,\theta_0(0))} = \frac{1}{5\sqrt{3}} \begin{pmatrix} -a_1 - a_2 + 2a_3 \\ a_1 - 2a_2 + a_3 \end{pmatrix}. \tag{5.3.6}$$

The idea is now to consider the first order approximation

$$\bar\theta(t) = \theta_0(0) + \theta_0'(0)t = \begin{pmatrix} 2/3\pi \\ -2/3\pi \end{pmatrix} + \frac{1}{5\sqrt{3}} \begin{pmatrix} -a_1 - a_2 + 2a_3 \\ a_1 - 2a_2 + a_3 \end{pmatrix} t$$

and the perturbed cost

$$h(t) = G\big(t, \bar\theta(t)\big).$$

We claim that $h(t) = g(t) + o(t^3)$, namely

$$h(0) = g(0), \qquad h'(0) = g'(0), \qquad h''(0) = g''(0), \qquad h'''(0) = g'''(0).$$

The first two are clearly true, since $\bar\theta(0) = \theta_0(0)$ and $\bar\theta'(0) = \theta_0'(0)$ by definition. Now consider the function $t \mapsto G\big(t, \theta(t)\big)$, where $\theta$ is either $\theta_0$ or $\bar\theta$. To prove the claim, we show that its second and third derivatives at $t = 0$ depend only on $\theta'(0)$ and not on the second and third derivatives of $\theta$.

As a matter of fact, we have

$$\left.\frac{d^2 G\big(t, \theta(t)\big)}{dt^2}\right|_{t=0} = G_{tt} + 2G_{t\theta}\theta' + G_{\theta\theta}\theta'\theta' + G_\theta\theta''\Big|_{t=0},$$

but $G_\theta\big(0, \theta(0)\big) = 0$, so the second derivative does not depend on $\theta''(0)$. In a similar fashion, we have

$$\begin{aligned}\left.\frac{d^3 G\big(t, \theta(t)\big)}{dt^3}\right|_{t=0} &= G_{ttt} + 3G_{tt\theta}\theta' + 3G_{t\theta\theta}(\theta')^2 + G_{\theta\theta\theta}(\theta')^3 \\ &\quad + 3\left(G_{t\theta} + G_{\theta\theta}\theta'\right)\theta'' + G_\theta\theta'''\Big|_{t=0}.\end{aligned}$$

Again, $G_\theta\big(0, \theta(0)\big) = 0$, therefore $\theta'''(0)$ doesn't contribute. Furthermore, we have $G_\theta\big(t, \theta_0(t)\big) = 0$, so that differentiating in $t$ yields

$$G_{t\theta}\big(0, \theta_0(0)\big) + G_{\theta\theta}\big(0, \theta_0(0)\big)\theta_0'(0) = 0.$$

But then also

$$G_{t\theta}\big(0, \bar\theta(0)\big) + G_{\theta\theta}\big(0, \bar\theta(0)\big)\bar\theta'(0) = 0,$$

since $\bar\theta'(0) = \theta_0'(0)$. Therefore we see that in both cases the coefficient of $\theta''$ vanishes. This concludes the proof of the claim because we have shown that the first three derivatives of $h$ and $g$ coincide at $t = 0$.

At this point the derivatives of $h$ can be computed directly, since $h(a_1, a_2, a_3, \cdot\,)$ is an explicit function of the last variable. □

In Lemma 5.3.1 we found the first nontrivial Taylor term in the expansion of $g(t)$. We employ this computation to obtain information on the $c$-monotonicity of points with linearly spaced radii close to $t = 0$.

**Lemma 5.3.2.** *For every $t > 0$, consider six linearly spaced radii*

$$(r_1, r_2, r_3, r_4, r_5, r_6) = (1, 1+t, 1+2t, 1+3t, 1+4t, 1+5t). \tag{5.3.7}$$

*Then there exists $t_0 > 0$ such that, for every $t \le t_0$,*

$$c(r_1, r_4, r_6) + c(r_2, r_3, r_5) < c(r_1, r_4, r_5) + c(r_2, r_3, r_6).$$

*Proof.* Let us define

$$F(t) = g(0, 3, 5, t) + g(1, 2, 4, t) - g(0, 3, 4, t) - g(1, 2, 5, t)$$

Applying Lemma 5.3.1 we can compute the derivatives of $F$ and find that

$$F(0) = 0, \qquad F'(0) = 0, \qquad F''(0) = 0, \qquad F'''(0) = -\frac{284\sqrt{3}}{125} < 0;$$

this shows that $F(t) < 0$ for $t$ sufficiently small and proves the lemma. □

*Remark* 5.3.3. Considering $r_1, ..., r_6$ as in (5.3.7), one could prove that the choice 146-235 is optimal between all possible choices, namely

$$\begin{aligned} &c(r_1, r_4, r_6) + c(r_2, r_3, r_5) \\ &\qquad = \min\left\{\, c(p_1, p_2, p_3) + c(p_4, p_5, p_6) : \{p_1, \dots, p_6\} = \{r_1, \dots, r_6\}\,\right\}, \end{aligned} \tag{5.3.8}$$

for $t$ small enough. Moreover, one could see that (5.3.8) holds also if we replace $c$ with $c_\triangle$ defined in (5.3.1). This is, however, not needed for our counterexamples.

*Remark* 5.3.4 (Asymptotic expansion of the cost at infinity). Although they will not be used in the proofs of the main results, we report the following formulas since they might help in future studies to gain more insight into the structure of $c$-monotone sets. We are interested in the asymptotic expansion of the cost as some of the radii go to infinity and the others remain fixed.

For $(r_1, r_2, r_3) = (1, 1, r)$, the optimal angles are

$$\theta_2(r) = \pi - \frac{8}{r^2} + o\left(\frac{1}{r^3}\right), \qquad \theta_3(r) = -\frac{\pi}{2} - \frac{4}{r^2} + o\left(\frac{1}{r^3}\right).$$

In comparison to (5.3.6), this expansion is harder to justify (but can be easily verified numerically). However, from this fact it follows rigorously that the cost has the following asymptotic behaviour:

$$\begin{aligned} c(1,1,r) &= C(1,1,r,\pi,-\pi/2) - \frac{4}{r^4} + o\left(\frac{1}{r^4}\right) \\ &= \left(\frac{1}{2} + \frac{1}{\sqrt{1+r^2}}\right) - \frac{4}{r^4} + o\left(\frac{1}{r^4}\right). \end{aligned}$$

Similarly, for $(r_1, r_2, r_3) = (1, r, r)$, the optimal angles are

$$\theta_2(r) = \frac{\pi}{2} + \frac{4}{r} + o\left(\frac{1}{r^2}\right), \qquad \theta_3(r) = -\frac{\pi}{2} - \frac{4}{r} + o\left(\frac{1}{r^2}\right),$$

and the cost is

$$\begin{aligned} c(1,r,r) &= C(1,r,r,\pi/2,-\pi/2) - \frac{4}{r^3} + o\left(\frac{1}{r^4}\right) \\ &= \frac{1}{2r} + \frac{2}{\sqrt{1+r^2}} - \frac{4}{r^3} + o\left(\frac{1}{r^4}\right). \end{aligned}$$

Furthermore, one can verify that

$$c(1,r,r) = C\left(1, r, r, \frac{\pi}{2} + \frac{4}{r}, -\frac{\pi}{2} - \frac{4}{r}\right) - O\left(\frac{1}{r^7}\right).$$

## 5.4 Condition for $c = c_\pi$ and $c_\pi$-monotonicity

When the radii are spread apart, a reasonable approximate cost appears to be

$$c_\pi(r_1, r_2, r_3) = \frac{1}{r_1 + r_2} + \frac{1}{r_2 + r_3} + \frac{1}{r_3 - r_1},$$

which arises from collocating the charges at angles $\theta_2 = \pi$ and $\theta_3 = 0$ (see Figure 5.3b). In the first part of this section we want to study under which condition on the radii $r_1$, $r_2$ and $r_3$ we have

$$c(r_1, r_2, r_3) = c_\pi(r_1, r_2, r_3).$$

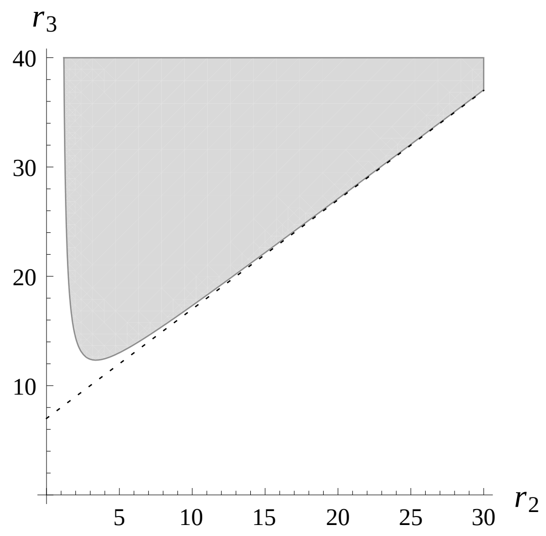



Figure 5.4: The region in the $(r_2, r_3)$ plane where $C_{\theta\theta}(r_1, r_2, r_3, \pi, 0) \geq 0$, with $r_1 = 1$. The dotted line is $r_3 = r_2 + 7$.

We start with a heuristic argument involving a necessary condition. Up to permutations, we may assume $r_1 \leq r_2 \leq r_3$. It is simple to check that

$$C_\theta(r_1, r_2, r_3, \pi, 0) = 0,$$

where $C$ has been defined in (5.3.4), either by direct computation or by a symmetry argument.[1] If $(\theta_2, \theta_3) = (\pi, 0)$ must be a minimum, then a necessary condition is

$$C_{\theta\theta}(r_1, r_2, r_3, \pi, 0) \geq 0,$$

in the sense that the Hessian matrix is positive-definite. We have

$$C_{\theta\theta}(r_1, r_2, r_3, \pi, 0) = \begin{pmatrix} r_2\left(\frac{r_1}{(r_1+r_2)^3} + \frac{r_3}{(r_2+r_3)^3}\right) & -\frac{r_2 r_3}{(r_2+r_3)^3} \\ -\frac{r_2 r_3}{(r_2+r_3)^3} & r_3\left(\frac{r_2}{(r_2+r_3)^3} - \frac{r_1}{(r_3-r_1)^3}\right) \end{pmatrix}$$

since the first entry is positive, this $2 \times 2$ matrix is positive-definite if and only if the determinant is positive too, namely

$$\det C_{\theta\theta}(r_1, r_2, r_3, \pi, 0) = -\frac{r_1 r_2 r_3 [r_2 r_3 (r_2 - r_3) + r_1(r_2^2 + 5 r_2 r_3 + r_3^2) + r_1^3]}{(r_1 + r_2)^3 (r_2 + r_3)^2 (r_3 - r_1)^3} \geq 0,$$

or equivalently

$$r_1(r_2^2 + 5r_2 r_3 + r_3^2) + r_1^3 < r_2 r_3 (r_3 - r_2).$$

Figure 5.4 depicts the region where the Hessian is positive.

We partially justify the previous argument in the following lemma which, despite not being quantitative, will suffice for our purposes.

[1] In fact, the four configurations with $\theta_2, \theta_3 \in \{0, \pi\}$ are always stationary.

**Lemma 5.4.1.** *If* $0 < r_1^- \le r_1^+ < r_2^- \le r_2^+$, *then there exists* $r_3^-(r_1^-, r_1^+, r_2^-, r_2^+)$ *such that for every* $r_1 \in [r_1^-, r_1^+]$, $r_2 \in [r_2^-, r_2^+]$ *and* $r_3 \ge r_3^-$ *we have*

$$c(r_1, r_2, r_3) = c_\pi(r_1, r_2, r_3).$$

*Proof.* We denote by $\mathbb{T}^2$ the 2-dimensional torus $\mathbb{R}^2/(2\pi\mathbb{Z})^2$. The idea of the proof is the following: we claim that for sufficiently large $r_3$ there are exactly four stationary points $(\theta_2, \theta_3) \in \mathbb{T}^2$ for $C(r_1, r_2, r_3, \theta_2, \theta_3)$, corresponding to $\theta_2, \theta_3 \in \{0, \pi\}$. Therefore $c(r_1, r_2, r_3)$ must coincide with the value achieved at one of them and by comparing the four values we arrive at the desired conclusion.

First of all, we compute the gradient

$$C_\theta(r_1, r_2, r_3, \theta_2, \theta_3) = \begin{pmatrix} -\frac{r_1 r_2 \sin(\theta_2)}{\left(r_1^2+r_2^2-2r_1r_2\cos(\theta_2)\right)^{3/2}} - \frac{r_2 r_3 \sin(\theta_2-\theta_3)}{\left(r_2^2+r_3^2-2r_2r_3\cos(\theta_2-\theta_3)\right)^{3/2}} \\ -\frac{r_1 r_3 \sin(\theta_3)}{\left(r_1^2+r_3^2-2r_1r_3\cos(\theta_3)\right)^{3/2}} + \frac{r_2 r_3 \sin(\theta_2-\theta_3)}{\left(r_2^2+r_3^2-2r_2r_3\cos(\theta_2-\theta_3)\right)^{3/2}} \end{pmatrix}.$$

The gradient vanishes if and only if the following equations are simultaneously satisfied:

$$\frac{r_1 r_2 \sin(\theta_2)}{\left(r_1^2+r_2^2-2r_1r_2\cos(\theta_2)\right)^{3/2}} + \frac{r_1 r_3 \sin(\theta_3)}{\left(r_1^2+r_3^2-2r_1r_3\cos(\theta_3)\right)^{3/2}} = 0, \tag{5.4.1}$$

$$-\frac{r_1 r_3 \sin(\theta_3)}{\left(r_1^2+r_3^2-2r_1r_3\cos(\theta_3)\right)^{3/2}} + \frac{r_2 r_3 \sin(\theta_2-\theta_3)}{\left(r_2^2+r_3^2-2r_2r_3\cos(\theta_2-\theta_3)\right)^{3/2}} = 0. \tag{5.4.2}$$

To show that there are exactly four stationary points, the idea is that, for $r_3$ sufficiently large, equations (5.4.1) and (5.4.2) define two pairs of closed curves on $\mathbb{T}^2$, of type $(0,1)$ and $(1,1)$ respectively, with the property that every curve from the first family intersects each curve of the second family in a single point. The situation is represented in Figure 5.5.

***Step 1.*** Given $r_1$, $r_2$ and a sufficiently large $r_3$, we claim that for every $\theta_3 \in S^1$ there are exactly two values $\tilde{\theta}_2^0(\theta_3), \tilde{\theta}_2^\pi(\theta_3) \in S^1$ which satisfy (5.4.1); moreover $\tilde{\theta}_2^0(\theta_3)$ and $\tilde{\theta}_2^\pi(\theta_3)$ are close to 0 and $\pi$ respectively by less than $O\big(r_3^{-2}\big)$, uniformly in $\theta_3$, and their derivatives go to to zero uniformly in $\theta_3$ for $r_3 \to \infty$.[2] These functions correspond to the solid, almost vertical, lines in Figure 5.5.

We begin by finding a useful bound on $|\sin(\theta_2)|$. The two terms of (5.4.1) can be estimated by

$$\Big|\frac{r_1 r_2 \sin(\theta_2)}{\left(r_1^2+r_2^2-2r_1r_2\cos(\theta_2)\right)^{3/2}}\Big| \ge \frac{r_1^- r_2^- |\sin(\theta_2)|}{(r_1^+ + r_2^+)^3},$$
$$\Big|\frac{r_1 r_3 \sin(\theta_3)}{\left(r_1^2+r_3^2-2r_1r_3\cos(\theta_3)\right)^{3/2}}\Big| \le \frac{r_1^+ r_3}{(r_3 - r_1^+)^3},$$

[2] More precisely, they are close to zero by less than $O\big(r_3^{-2}\big)$, uniformly in $\theta_3$.

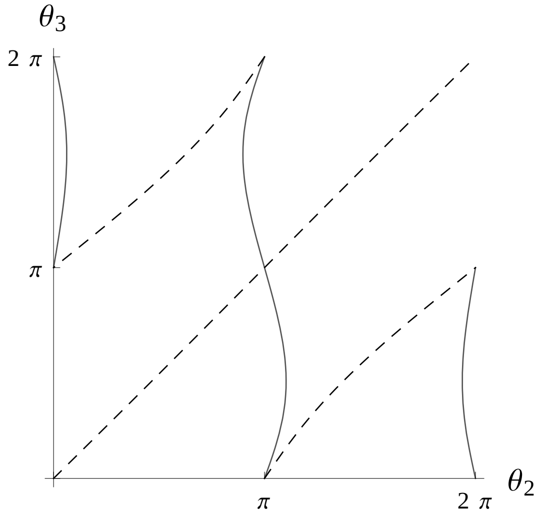



Figure 5.5: The curves in $\mathbb{T}^2$ whose four intersections correspond to stationary points of $C(r_1, r_2, r_3, \theta_2, \theta_3)$. The two solid curves are defined by (5.4.1). The dashed curves are defined by (5.4.2).

therefore, in order to have equality (5.4.1), it must be that

$$\frac{r_1^- r_2^- |\sin(\theta_2)|}{(r_1^+ + r_2^+)^3} \le \frac{r_1^+ r_3}{(r_3 - r_1^+)^3},$$

that is

$$|\sin(\theta_2)| \le \frac{r_1^+ (r_1^+ + r_2^+)^3}{r_1^- r_2^-} \cdot \frac{r_3}{(r_3 - r_1^+)^3} = O\big(r_3^{-2}\big) \tag{5.4.3}$$

as $r_3 \to \infty$, where the implied constant depends only on $r_1^\pm$ and $r_2^\pm$.

We have already discussed that, for every $\theta_3 \in S^1$, the second term in (5.4.1) is smaller than $r_3(r_3 - r_1^+)^{-3}$ in magnitude. On the other hand, the first term vanishes for $\theta_2 = 0, \pi$ and is equal to $\pm r_1 r_2 (r_1^2 + r_2^2)^{3/2}$ for $\theta_2 = \pm\pi/2$. Therefore, by continuity, for $r_3$ large we have at least two solutions to (5.4.1).

The estimate on $|\sin(\theta_2)|$ proves that the solutions must be located near 0 and $\pi$. Now we want to prove that there are exactly two of them. To do so, we verify that the partial derivative with respect to $\theta_2$ of the first term in (5.4.1) is different from zero for $\theta_2$ in the prescribed intervals around 0 and $\pi$. Indeed, the derivative is

$$\frac{\partial}{\partial\theta_2}\bigg|_{\theta_2=0} \left( \frac{r_1 r_2 \sin(\theta_2)}{\big(r_1^2 + r_2^2 - 2 r_1 r_2 \cos(\theta_2)\big)^{3/2}} \right) = \frac{r_1 r_2}{(r_2 - r_1)^3},$$

$$\frac{\partial}{\partial\theta_2}\bigg|_{\theta_2=\pi} \left( \frac{r_1 r_2 \sin(\theta_2)}{\big(r_1^2 + r_2^2 - 2 r_1 r_2 \cos(\theta_2)\big)^{3/2}} \right) = -\frac{r_2}{(r_1 + r_2)^3},$$

therefore it is different from zero around the two points and the two solutions are simple.

The claim is almost entirely proved. We now have the two functions $\tilde{\theta}_2^0(\,\cdot\,), \tilde{\theta}_2^\pi(\,\cdot\,)$ and the last thing that we want to derive is the estimate of their first derivatives. Let $\theta_2(\,\cdot\,)$ be one of the two functions. Thanks to the implicit function theorem, we know that $\theta_2(\,\cdot\,)$ is at least $C^1$ and we can compute

$$\theta_2'(\theta_3) = -\frac{r_3}{r_2}\cdot\frac{2(r_1^2+r_3^2)\cos(\theta_3)+r_1r_3[-5+\cos(2\theta_3)]}{2(r_1^2+r_2^2)\cos\big(\theta_2(\theta_3)\big)+r_1r_2\big[-5+\cos\big(2\theta_2(\theta_3)\big)\big]} \cdot\left(\frac{r_1^2+r_2^2-2r_1r_2\cos\big(\theta_2(\theta_3)\big)}{r_1^2+r_3^2-2r_1r_3\cos(\theta_3)}\right)^{5/2}.$$

All the terms are fairly easy to deal with, apart from the denominator of the second fraction. However, we have that

$$\begin{aligned} 2(r_1^2+r_2^2)\cos(\theta_2)+r_1r_2[-5+\cos(2\theta_2)]\big|_{\theta_2=0} &= 2(r_1^2-2r_1r_2+r_2^2)\geq 2(r_2^- - r_1^+)^2,\\ -2(r_1^2+r_2^2)\cos(\theta_2)-r_1r_2[-5+\cos(2\theta_2)]\big|_{\theta_2=\pi} &= 2(r_1^2+2r_1r_2+r_2^2)\geq 2(r_2^- + r_1^-)^2, \end{aligned}$$

therefore, by the continuity of the functions involved and by compactness, there exists a neighbourhood $U$ of $\{0,\pi\}$ such that if $r_1\in[r_1^-,r_1^+]$, $r_2\in[r_2^-,r_2^+]$ and $\theta_2\in U$ then

$$|2(r_1^2+r_2^2)\cos(\theta_2)+r_1r_2[-5+\cos(2\theta_2)]| > (r_2^- - r_1^+)^2.$$

From this and (5.4.3), which ensures that $\theta_2(\theta_3)\in U$, we deduce that for $r_3$ large

$$|\theta_2'(\theta_3)| \leq \frac{r_3}{r_2^-}\cdot\frac{2(r_1^+)^2+2r_3^2}{(r_2^- - r_1^+)^2}\cdot\frac{(r_1^+ + r_2^+)^5}{(r_3-r_1^+)^5} = O\left(r_3^{-2}\right).$$

***Step 2.*** Next we perform the same analysis for (5.4.2). We prove that there exist two $C^1$ functions $\hat{\theta}_2^0(\theta_3)$ and $\hat{\theta}_2^\pi(\theta_3)$ which are the only solutions of (5.4.2) when $\theta_3$ is prescribed and that their derivatives are strictly positive. First of all, we introduce the new variable $\psi=\theta_2-\theta_3$. Equation (5.4.2) reads as

$$-\frac{r_1\sin(\theta_3)}{\big(r_1^2+r_3^2-2r_1r_3\cos(\theta_3)\big)^{3/2}}+\frac{r_2\sin(\psi)}{\big(r_2^2+r_3^2-2r_2r_3\cos(\psi)\big)^{3/2}}=0. \tag{5.4.4}$$

- **The solutions lie in two strips.** From equation (5.4.4) we get

$$\begin{aligned}\frac{r_1^+}{(r_3-r_1^+)^3} &\geq \Big|\frac{r_1\sin(\theta_3)}{\big(r_1^2+r_3^2-2r_1r_3\cos(\theta_3)\big)^{3/2}}\Big|\\ &= \Big|\frac{r_2\sin(\psi)}{\big(r_2^2+r_3^2-2r_2r_3\cos(\psi)\big)^{3/2}}\Big| \geq \frac{r_2^-|\sin(\psi)|}{(r_2^+ + r_3)^3}.\end{aligned}$$

  Therefore we have

$$|\sin(\psi)|\leq\left(\frac{r_3+r_2^+}{r_3-r_1^+}\right)^3\frac{r_1^+}{r_2^-},$$

  which, for $r_3$ sufficiently large, implies $|\sin(\psi)|<\eta$ for a fixed $\eta\in(r_1^+/r_2^-,1)$.

- **There are at least two solutions.** The first term of (5.4.4) is bounded by
$$|\frac{r_1 \sin(\theta_3)}{(1 + r_3^2 - 2r_3 \cos(\theta_3))^{3/2}}| \leq \frac{r_1}{(r_3 - 1)^3}.$$
On the other hand, when $\psi = \pm\pi/2$ the second term equals
$$\pm\frac{r_2}{(r_2^2 + r_3^2)^{3/2}},$$
which is bigger for $r_3$ large enough. This tells us that for every $\theta_3$ there are at least two distinct values of $\psi$ which solve (5.4.4), because the second term is a continuous periodic function of $\psi$.

- **There are exactly two solutions.** The derivative of the second term is
$$\frac{\partial}{\partial\psi}\left(\frac{r_2 \sin(\psi)}{(r_2^2 + r_3^2 - 2r_2 r_3 \cos(\psi))^{3/2}}\right) = \frac{-3r_2^2 r_3 + (r_2^3 + r_2 r_3^2) \cos(\psi) + r_2^2 r_3 \cos(\psi)^2}{(r_2^2 + r_3^2 - 2r_2 r_3 \cos(\psi))^{5/2}}.$$
We observe that the denominator is always positive. We study the sign of the numerator. The equation
$$-3r_2^2 r_3 + (r_2^3 + r_2 r_3^2)t + r_2^2 r_3 t^2 = 0$$
for the unknown $t$ has the two solutions
$$\frac{-r_2^2 - r_3^2 + \sqrt{r_2^4 + 14r_2^2 r_3^2 + r_3^4}}{2r_2 r_3}, \qquad \frac{-r_2^2 - r_3^2 - \sqrt{r_2^4 + 14r_2^2 r_3^2 + r_3^4}}{2r_2 r_3}.$$
However, only the first one lies in the range $[-1, 1]$, whereas the second is less than $-2$. In fact,
$$r_2^2+r_3^2+\sqrt{r_2^4 + 14r_2^2 r_3^2 + r_3^4} \geq r_2^2+r_3^2+\sqrt{r_2^4 + 2r_2^2 r_3^2 + r_3^4} = 2(r_2^2+r_3^2) \geq 4r_2 r_3.$$
Therefore the function has exactly two stationary points and is monotone between them.

- **Derivative of the solutions.** At this point we know that there exist two functions $\psi_0(\theta_3)$ and $\psi_\pi(\theta_3)$ such that the corresponding $\hat{\theta}_2^0(\theta_3) = \psi_0(\theta_3) + \theta_3$ and $\hat{\theta}_2^\pi(\theta_3) = \psi_\pi(\theta_3) + \theta_3$ parametrize the solutions of (5.4.2).

  The goal is to show that for $r_3$ sufficiently large we have $\theta_2'(\theta_3) \geq C > 0$ for some constant $C$ independent of $r_3$, where $\theta_2(\,\cdot\,)$ is either $\hat{\theta}_2^0(\,\cdot\,)$ or $\hat{\theta}_2^\pi(\,\cdot\,)$.

Thanks to the implicit function theorem we can compute the derivative

$$\theta_2'(\theta_3) = \frac{(r_2^2 + r_3^2 - 2r_2 r_3 \cos(\psi))^{5/2}}{-3r_2^2 r_3 + (r_2^3 + r_2 r_3^2)\cos(\psi) + r_2^2 r_3 \cos(\psi)^2} \cdot \left( \frac{r_1 \cos(\theta_3)}{(r_1^2 + r_3^2 - 2r_1 r_3 \cos(\theta_3))^{3/2}} + \frac{r_2 \cos(\psi)}{(r_2^2 + r_3^2 - 2r_2 r_3 \cos(\psi))^{3/2}} - \frac{3r_1^2 r_3 \sin(\theta_3)^2}{(r_1^2 + r_3^2 - 2r_1 r_3 \cos(\theta_3))^{5/2}} - \frac{3r_2^2 r_3 \sin(\psi)^2}{(r_2^2 + r_3^2 - 2r_2 r_3 \cos(\psi))^{5/2}} \right),$$

where $\psi = \theta_2 - \theta_3$ as before. We introduce the parameter $\kappa = 1/r_3$ and write the derivative in terms of it. We have that

$$\theta_2'(\theta_3) = f(r_1, r_2, 1/r_3, \theta_2 - \theta_3, \theta_3)$$

where

$$f(r_1, r_2, \kappa, \psi, \theta_3) = \frac{(1 - 2r_2\kappa \cos(\psi) + r_2^2\kappa^2)^{5/2}}{-3r_2^2\kappa + (r_2^3\kappa^2 + r_2)\cos(\psi) + r_2^2\kappa\cos(\psi)^2} \cdot \left( \frac{r_1 \cos(\theta_3)}{(1 + r_1^2\kappa^2 - 2r_1\kappa\cos(\theta_3))^{3/2}} + \frac{r_2 \cos(\psi)}{(1 + r_2^2\kappa^2 - 2r_2\kappa\cos(\psi))^{3/2}} - \frac{3r_1^2\kappa \sin(\theta_3)^2}{(1 + r_1^2\kappa^2 - 2r_1\kappa\cos(\theta_3))^{5/2}} - \frac{3r_2^2\kappa\sin(\psi)^2}{(1 + r_2^2\kappa^2 - 2r_2\kappa\cos(\psi))^{5/2}} \right). \quad (5.4.5)$$

Observe that the only singularities are due to the denominator of the first fraction. However, the singular values of $\psi$ lie outside the two intervals

$$S = [-\arcsin(\eta), \arcsin(\eta)] \cup [\pi - \arcsin(\eta), \pi + \arcsin(\eta)]$$

for $\kappa$ sufficiently small ($r_3$ large enough), because they converge to $\pm\pi/2$. Therefore there exists $\kappa^+ > 0$ such that the function $f$ is continuous in the domain

$$D = [r_1^-, r_1^+]_{r_1} \times [r_2^-, r_2^+]_{r_2} \times [0, \kappa^+]_\kappa \times S_\psi \times [0, 2\pi]_{\theta_3}.$$

- **Limit case.** We rewrite equation (5.4.4) in terms of $\kappa$ as

$$-\frac{r_1 \sin(\theta_3)}{(1 + r_1^2\kappa^2 - 2r_1\kappa\cos(\theta_3))^{3/2}} + \frac{r_2\sin(\psi)}{(1 + r_2^2\kappa^2 - 2r_2\kappa\cos(\psi))^{3/2}} = 0. \quad (5.4.6)$$

Let $\Gamma_{r_1,r_2,\kappa}$ denote the set of solutions $(\psi, \theta_3) \in S_\psi \times [0, 2\pi]_{\theta_3}$ to (5.4.6). By the continuity of (5.4.6) we know that

$$\Gamma = \bigcup_{r_1 \in [r_1^-, r_1^+]} \bigcup_{r_2 \in [r_2^-, r_2^+]} \bigcup_{\kappa \in [0, \kappa^+]} \Gamma_{r_1,r_2,\kappa} \subset D$$

is a closed set. Our ultimate goal is to show that $f$ is positive on $\Gamma_{r_1,r_2,\kappa}$ when $\kappa$ is small enough.

We start by studying the limit case $\kappa = 0$. The limit curve $\Gamma_{r_1,r_2,0}$ is given by the equation

$$r_1 \sin(\theta_3) = r_2 \sin(\psi). \tag{5.4.7}$$

For $\kappa = 0$, the function $f$ equals

$$f(r_1, r_2, 0, \psi, \theta_3) = \frac{1}{r_2 \cos(\psi)}\big(r_1 \cos(\theta_3) + r_2 \cos(\psi)\big) = 1 + \frac{r_1 \cos(\theta_3)}{r_2 \cos(\psi)}.$$

We claim that this function is positive on the curve defined by (5.4.7). Indeed, positivity is guaranteed if we are able to prove that

$$|\frac{r_1 \cos(\theta_3)}{r_2 \cos(\psi)}| < 1.$$

But, by squaring, this is equivalent to

$$r_1^2 \cos(\theta_3)^2 < r_2 \cos(\psi)^2,$$

which, thanks to (5.4.7), reduces to the true inequality $r_1^2 < r_2^2$.

- **Conclusion.** Finally, we prove that $f \geq C > 0$ on $\Gamma_{r_1,r_2,\kappa}$ for $\kappa$ close to zero, where $C$ is a constant depending only on $r_1^\pm$ and $r_2^\pm$.

  We know that $f$ is positive on the compact set

$$K = \bigcup_{r_1 \in [r_1^-, r_1^+]} \bigcup_{r_2 \in [r_2^-, r_2^+]} \Gamma_{r_1,r_2,0}.$$

  Therefore there exists a positive constant $C$ and an open neighbourhood $U$ of $K$ in $D$ such that $f > C$ on $U$. Since $\Gamma$ is closed, a compactness argument shows that $\Gamma_{r_1,r_2,\kappa} \subset U$ for $\kappa$ close to zero and this concludes the proof.

***Step 3.*** The previous steps tell us that (5.4.1) defines two vertical curves and (5.4.2) two diagonal curves. The estimates on the derivatives of such curves prove that the intersections are simple, therefore there are exactly four stationary points. But we already know four stationary points, namely

$$(\theta_2, \theta_3) = (0, 0),\ (0, \pi),\ (\pi, 0),\ (\pi, \pi).$$

To conclude, we can just compare the costs associated to each of them and pick the smallest one. It is easy to see that $(\theta_2, \theta_3) = (\pi, 0)$ is the optimal choice. In fact, $(0, 0)$ is clearly the worst. Among the three cases left, we can say that $(\pi, 0)$ always beats $(\pi, \pi)$, that is

$$C(r_1, r_2, r_3, \pi, \pi) - C(r_1, r_2, r_3, \pi, 0) \\ = \left(\frac{1}{r_3 - r_2} - \frac{1}{r_3 - r_1}\right) + \left(\frac{1}{r_2 + r_1} - \frac{1}{r_3 + r_2}\right) > 0,$$

as both the differences in parenthesis are positive. Finally, $(\pi, 0)$ beats $(0, \pi)$ too because

$$C(r_1, r_2, r_3, 0, \pi) - C(r_1, r_2, r_3, \pi, 0) = \frac{2r_1(r_3^2 - r_2^2)}{(r_2^2 - r_1^2)(r_3^2 - r_1^2)} > 0. \qquad \square$$

In the following lemma, we prove that, with the frozen cost $c_\pi$, given six increasing radii numbered $1, \dots, 6$ the choice of two disjoint subsets of three elements which minimizes the cost is always given by 145 and 236. Actually, we prove only some comparisons that are enough for our examples, but one could show in general that

$$\begin{aligned} c_\pi(r_1, r_4, r_5) + c_\pi(r_2, r_3, r_6) &= \\ &= \min \{ \, c_\pi(p_1, p_2, p_3) + c_\pi(p_4, p_5, p_6) : \{p_1, \dots, p_6\} = \{r_1, \dots, r_6\} \, \} \, . \end{aligned}$$

The proof of this fact reduces to the characterization of $c$-monotonicity with Coulomb cost performed in [CDD15, Proposition 2.4].

**Lemma 5.4.2.** *Let $0 < r_1 < \dots < r_6$. Then we have that*

$$\begin{aligned} c_\pi(r_1, r_4, r_5) + c_\pi(r_2, r_3, r_6) \le \min \big\{ & c_\pi(r_1, r_4, r_6) + c_\pi(r_2, r_3, r_5), \\ & c_\pi(r_1, r_3, r_6) + c_\pi(r_2, r_4, r_5), \; c_\pi(r_1, r_3, r_5) + c_\pi(r_2, r_4, r_6) \big\}. \end{aligned} \tag{5.4.8}$$

*Proof.* Let us consider the one dimensional Coulomb cost defined in $\mathbb{R}$

$$\bar{c}(v_1, v_2, v_3) = \frac{1}{|v_2 - v_1|} + \frac{1}{|v_3 - v_2|} + \frac{1}{|v_1 - v_3|} \qquad \forall v_1, v_2, v_3 \in \mathbb{R}.$$

We notice that $c_\pi(r_1, r_4, r_5) = \bar{c}(r_1, -r_4, r_5)$ and, more in general, for all the 3-uples appearing in (5.4.8) the $c_\pi$-cost and the $\bar{c}$-cost satisfy the same relation. In [CDD15, Proposition 2.4] it is proved that, given the six points $-r_4, -r_3, r_1, r_2, r_5, r_6$ the best way to choose two 3-uples to minimize the one dimensional Coulomb cost is to take the points in odd position and the points in even position; in particular, we have

$$\begin{aligned} \bar{c}(-r_4, r_1, r_5) + \bar{c}(-r_3, r_2, r_6) \le \min \big\{ & \bar{c}(-r_4, r_1, r_6) + \bar{c}(-r_3, r_2, r_5), \\ & \bar{c}(-r_3, r_1, r_6) + \bar{c}(-r_4, r_2, r_5), \; \bar{c}(-r_3, r_1, r_5) + \bar{c}(-r_4, r_2, r_6) \big\}, \end{aligned}$$

which proves (5.4.8). $\square$

*Remark* 5.4.3. The previous lemma allows to prove that, for the cost $c_\pi$, the symmetrized optimal plan for the problem (5.2.3) is unique and coincides with the symmetrization of the *DDI*-map.

## 5.5 Proofs of examples and counterexamples

*Proof of Counterexample 5.2.6.* Let $t_0$ be given by Lemma 5.3.2 and let us choose $\varepsilon \leq t_0/2$. If, by contradiction, the $DDI$-map $T$ associated to $\rho_\varepsilon$ is optimal, by Proposition 5.2.4 its support is $c$-monotone. Let us consider $1+\varepsilon$, $1+3\varepsilon$ and the images of these points through $T$ and $T \circ T$:

$$T(1+\varepsilon) = 1+7\varepsilon, \quad T \circ T(1+\varepsilon) = 1+9\varepsilon,$$

$$T(1+3\varepsilon) = 1+5\varepsilon, \quad T \circ T(1+3\varepsilon) = 1+11\varepsilon,$$

We notice that these points

$$(r_1, ..., r_6) = (1+\varepsilon, 1+3\varepsilon, 1+5\varepsilon, 1+7\varepsilon, 1+9\varepsilon, 1+11\varepsilon),$$

are equally spaced; hence, we can apply the scaling properties of the cost function and Lemma 5.3.2 with $t = 2\varepsilon/(1+\varepsilon) \leq t_0$ to deduce that,

$$\begin{aligned} c(r_1, r_4, r_6) &+ c(r_2, r_3, r_5) \\ &= \frac{1}{1+\varepsilon}\Big[c\Big(\frac{r_1}{1+\varepsilon}, \frac{r_4}{1+\varepsilon}, \frac{r_6}{1+\varepsilon}\Big) + c\Big(\frac{r_2}{1+\varepsilon}, \frac{r_3}{1+\varepsilon}, \frac{r_5}{1+\varepsilon}\Big)\Big] \\ &< \frac{1}{1+\varepsilon}\Big[c\Big(\frac{r_1}{1+\varepsilon}, \frac{r_4}{1+\varepsilon}, \frac{r_5}{1+\varepsilon}\Big) + c\Big(\frac{r_2}{1+\varepsilon}, \frac{r_3}{1+\varepsilon}, \frac{r_6}{1+\varepsilon}\Big)\Big] \\ &= c(r_1, r_4, r_5) + c(r_2, r_3, r_6). \end{aligned}$$

This contradicts the $c$-monotonicity of the support by taking $p = \{3\}$. ☐

*Remark* 5.5.1. In the paper in preparation [DNG] it is shown that, in the setting of Counterexample 5.2.6, none of the maps in the $\{D, I\}^3$-class associated to $\rho_\varepsilon$ is optimal in problem (5.2.2), by considering the limit problem as $\varepsilon \to 0$ of a suitably rescaled problem and analyzing the optimal maps with the cost $c_0(x_1, x_2, x_3) = |x_1 + x_2 + x_3|^2$.

*Proof of Counterexample 5.2.7.* ***Step 1.*** By choosing $\varepsilon$ sufficiently small (independently of $M$), we exclude that the $DDI$-map is optimal in problem (5.2.2) for every $M > 2$.

Let $T$ be the piecewise continuous $DDI$-map. Consider the following two points in the support of the plan associated to $T$ (recall that the support is a closed set):

$$\left(1+\frac{\varepsilon}{2}, T\left(1+\frac{\varepsilon}{2}\right), T^{(2)}\left(1+\frac{\varepsilon}{2}\right)\right) = \left(1+\frac{\varepsilon}{2}, 1+\frac{7\varepsilon}{2}, 1+\frac{9\varepsilon}{2}\right),$$
$$\lim_{r \to 1+\varepsilon^-} \left(r, T(r), T^{(2)}(r)\right) = (1+\varepsilon, 1+3\varepsilon, 1+5\varepsilon).$$

We claim that they violate the $c$-monotonicity property (Proposition 5.2.4) with $p = \{3\}$, namely

$$f(\varepsilon) = c\left(1+\frac{\varepsilon}{2}, 1+\frac{7\varepsilon}{2}, 1+\frac{9\varepsilon}{2}\right) + c(1+\varepsilon, 1+3\varepsilon, 1+5\varepsilon)$$
$$-\left[c\left(1+\frac{\varepsilon}{2}, 1+\frac{7\varepsilon}{2}, 1+5\varepsilon\right) + c\left(1+\varepsilon, 1+3\varepsilon, 1+\frac{9\varepsilon}{2}\right)\right] > 0$$

for $\varepsilon$ sufficiently small. The proof is similar to that of Lemma 5.3.2. Using the formulas obtained in Lemma 5.3.1 we just compute the derivatives

$$f(0) = f'(0) = f''(0) = 0,$$
$$f'''(0) = \frac{71\sqrt{3}}{100} > 0.$$

***Step 2.*** We exclude that the maps $DID$, $IDD$, $III$ in the $\{D, I\}^3$-class are optimal in problem (5.2.2) for $M$ large enough.

We present the argument to exclude the $DID$-map, the others being similar. Let us fix $x, y \in (M + 1/4, M + 3/4)$, $x < y$, and let us consider their orbits through $T$, that is $T(x), T(y) \in (1, 1+\varepsilon_0)$ and $T^{(2)}(x), T^{(2)}(y) \in (1+3\varepsilon_0, 1+4\varepsilon_0)$. Let us consider the increasingly ordered points

$$(r_1, ..., r_6) = \Big(T(y), T(x), T^{(2)}(x), T^{(2)}(y), x, y\Big);$$

the couples of points $(r_1, r_4, r_6)$ and $(r_2, r_3, r_5)$ belong to the support of the plan associated to the $DID$-map. By Lemma 5.4.1, we can choose $M$ sufficiently large so that the previous points, as well as the points $(r_1, r_4, r_5)$ and $(r_2, r_3, r_6)$, have the same $c$ and $c_\pi$ cost. By Lemma 5.4.2, which describes the $c_\pi$ monotonicity, we have

$$\begin{aligned} c(r_1, r_4, r_5) + c(r_2, r_3, r_6) &= c_\pi(r_1, r_4, r_5) + c_\pi(r_2, r_3, r_6) \\ &\le c_\pi(r_1, r_4, r_6) + c_\pi(r_2, r_3, r_5) \\ &= c(r_1, r_4, r_6) + c(r_2, r_3, r_5). \end{aligned}$$

This shows, by Proposition 5.2.4, that the $DID$-map cannot be optimal. □

*Remark* 5.5.2. Our method can be applied to the 4-marginal problem to show that there exists $\varepsilon > 0$ such that, setting

$$\rho_\varepsilon = \frac{1}{16\varepsilon} 1_{[1,1+16\varepsilon]}\, dr \in \mathscr{M}(\mathbb{R}_+),$$

any map in the $\{D, I\}^4$-class associated to $\rho_\varepsilon$ is not optimal in problem (5.2.2). Indeed, let $T$ be any such map. Pick two points in $[1, 1+16\varepsilon]$ such that the union of their two orbits is

$$\{r_1, \dots, r_8\} = \{1+\varepsilon, 1+3\varepsilon, 1+5\varepsilon, 1+7\varepsilon, 1+9\varepsilon, 1+11\varepsilon, 1+13\varepsilon, 1+15\varepsilon\}.$$

We claim that $T$ is not $c$-monotone because the partitioning of $\{r_1, \dots, r_8\}$ into two quartets that minimizes

$$c(r_{i_1}, r_{i_2}, r_{i_3}, r_{i_4}) + c(r_{i_5}, r_{i_6}, r_{i_7}, r_{i_8})$$

is $\{(r_1, r_5, r_6, r_7), (r_2, r_3, r_4, r_8)\}$ and such partition doesn't correspond to any of the maps in the $\{D, I\}^4$-class.

The way to see this is to extend the results of Section 5.3 to the 4-marginal case. Consider four radii

$$(r_1, r_2, r_3, r_4) = (1 + a_1 t, 1 + a_2 t, 1 + a_3 t, 1 + a_4 t).$$

Following the same derivation, we find that the angles that give the cost $c$ are

$$\begin{pmatrix} \theta_2(t) \\ \theta_3(t) \\ \theta_4(t) \end{pmatrix} = \begin{pmatrix} \pi/2 \\ \pi \\ 3/3\pi \end{pmatrix} + \frac{6 - \sqrt{2}}{34} \begin{pmatrix} -a_1 - a_2 + a_3 + a_4 \\ 2a_4 - 2a_2 \\ a_1 - a_2 - a_3 + a_4 \end{pmatrix} t + o(t).$$

In turn, this provides the expansion of the cost up to the third order and this information can be used to verify the asymptotic optimality of any given partition. We omit the formulas, since this computations are better performed with the aid of a computer algebra system.

*Proof of Proposition 5.2.9.* Let $M$ be chosen, thanks to Lemma 5.4.1, so that

$$c(r_1, r_2, r_3) = c_\pi(r_1, r_2, r_3) \qquad \text{for every } r_1 \in [1, 2],\ r_2 \in [3, 4],\ r_3 \in [M, \infty). \tag{5.5.1}$$

In order to prove the $c$-monotonicity property, since the map $T$ is cyclical and since its orbits take exactly one point in each interval $[1, 2]$, $[3, 4]$, and $[M, \infty)$, it is enough to show that, given $x, y \in [1, 2]$, $x < y$, we have

$$c\big(x, T(x), T^{(2)}(x)\big) + c\big(y, T(y), T^{(2)}(y)\big) \le c(x, A, B) + c(y, C, D) \tag{5.5.2}$$

for every possible choice of $A, B, C, D$ such that $\{A, C\} = \{T(x), T(y)\}$ and $\{B, D\} = \{T^{(2)}(x), T^{(2)}(y)\}$. By definition, we have that

$$1 \le x < y \le 2 \le 3 \le T(y) < T(x) \le 4 \le M \le T^{(2)}(x) < T^{(2)}(y);$$

hence by (5.5.1) we have that $c\big(x, T(x), T^{(2)}(x)\big) = c_\pi\big(x, T(x), T^{(2)}(x)\big)$ (and similarly for $y$ and for the other 3-uples) and by Lemma 5.4.2 we have that

$$\begin{aligned} c\big(x, T(x), T^{(2)}(x)\big) &+ c\big(y, T(y), T^{(2)}(y)\big) \\ &= c_\pi\big(x, T(x), T^{(2)}(x)\big) + c_\pi\big(y, T(y), T^{(2)}(y)\big) \\ &\le c_\pi(x, A, B) + c_\pi(y, C, D) = c(x, A, B) + c(y, C, D), \end{aligned}$$

for every possible choice of $A, B, C, D$ such that $\{A, C\} = \{T(x), T(y)\}$ and $\{B, D\} = \{T^{(2)}(x), T^{(2)}(y)\}$; this proves (5.5.2). □

# Chapter 6

# Finiteness and continuity of multi-marginal optimal transport with repulsive cost

## 6.1 Introduction

In this chapter we prove the finiteness and continuity of multi-marginal optimal transport with repulsive cost under the assumption that the measure does not concentrate too much. This chapter is based on the article in preparation [CDS] and is a refinement of the results presented in [BCP16], especially from the point of view of the assumptions, which in our work are shown to be sharp.

The setting is as follows. The ambient space is a complete and separable (Polish) metric space $(X, \mathsf{d})$. We consider a repulsive interaction cost given by a symmetric lower semi-continuous function $c : X \times X \to [0, \infty]$ such that $c(x, x) = \infty$ for all $x \in X$ and for which there exist two right-continuous non-increasing[1] functions $m, M : (0, \infty) \to [0, \infty)$ satisfying

$$m\big(\mathsf{d}(x_1, x_2)\big) \le c(x_1, x_2) \le M\big(\mathsf{d}(x_1, x_2)\big), \qquad \text{for all } x_1 \neq x_2 \in X,$$

and

$$\lim_{r\to 0^+} m(r) = \lim_{r\to 0^+} M(r) = \infty.$$

If we wish, we can extend $m(0) = M(0) = \infty$, so that the preceding inequality holds for all $x_1, x_2 \in X$. For $a > 0$ define the "enlarged diagonal"

$$D_\alpha = \big\{x = (x_1, \dots, x_N) \in (\mathbb{R}^d)^N : \mathsf{d}(x_i, x_j) < \alpha \text{ for some } i \neq j\big\},$$
$$\bar{D}_\alpha = \big\{x = (x_1, \dots, x_N) \in (\mathbb{R}^d)^N : \mathsf{d}(x_i, x_j) \le \alpha \text{ for some } i \neq j\big\}.$$

Notice that in general $\bar{D}_\alpha$ is not the closure of $D_\alpha$ (which would be denoted by $\overline{D_\alpha}$ if needed), but rather contains it.

[1] Hence lower semi-continuous.

### 6.1.1 Examples

We summarize here three particular examples that fall inside this setting:

- Coulomb in $\mathbb{R}^d$,
- $c = \phi \circ \mathsf{d}$,
- $c = G$ Green function of $\Delta$ on a manifold.

**Coulomb in $\mathbb{R}^d$.** The model case is the Coulomb interaction in $\mathbb{R}^3$. This is how the problem originated in the context of Density Functional Theory. The ambient space is $\mathbb{R}^d$ and the cost $c(x, y) = 1/|x - y|$.

**Case $c = \phi \circ \mathsf{d}$.** A specific instance of this kind would be a cost of the form $c(x_1, x_2) = \phi\big(\mathsf{d}(x_1, x_2)\big)$, where $\phi : [0, \infty) \to [0, \infty]$ is a lower semi-continuous function such that

- $\phi(0) = \infty$, hence $\lim_{r\to 0^+} \phi(r) = \infty$,
- and $\phi|_{[r,\infty)}$ is bounded for every $r > 0$.

In this case, $m$ and $M$ could be given by

$$m(r) \coloneqq \min_{r'\in[0,r]} \phi(r'), \qquad M(r) \coloneqq \sup_{r'\in[r,\infty)} \phi(r').$$

From the definition follows that $m$ and $M$ are non-increasing and right-continuous, $m(r) \le \phi(r) \le M(r)$ and $\lim_{r\to 0^+} m(r) = \infty$. We define also the pseudo-inverse $m^{-1} : [0, \infty) \to (0, \infty]$ by

$$m^{-1}(t) \coloneqq \max\{r \in (0, \infty] : m(r) \ge t\}.$$

Then $m^{-1}$ is non-increasing, left-continuous and satisfies the important relation $m\big(m^{-1}(t)\big) \ge t$.

**Green function of $\Delta$.** Noticing that the potential $1/|x - y|$ is the fundamental solution of the Laplacian in $\mathbb{R}^3$, the first case can be generalized to a Riemannian manifold $M$ where the cost is given by $c(x, y) = G(x, y)$, the fundamental solution of $\Delta_x G(x, y) = \delta_y$. If the manifold is compact then it is clear that $c$ satisfies the previous hypotheses, but they could be verified also on some non-compact manifolds, like they are in $\mathbb{R}^d$ because of the translation invariance.

### 6.1.2 Notation

For every integer $N \geq 2$, define the symmetric interaction cost $c : (\mathbb{R}^d)^N \to [0, \infty]$ by

$$c(x_1, \dots, x_N) \coloneqq \sum_{1 \leq i < j \leq N} c(x_i, x_j),$$

the cost of a plan $C : \mathscr{P}\big((\mathbb{R}^d)^N\big) \to [0, \infty]$ by

$$C(\pi) \coloneqq \int_{(\mathbb{R}^d)^N} c(x_1, \dots, x_N) \, \mathrm{d}\pi(x_1, \dots, x_N)$$

and lastly the optimal transport cost $\mathscr{C}_N : \mathscr{P}(\mathbb{R}^d) \to [0, \infty]$ associated to a marginal by

$$\mathscr{C}_N(\rho) \coloneqq \inf\{C(\pi) : \pi \in \Pi_N(\rho)\},$$

where

$$\Pi_N(\rho) \coloneqq \big\{\pi \in \mathscr{P}\big((\mathbb{R}^d)^N\big) : P^i_{\#}\pi = \rho \text{ for } i = 1, \dots, N\big\}$$

denotes the admissible transport plans.

Our results depend on assumptions regarding the concentration of mass of the marginal $\rho$, therefore we introduce two quantities measuring it. Given $\mu \in \mathscr{P}(X)$, we consider the biggest atom of $\mu$

$$a(\mu) \coloneqq \max_{x \in X} \mu(\{x\}),$$

and the concentration on balls defined as

$$\kappa(\mu, r) \coloneqq \sup_{x \in X} \mu\big(\bar{B}(x, r)\big),$$

which will be needed for the uniform quantitative version of the results.

We will use the notation $P^i : X^N \to X$ to denote the projection on the $i$-th coordinate and also $P^{i_1, \dots, i_k} : X^N \to X^k$ to denote the projection on the coordinates $i_1, \dots, i_k$.

## 6.2 Preliminary results

**Definition 6.2.1.** A measure $\pi \in \mathscr{M}_+(\mathbb{R} \times \mathbb{R})$ is said to be *increasing* if $(x' - x)(y' - y) \geq 0$ for $\pi \otimes \pi$-a.e. $\big((x, y), (x', y')\big) \in (\mathbb{R} \times \mathbb{R})^2$, that is, $\pi \otimes \pi(R) = 0$ where

$$R = \big\{\big((x, y), (x', y')\big) \in (\mathbb{R} \times \mathbb{R})^2 : (x' - x)(y' - y) < 0\big\}.$$

**Lemma 6.2.2.** *Given $\mu, \nu \in \mathscr{P}(\mathbb{R})$, there exists a unique increasing plan $\pi \in \Pi(\mu, \nu)$.*

*Proof.* Assume $\mu = u\mathscr{L}^1$ and $\nu = v\mathscr{L}^1$ with strictly positive densities $u$ and $v$. Consider the repartition functions $F(x) = \mu\big((-\infty, x]\big)$ and $G(x) = \nu\big((-\infty, x]\big)$, which are continuous and strictly increasing. Then $\nu = T_\#\mu$ where $T = g^{-1} \circ f$ is increasing. Therefore $\pi = (\mathrm{Id}, T)_\#\mu \in \Pi(\mu, \nu)$ is increasing, since it is concentrated on the graph of $T$.

In the general case, consider $\mu_n = \mu * g_n$ and $\nu_n = \nu * g_n$, where $g \in L^1(\mathbb{R})$ is a strictly positive probability density and $g_n(x) = ng(nx)$. When $n \to \infty$, we have $\mu_n \rightharpoonup \mu$ and $\nu_n \rightharpoonup \nu$. We know that there are increasing plans $\pi_n \in \Pi(\mu_n, \nu_n)$. By a standard compactness argument, up to a subsequence, we have $\pi_n \rightharpoonup \pi \in \Pi(\mu, \nu)$. But then $\pi$ is increasing because $\pi_n \otimes \pi_n \rightharpoonup \pi \otimes \pi$ and $R$ is open, hence

$$\pi \otimes \pi(R) \leq \liminf_{n\to\infty} \pi_n \otimes \pi_n(R) = 0.$$

As for uniqueness (which will not be needed in the sequel, however), notice that $\pi$ is completely characterized by the property

$$\pi\big((-\infty, x] \times (-\infty, y]\big) = F(x) \wedge G(y), \qquad \text{for all } x, y \in \mathbb{R}. \qquad \square$$

The previous definition and lemma can be generalized straightforwardly to more than two marginals and in the sequel they will be used this way.

Clearly the uniform concentration condition measured by $\kappa$ is stronger than the pointwise one encoded by $a$. However, thanks to a compactness argument, the next lemma shows that the two are in fact almost equivalent.

**Lemma 6.2.3.** *Let $\rho \in \mathscr{P}(X)$ and assume that $a(\rho) < \delta$. Then there exists $r > 0$ such that $\kappa(\rho, r) < \delta$.*

*Proof.* Fix $a(\rho) < \delta' < \delta$. Since $\rho$ is tight, we can find a compact subset $K \subset X$ such that $\rho(K^c) < \delta'$. Given $x \in X$, one has $\lim_{r\to 0^+} \rho\big(\bar{B}(x, r)\big) = \rho(\{x\}) \leq a(\rho) < \delta'$, therefore for every $x$ there exists a positive radius $r_x$ such that

$$\rho\big(\bar{B}(x, 3r_x)\big) < \delta'.$$

Since $K$ is compact, we can find a finite number of points $x_1, \dots, x_k$ such that $K \subset \bigcup_{i=1}^k \bar{B}(x_i, r_{x_i})$. Let $r = \min\{r_{x_1}, \dots, r_{x_k}\}$. If $\mathsf{d}(x, K) > r$, then $\bar{B}(x, r) \subset K^c$, hence $\rho\big(\bar{B}(x, r)\big) < \delta'$. If $\mathsf{d}(x, K) \leq r$, then $\mathsf{d}(x, x_i) \leq 2r_{x_i}$ for some $i = 1, \dots, k$, therefore $\bar{B}(x, r) \subset \bar{B}(x_i, 3r_{x_i})$, hence $\rho\big(\bar{B}(x, r)\big) < \delta'$. This implies that $\kappa(\rho, r) \leq \delta' < \delta$. $\square$

**Lemma 6.2.4.** *Assume that $\rho \in \mathscr{P}(X)$ satisfies $\kappa(\rho, r) < \delta$ for some $r > 0$ and let $\rho_n \rightharpoonup \rho$. Then for every $r' \in (0, r/2)$ one has $\kappa(\rho_n, r') < \delta$ for $n$ large enough. If $X$ si proper, then we can take $r' \in (0, r)$.*

*In particular, if $a(\rho) < \delta$, then $a(\rho_n) < \delta$ definitely in $n$.*

*Proof.* Fix $\kappa(\rho, r) < \delta' < \delta$. Since the family $(\rho_n)$ is tight, we can find a compact subset $K \subset X$ such that $\rho_n(K^c) < \delta'$ for all $n$. Take $\varepsilon \in (0, r - 2r']$. The compact set $K$ can be covered by a finite number of balls $K \subset \bigcup_{i=1}^k \bar{B}(x_i, \varepsilon)$. For each $i = 1, \dots, k$ one has

$$\limsup_{n\to\infty} \rho_n\big(\bar{B}(x_i, r)\big) \leq \rho\big(\bar{B}(x_i, r)\big) \leq \kappa(\rho, r) < \delta'.$$

This means that there exists $\bar{n} \in \mathbb{N}$ such that for all $n \geq \bar{n}$ and for every $i = 1, \dots, k$ one has

$$\rho_n\big(\bar{B}(x_i, r)\big) < \delta'.$$

Let now $n \geq \bar{n}$. If $\mathsf{d}(x, K) > r'$, then $\bar{B}(x, r') \subset K^c$, hence $\rho_n\big(\bar{B}(x, r')\big) \leq \rho_n(K^c) < \delta'$. Otherwise, if $\mathsf{d}(x, K) \leq r'$, then $\mathsf{d}(x, x_i) \leq r' + \varepsilon$ for some $i = 1, \dots, k$, therefore $\bar{B}(x, r') \subset \bar{B}(x_i, 2r' + \varepsilon) \subset \bar{B}(x_i, r)$, from which $\rho_n\big(\bar{B}(x, r')\big) < \delta'$. This implies that $\kappa(\rho_n, r') \leq \delta' < \delta$ for $n \geq \bar{n}$.

Assume that $X$ is proper and take $\delta'$ and $K$ as before. Fix $\varepsilon \in (0, r - r']$. The set $H = \{x \in X : \mathsf{d}(x, K) \leq r'\}$ is compact because it is closed and bounded, therefore it can be covered by a finite number of balls $H \subset \bigcup_{i=1}^k \bar{B}(x_i, \varepsilon)$. For each $i = 1, \dots, k$ one has

$$\limsup_{n\to\infty} \rho_n\big(\bar{B}(x_i, r)\big) \leq \rho\big(\bar{B}(x_i, r)\big) \leq \kappa(\rho, r) < \delta'.$$

This means that there exists $\bar{n} \in \mathbb{N}$ such that for all $n \geq \bar{n}$ and for every $i = 1, \dots, k$ one has

$$\rho_n\big(\bar{B}(x_i, r)\big) < \delta'.$$

Let now $n \geq \bar{n}$. If $\mathsf{d}(x, K) > r'$, then $\bar{B}(x, r') \subset K^c$, hence $\rho_n\big(\bar{B}(x, r')\big) \leq \rho_n(K^c) < \delta'$. Otherwise, if $\mathsf{d}(x, K) \leq r'$, then $x \in H$ and $\mathsf{d}(x, x_i) \leq \varepsilon$ for some $i = 1, \dots, k$, therefore $\bar{B}(x, r') \subset \bar{B}(x_i, r' + \varepsilon) \subset \bar{B}(x_i, r)$, from which $\rho_n\big(\bar{B}(x, r')\big) < \delta'$. This implies that $\kappa(\rho_n, r') \leq \delta' < \delta$ for $n \geq \bar{n}$. □

The next lemma is the one dimensional version of the finiteness of the cost and will be used later to prove the general case, together with Proposition 6.2.7.

**Lemma 6.2.5.** *Let $\rho \in \mathscr{P}(\mathbb{R})$ be such that $a(\rho) < 1/N$. Then $\mathscr{C}(\rho) < \infty$.*

*Proof.* An immediate consequence of Lemma 6.2.3 and Lemma 6.2.6. □

**Lemma 6.2.6.** *Let $\rho \in \mathscr{P}(\mathbb{R})$ be such that $\kappa(\rho, r) < 1/N$. Then the optimal plan is distant from the diagonal: more precisely $\pi(D_{2r}) = 0$ and $\mathscr{C}(\rho) \leq \binom{N}{2} M(2r)$.*

*Proof.* Let $-\infty \leq t_0 \leq t_1 \leq \cdots \leq t_N \leq \infty$ and $\rho_1, \dots, \rho_N \in \mathscr{M}_+(\mathbb{R})$ be such that $\rho = \rho_1 + \cdots + \rho_N$, $\rho_i(\mathbb{R}) = 1/N$ and $\rho_i$ is supported on $[t_{i-1}, t_i]$. By Lemma 6.2.2, for $1 \leq i < j \leq N$ there exists an increasing plan $\pi_{i,j} \in \Pi(\rho_i, \rho_j)$.

Let $\rho_i^\varepsilon \rightharpoonup \rho_i$ be measures with strictly positive densities. Then there are maps $T_i^\varepsilon : [0, 1/N] \to \mathbb{R}$ such that $\rho_i^\varepsilon = {T_i^\varepsilon}_\#(\mathscr{L}^1 \llcorner [0, 1/N])$. Letting $\pi^\varepsilon = (T_1^\varepsilon, \dots, T_N^\varepsilon)$, by a standard compactness argument we have that up to a subsequence $\pi^\varepsilon \rightharpoonup \tilde{\pi}$

as $\varepsilon \to 0$ for some $\tilde{\pi} \in \mathscr{M}_+(\mathbb{R}^d)$ with total mass $1/N$. Finally, define the cyclic version

$$\pi = \sum_{i=1}^{N} P_{\#}^{i,\dots,N,1,\dots,i-1} \tilde{\pi}.$$

Then $\pi \in \Pi(\rho)$ because all the marginals $\rho_i^\varepsilon$ pass to the limit in the correct way. This is the optimal plan according to [CDD15]. Notice that by the concentration assumption one must have $\mathsf{d}(x_{i,j}) \geq 2r$ for $i \neq j$ and all $x \in \operatorname{supp} \pi$, otherwise the ball of radius $r$ centered at the midpoint $(x_i + x_j)/2$ would contain more than $1/N$ of the mass of $\rho$. But then this fact implies □

**Proposition 6.2.7** (Good projection). *Let $\rho \in \mathscr{P}(X)$ with $a(\rho) < \delta$. Then there exists $P \in \mathrm{Lip}_1(X)$ such that $a(P_\# \rho) < \delta$. Such a $P$ will be called a good projection.*

*Proof.* We start from the case where $X$ is a finite-dimensional normed vector space, i.e. $X \simeq \mathbb{R}^d$. It is sufficient to show that there exists $P_d \in \mathrm{Lip}(\mathbb{R}^d; \mathbb{R}^{d-1})$ such that $a(P_{d\#}\rho) < \delta$. Then we conclude by taking $P = P_2 \circ \cdots \circ P_d$. The statement is true if we are able to find a direction $v \in \mathbb{R}^d$ such that $\rho(l) < \delta$ for every line $l$ parallel to $v$. In fact, then we can write $\mathbb{R}^d \simeq \mathbb{R}^{d-1} \oplus \langle v \rangle$ and take $P_d$ to be the projection onto the first factor. Fix a positive $\varepsilon < [\delta - a(\rho)]/2$. Let $\{x_i\}_i$ be the at most countable set of atoms of $\rho$. Take out a finite number of them, $x_1, \dots, x_n$, such that the mass of the remaining ones is small, namely

$$\sum_{i>n} \rho(\{x_i\}) < \varepsilon.$$

The directions $v_{ij} = x_i - x_j$ are forbidden. Consider the non-atomic measure

$$\tilde{\rho} = \rho - \sum_{i \geq 1} \rho(\{x_i\}) \delta_{x_i}.$$

This measure is additive on finite unions of distinct lines, because the intersections are finite sets of points, which have zero measure w.r.t. $\tilde{\rho}$. Therefore there is only a finite number of lines $l_1, \dots, l_k$ with $\tilde{\rho}(l_i) \geq \varepsilon$. Let $v_i$ denote a direction parallel to $l_i$. This procedure rules out another finite number of directions, $v_1, \dots, v_k$. Now take a direction $v$ which is not parallel to any of the $v_{ij}$ or $v_i$. If $l$ is a line parallel to $v$, $l$ can contain at most one of the points $x_1, \dots, x_n$ (otherwise $v$ would be parallel to some $v_{ij}$) and $\tilde{\rho}(l) < \varepsilon$ (otherwise $v$ would be parallel to some $v_i$). Therefore

$$\rho(l) \leq \tilde{\rho}(l) + \max_{i=1,\dots,n} \rho(\{x_i\}) + \sum_{i>n} \rho(\{x_i\}) < \varepsilon + a(\rho) + \varepsilon < \delta.$$

Assume now that $X = \ell^\infty$ and $\rho \in \mathscr{P}(\ell^\infty)$ is tight. It is well know (see for instance [PS12, Lemma 5.7]) that $\ell^\infty$ has the metric approximation property, that is, for every compact set $K \subset \ell^\infty$ and every $\varepsilon > 0$ there is a linear operator $T : \ell^\infty \to \ell^\infty$ of finite rank with operator norm $\|T\| \leq 1$ and $\sup_{x \in K} \|Tx - x\|_\infty \leq \varepsilon$. Since $\rho$ is tight, there are increasing compact sets $K_n$ such that $\rho(K_n^c) < 1/n$. $\rho$ is clearly concentrated on the set $H = \bigcup_n K_n$. Let $T_n : \ell^\infty \to \ell^\infty$ be a finite-rank linear operator with $\|T_n\| \leq 1$ and $\sup_{x \in K_n} \|T_n x - x\|_\infty \leq 1/n$. For every $x \in H$ we have $T_n x \to x$ as $n \to \infty$, therefore $T_{n\#}\rho \rightharpoonup \rho$.[2] But then, by Lemma 6.2.4, $a(T_{n\#}\rho) < \delta$ for $n$ sufficiently large. The measure $T_{n\#}\rho$ is supported on a finite-dimensional vector subspace of $\ell^\infty$ (the image of $T_n$), therefore we already know that there is a good projection $Q$ for it. A good projection for $\rho$ itself is then given by $P = Q \circ T_n$.

In the general case of a Polish space $(X, \mathsf{d})$, we simply need to embed it isometrically $\iota : X \to \ell^\infty$ by means of $\iota(x) = (\varphi_n(x))_n$, where $\varphi_n(x) = \mathsf{d}(x, x_n) - \mathsf{d}(x, x_0)$ and $\{x_n\}_n \subset X$ is a countable dense set. By Ulam lemma $\rho$ is tight, and so is $\iota_\# \rho \in \mathscr{P}(\ell^\infty)$. Clearly $a(\iota_\#\rho) = a(\rho) < \delta$, therefore we can find a good projection $Q$ for $\iota_\#\rho$ and a good projection for $\rho$ is given by $P = Q \circ \iota$. □

*Remark* 6.2.8. The previous proposition remains true when $\rho$ is a tight finite non-negative measure on a generic metric space $X$. The only modification is to observe that we just need to embed only $\operatorname{supp}(\rho) \hookrightarrow \ell^\infty$, which is $\sigma$-compact and closed, thus Polish.

Proposition 6.2.7 will be used to prove the finiteness of the cost under the assumption that $a(\rho) < 1/N$. To deal with the other concentration condition $\kappa(\rho, r) < 1/N$, one could hope to extend the good projection in the following way. However we have not been able to establish the truth of the next conjecture, therefore we had to find another way to get the bound of the cost (see Theorem 6.3.6). The conjecture, however, seems interesting enough from the measure teoretic perspective, so we state it anyway.

**Conjecture 6.2.9** (Good projection, quantitative version). *Let $\rho \in \mathscr{P}(\mathbb{R}^d)$ with $\kappa(\rho, r) < \delta$. Then for every $\varepsilon > 0$ there exists $P \in \mathrm{Lip}_1(\mathbb{R}^d)$ such that $\kappa(P_\#\rho, r') < \delta + \varepsilon$ for some $r'(r, d, \delta, \varepsilon) > 0$.*

## 6.3 Main results

Apart from proving that if the concentration of a measure is below $1/N$ then the cost is finite (see Lemma 6.3.3 and Theorem 6.3.6), we are also able to show that this threshold is sharp, as illustrated by the next simple theorem.

**Theorem 6.3.1.** *Let $\rho \in \mathscr{P}(X)$ with $a(\rho) > 1/N$. Then $\mathscr{C}(\rho) = \infty$.*

*Proof.* We prove the contrapositive. Let $\pi \in \Pi(\rho)$ be an optimal plan. Since $\mathscr{C}(\rho) = C(\pi) < \infty$, we infer that $\pi(D) = 0$. Let $\bar{x} \in \arg\max\{\rho(x) : x \in X\}$, so

[2] Indeed, if $f \in C_b(\ell^\infty)$, one has $\int f \,\mathrm{d}T_{n\#}\rho = \int f \circ T_n \,\mathrm{d}\rho \to \int f \,\mathrm{d}\rho$ by dominated convergence.

that $\rho(\{\bar{x}\}) = a(\rho)$, and define $X_* = \{\bar{x}\}^c$. For every $i = 1, \dots, N$ one has

$$\rho(\{\bar{x}\}) = P^i_\# \pi(\{\bar{x}\}) = \pi\big(X^{N-1} \times_i \{\bar{x}\}\big) = \pi\big(X_*^{N-1} \times_i \{\bar{x}\}\big).$$

Notice that the $N$ sets $X_*^{N-1} \times_i \{\bar{x}\}$ are disjoint, therefore, adding over $i = 1, \dots, N$, we get

$$N\rho(\{\bar{x}\}) = \sum_{i=1}^N \pi\big(X_*^{N-1} \times_i \{\bar{x}\}\big) = \pi\left(\bigcup_{i=1}^N X_*^{N-1} \times_i \{\bar{x}\}\right) \le \pi\big(X^N\big) = 1,$$

from which $a(\rho) \le 1/N$. □

At the threshold level $1/N$ anything can happen: the cost can be finite or infinite, depending on the specific distribution of the mass.

**Theorem 6.3.2.** *Let $X$ be a space with at least one accumulation point. There exists $\rho \in \mathscr{P}(X)$ such that $a(\rho) = 1/N$ and $\operatorname{supp}(\pi) \cap D \neq \emptyset$ for every $\pi \in \Pi(\rho)$ (thus $\pi(D_\alpha) > 0$ for every $\alpha > 0$). Moreover, there is one such $\rho$ with $\mathscr{C}(\rho) < \infty$ and one with $\mathscr{C}(\rho) = \infty$.*

*Proof.* Let $x \in X$ be a limit point and let $(x_n)_{n\in\mathbb{N}} \subset X \setminus \{x\}$ be a sequence of distinct points converging to $x$. Consider the probability measure

$$\rho = \frac{1}{N}\delta_x + \frac{N-1}{N}\sum_n p_n \delta_{x_n},$$

where $(p_n)_{n\in\mathbb{N}} \in \ell^1$ with $p_n > 0$ and $\|p\|_1 = 1$. Let $\pi \in \Pi(\rho)$ and assume by contradiction that $\pi(D_\alpha) = 0$ for some $\alpha > 0$. For $i = 1, \dots, N$ define the restricted measures

$$\eta_i = \pi \llcorner (X^{N-1} \times_i \{x\}).$$

We have that

$$\eta_i(X^N) = \pi(X^{N-1} \times_i \{x\}) = \rho(\{x\}) = 1/N.$$

Define the sets $X_* = X \setminus B(x, \alpha)$ and $B_* = B(x, \alpha) \setminus \{x\}$. The measure $\eta_i$ is actually concentrated on $X_*^{N-1} \times_i \{x\}$, in fact

$$\eta_i\big((X_*^{N-1} \times_i \{x\})^c\big) = \pi\left(\bigcup_{j\neq i} X_*^{N-2} \times_i \{x\} \times_j B(x,\alpha)\right) \le \pi(D_\alpha) = 0.$$

These sets are disjoint, therefore $\eta_i \wedge \eta_j = 0$ for $i \neq j$ and $\pi = \sum_{i=1}^N \eta_i$. Notice that both $B_* \cap \{x\} = \emptyset$ and $B_* \cap X_* = \emptyset$, therefore

$$\begin{aligned} P^1_\# \eta_1(B_*) &= \pi\big((B_* \cap \{x\}) \times X_*^{N-1}\big) = \pi(\emptyset) = 0, \\ P^1_\# \eta_i(B_*) &= \pi\big((B_* \cap X_*) \times X_*^{N-2} \times_i \{x\}\big) = \pi(\emptyset) = 0, \end{aligned}$$

but this leads

$$\rho(B_*) = P^1_\# \pi(B_*) = \sum_{i=1}^N P^1_\# \eta_i(B_*) = 0,$$

which is a contradiction since $x \in \operatorname{supp}(\rho \llcorner \{x\}^c)$.

Finally, one can fiddle with the choice of the weights $(p_n)_n$ in order to make the cost finite or infinite. $\square$

We present here a simple proof of the finiteness of the cost depending on the existence of good projections, before moving on to the more powerful, but maybe less intuitive, Theorem 6.3.6.

**Lemma 6.3.3.** *Let $\rho \in \mathscr{P}(X)$ be such that $a(\rho) < 1/N$. Then there exists a plan $\pi \in \Pi(\rho)$ such that $\pi(D_\alpha) = 0$ for some $\alpha > 0$. In particular,*

$$\mathscr{C}(\rho) \le C(\pi) \le \binom{N}{2} M(\alpha) < \infty.$$

*Proof.* Take a good projection $P \in \operatorname{Lip}_1(X)$ given by Proposition 6.2.7 and consider the measure $\nu = P_\# \mu$. By the disintegration theorem there are probabilities $\mu_t \in \mathscr{P}(X)$ such that $\mu = \mu_t \otimes \nu(t)$. Let $\tilde{\pi} \in \Pi(\nu)$ be the optimal monotone plan and let $\pi \in \Pi(\mu)$ be any plan such that $(P, \dots, P)_\# \pi = \tilde{\pi}$. Such a plan can be build by mapping arbitrarily the measures $\mu_t$ on one another. If $x \in \operatorname{supp} \mu_t$ and $y \in \operatorname{supp} \mu_s$, then $\mathsf{d}(x, y) \ge |t - s|$ by the Lipschitzianity of $P$, because $t = P(x)$ and $s = P(y)$. Therefore $c(x, y) \le M(|t - s|)$. But in proving Lemma 6.2.5 we showed that $|t - s| \ge \alpha$ for some $\alpha > 0$ if the points $t$ and $s$ are coupled by the optimal plan $\tilde{\pi}$. Therefore $c(x, y) \le M(\alpha)$ if the points $x$ and $y$ are coupled by $\pi$ and tis leads to $\mathscr{C}(\rho) \le C(\pi) \le \binom{N}{2} M(\alpha)$. $\square$

**Proposition 6.3.4** (Local boundedness of the cost)**.** *Let $\rho \in \mathscr{P}(X)$ be such that $a(\rho) < 1/N$. Then $\mathscr{C}$ is locally bounded around $\rho$ w.r.t. weak convergence. In particular, $\mathscr{C}(\rho) < \infty$.*

*Proof.* We start by taking a good projection $P \in \operatorname{Lip}_1(X)$ provided by Proposition 6.2.7. By Lemma 6.2.3, the projected measure $\rho' = P_\# \rho$ satisfies $\kappa(\rho', r) < 1/N$ for some $r > 0$. If $\rho_n \rightharpoonup \rho$, then $\rho'_n = P_\# \rho_n \rightharpoonup \rho'$ and by Lemma 6.2.4 they all satisfy $\kappa(\rho, r/3) < 1/N$. Then the same argument of the previous lemma leads to $\mathscr{C}(\rho_n) \le \binom{N}{2} M(r/3)$. $\square$

**Corollary 6.3.5** (Boundedness of the cost)**.** *Let $\mathscr{F} \subset \mathscr{P}(X)$ be relatively compact, $r > 0$ and $\delta < 1/N$. Then there exists $C(r, \delta, \mathscr{F}) < \infty$ such that $\mathscr{C}(\rho) \le C(r, \delta, \mathscr{F})$ for all $\rho \in \mathscr{F}$ such that $\kappa(\rho, r) < \delta$.*

*Proof.* Assume by contradiction that there is a sequence $(\rho_n)_{n \in \mathbb{N}} \subset \mathscr{F}$ with $\kappa(\rho_n, r) < \delta$, but $\mathscr{C}(\rho_n) \to \infty$. Up to a subsequence we may assume that $\rho_n \rightharpoonup \rho \in \mathscr{P}(X)$. Moreover, given $r' \in (0, r)$ and $x \in X$, we have

$$\rho\big(\bar{B}(x, r')\big) \le \rho\big(B(x, r)\big) \le \liminf_{n \to \infty} \rho_n\big(B(x, r)\big) \le \liminf_{n \to \infty} \kappa(\rho_n, r) \le \delta,$$

therefore $\kappa(\rho, r') \leq \delta < 1/N$, and in particular $a(\rho) < 1/N$. The previous proposition asserts that the cost is locally bounded around $\rho$ and this provides a contradiction. $\square$

**Theorem 6.3.6** (Uniform bound on the cost)**.** *Let $\rho \in \mathscr{P}(\mathbb{R}^d)$ be such that $\kappa(\rho, r) \leq \frac{1}{N}$ for some $r > 0$. Then*

$$\mathscr{C}(\rho) \leq \binom{N}{2} M(r).$$

*Proof.* The proof exploits the duality formula for bounded costs. We want to show that there exists an admissible plan $\pi \in \Pi(\rho)$ such that $\pi(D_r) = 0$. In this case then clearly $\mathscr{C}(\rho) \leq C(\pi) \leq \binom{N}{2} M(r)$. Such a plan will be given as the minimizer of the multi-marginal optimal transport with respect to the following bounded cost:

$$\tilde{c}(x_1, \ldots, x_N) = \begin{cases} 0 & \text{if } x \in D_r^c, \\ \max\limits_{i \neq j}(r - |x_i - x_j|)_+ & \text{if } x \in D_r. \end{cases}$$

For this cost it is known that the duality formula holds ([De 15]):

$$\inf_{\pi \in \Pi(\rho)} \int_{\mathbb{R}^{Nd}} \tilde{c} \, \mathrm{d}\pi = \sup_{\varphi(x_1) + \cdots + \varphi(x_N) \leq \tilde{c}(x)} N \int_{\mathbb{R}^d} \varphi \, \mathrm{d}\rho.$$

The optimal $\pi \in \Pi(\rho)$ will satisfy $\pi(D_r) = 0$ if we show that

$$\int_{\mathbb{R}^d} \varphi \, \mathrm{d}\rho \leq 0 \qquad \text{for all admissible } \varphi.$$

In fact, in such case the optimal value of the previous problems must be 0, therefore $\pi$ has to be supported on $D_r^c$.

Actually, the crucial constraint on $\varphi$ that will be needed for the proof is

$$\varphi(x_1) + \cdots + \varphi(x_N) \leq 0 \qquad \text{if } x \in D_r^c.$$

The only role that the condition on $D_r$ plays is telling us that $\varphi$ is bounded from above, since $(x, \ldots, x) \in D_r$ and therefore $N\varphi(x) \leq \tilde{c}(x, \ldots, x) = r$; indeed one would like to consider the cost which takes the value $\infty$ in this region, if there were not the problem of the validity of the duality formula for such a cost and the boundedness of the potential.

After having fixed a small $\varepsilon > 0$, we do the following iterative construction of $\eta_i$, $z_i$ and $B_i$:

$$\begin{aligned}
&\eta_1 = \sup_{\mathbb{R}^d} \varphi, && z_1 \in \mathbb{R}^d,\ \varphi(z_1) \geq \eta_1 - \varepsilon, && B_1 = B(z_1, r), \\
&\eta_2 = \sup_{B_1^c} \varphi, && z_2 \in B_1^c,\ \varphi(z_2) \geq \eta_2 - \varepsilon, && B_2 = B(z_2, r), \\
&\quad\vdots && \qquad\vdots && \quad\vdots \\
&\eta_k = \sup_{(B_1 \cup \cdots \cup B_{k-1})^c} \varphi, && z_k \in (B_1 \cup \cdots \cup B_{k-1})^c,\ \varphi(z_k) \geq \eta_k - \varepsilon, && B_k = B(z_k, r).
\end{aligned}$$

Notice that we have the monotone sequence $r/N \geq \eta_1 \geq \eta_2 \geq \dots$ and so on.

At each step we check the sign of the quantity

$$\eta_1 + \cdots + \eta_{k-1} + (N-k+1)\eta_k - (k-1)\varepsilon.$$

As soon as it is non-positive we stop the process and estimate the quantity $\int_{\mathbb{R}^d} \varphi \, \mathrm{d}\rho$. Notice that this will surely happen by the time we reach $k = N$, because if $z \in (B_1 \cup \cdots \cup B_{N-1})^c$, then $(z_1, \dots, z_{N-1}, z) \in D_r^c$, so

$$(\eta_1 - \varepsilon) + \cdots + (\eta_{N-1} - \varepsilon) + \varphi(z) \leq \varphi(z_1) + \cdots + \varphi(z_{N-1}) + \varphi(z) \leq 0$$

and $\eta_1 + \cdots + \eta_N - (N-1)\varepsilon \leq 0$ follows by taking the supremum over $z$.

Calling $k$ the smallest integer for wich this happens, by constuction we have

$$\eta_k \leq -\frac{1}{N-k+1}\sum_{j=1}^{k-1}\eta_j + \frac{k-1}{N-k+1}\varepsilon, \tag{6.3.1}$$

while the preceding inequalities are reversed.

Letting $\tilde{B}_j = B_j \setminus (B_1 \cup \cdots \cup B_{k-1})$ so that they are disjoint, we can estimate

$$\begin{aligned}
\int_{\mathbb{R}^d} \varphi \, \mathrm{d}\rho &= \sum_{i=1}^{k-1} \int_{\tilde{B}_i} \varphi \, \mathrm{d}\rho + \int_{(B_1 \cup \cdots \cup B_{k-1})^c} \varphi \, \mathrm{d}\rho \\
&\leq \sum_{i=1}^{k-1} \eta_i \rho(\tilde{B}_i) + \eta_k \left(1 - \sum_{i=1}^{k-1} \rho(\tilde{B}_i)\right) \\
&\leq \sum_{i=1}^{k-1} \eta_i \rho(\tilde{B}_i) + \left(-\frac{1}{N-k+1}\sum_{i=j}^{k-1}\eta_j + \frac{k-1}{N-k+1}\varepsilon\right)\left(1 - \sum_{i=1}^{k-1}\rho(\tilde{B}_i)\right) \\
&= \sum_{i=1}^{k-1} \rho(\tilde{B}_i) \underbrace{\left(\eta_i + \frac{1}{N-k+1}\sum_{j=1}^{k-1}\eta_j - \frac{k-2}{N-k+1}\varepsilon\right)}_{\geq 0} \\
&\qquad - \frac{1}{N-k+1}\sum_{j=1}^{k-1}\eta_j + \frac{k-1}{N-k+1}\varepsilon - \frac{1}{N-k+1}\varepsilon\sum_{i=1}^{k-1}\rho(\tilde{B}_i), \\
&\leq \sum_{i=1}^{k-1} \frac{1}{N}\left(\eta_i + \frac{1}{N-k+1}\sum_{j=1}^{k-1}\eta_j - \frac{k-2}{N-k+1}\varepsilon\right) \\
&\qquad - \frac{1}{N-k+1}\sum_{j=1}^{k-1}\eta_j + \frac{k-1}{N-k+1}\varepsilon \\
&\leq \left(\frac{1}{N} + \frac{k-1}{N(N-k+1)} - \frac{1}{N-k+1}\right)\sum_{j=1}^{k-1}\eta_j + \frac{k-1}{N-k+1}\varepsilon \\
&= \frac{k-1}{N-k+1}\varepsilon \leq N\varepsilon,
\end{aligned}$$

where we used (6.3.1) in the second inequality and then

$$\begin{aligned}(N-k+1)\eta_i + \sum_{j=1}^{k-1}\eta_j - (k-2)\varepsilon \\ \geq (N-k+1)\eta_{k-1} + \sum_{j=1}^{k-1}\eta_j - (k-2)\varepsilon \\ \geq (N-(k-1)+1)\eta_{k-1} + \sum_{j=1}^{k-2}\eta_j - (k-2)\varepsilon \geq 0\end{aligned}$$

in the next step in order to substitute $\rho(\tilde{B}_i) \leq 1/N$. Letting $\varepsilon \to 0$ shows that $\int_{\mathbb{R}^d} \varphi \, \mathrm{d}\rho \leq 0$ as desired. □

This next theorem is a direct improvement of [BCP16, Theorem 2.4], and also its proof is based on their, with suitable modifications to reach the sharp hypothesis. In particular, most of the difference is in how we substitute their Lemma 2.3 with a better selection of competitor points.

**Theorem 6.3.7** (Diagonal bound)**.** *Let $\rho \in \mathscr{P}(X)$ be such that $\kappa(\rho, r) < 1/N$ for some $r > 0$ and let $\pi \in \Pi(\rho)$ be an optimal plan. Then there exist $\alpha, \beta > 0$ satisfying*

$$m(\alpha) > 2(N-1)M(\beta/2), \qquad m(\beta) > \frac{\mathscr{C}(\rho)}{1 - N\kappa(\rho, r)}, \qquad \beta/2 \leq r \tag{6.3.2}$$

*and for any such choice of $\alpha$ and $\beta$ we have*

$$\pi(\bar{D}_\alpha) = 0.$$

*Proof.* First of all, we can assume without loss of generality that the plan $\pi$ is symmetric, since $\pi^{\mathrm{sym}}$ has the same cost of $\pi$ and $\pi^{\mathrm{sym}}(\bar{D}_\alpha) = \pi(\bar{D}_\alpha)$ for every $\alpha \geq 0$.

Assume by contradiction that $\pi(\bar{D}_\alpha) > 0$. Then there exists $x \in \mathrm{supp}(\pi) \cap D_\alpha$. We may assume without loss of generality that $|x_1 - x_2| \leq \alpha$. For notational simplicity, let $\gamma = \beta/2 \leq r$. We claim that there is a point

$$y \in \mathrm{supp}(\pi) \setminus \bar{D}_\beta \cap \left(\bar{B}(x_1, \gamma)^c\right)^N.$$

To prove that such a point exists, it is sufficient to show that

$$\pi\Big(\bar{D}_\beta^c \cap \left(\bar{B}(x_1, \gamma)^c\right)^N\Big) > 0.$$

But this is true since we can estimate the mass of the complement as

$$\begin{aligned}\pi\Big(\Big[\bar{D}_\beta^c \cap \big(\bar{B}(x_1,\gamma)^c\big)^N\Big]^c\Big) &= \pi\Big(\bar{D}_\beta \cup \Big[\big(\bar{B}(x_1,\gamma)^c\big)^N\Big]^c\Big)\\ &\le \pi(\bar{D}_\beta) + \pi\left(\bigcup_{i=1}^N X^{N-1} \times_i \bar{B}(x_1,\gamma)\right)\\ &\le \frac{C(\pi)}{m(\beta)} + N\rho\big(\bar{B}(x_1,\gamma)\big)\\ &< 1 - N\kappa(\rho,r) + N\kappa(\rho,\gamma) \le 1.\end{aligned}$$

Next we prove that there exists $i \in \{1,\dots,N\}$ such that $|y_i - x_j| > \gamma$ for every $j = 1,\dots,N$. Indeed, by definition of $y$, the set $\bar{B}(x_1,\gamma)$ does not contain any of the points $y_i$; furthermore the $N-1$ sets $\bar{B}(x_2,\gamma), \bar{B}(x_3,\gamma),\dots,\bar{B}(x_N,\gamma)$ have diameter at most $2\gamma \le \beta$, therefore at least one of the $N$ points $y_i$ does not belong to any of them; otherwise by the pidgeonhole principle one of the aforementioned sets would contain two of the points $y_i$, which is impossible because they are pairwise spaced apart by more than $\beta$. Since we are dealing with a symmetric plan, we may assume that $|y_1 - x_j| > \gamma$ for every $j = 1,\dots,N$.

Now we introduce the two points $\tilde{x}$ and $\tilde{y}$ obtained by swapping the coordinates $x_1$ and $y_1$, namely

$$\tilde{x} = (y_1, x_2, \dots, x_N), \qquad \tilde{y} = (x_1, y_2, \dots, y_N),$$

which will be needed to construct a competitor plan contesting the optimality of $\pi$. For a fixed $\varepsilon > 0$, consider the four sets

$$\begin{aligned} X_\varepsilon &= \prod_{i=1}^N B(x_i,\varepsilon), & Y_\varepsilon &= \prod_{i=1}^N B(y_i,\varepsilon),\\ \tilde{X}_\varepsilon &= B(y_1,\varepsilon) \times \prod_{i=2}^N B(x_i,\varepsilon), & \tilde{Y}_\varepsilon &= B(x_1,\varepsilon) \times \prod_{i=2}^N B(y_i,\varepsilon).\end{aligned}$$

Since $x, y \in \operatorname{supp}(\pi)$, we have $\pi(X_\varepsilon) > 0$ and $\pi(Y_\varepsilon) > 0$, which allows us to define the two restrictions $\mu, \nu \in \mathscr{M}_+(X^N)$

$$\mu = [\pi(X_\varepsilon) \wedge \pi(Y_\varepsilon)]\frac{\pi \llcorner X_\varepsilon}{\pi(X_\varepsilon)}, \qquad \nu = [\pi(X_\varepsilon) \wedge \pi(Y_\varepsilon)]\frac{\pi \llcorner Y_\varepsilon}{\pi(Y_\varepsilon)}.$$

Clearly we have that $0 \le \mu, \nu \le \pi$ and $\mu(X^N) = \nu(X^N)$; moreover $\mu$ and $\nu$ are concentrated on disjoint sets for $\varepsilon < 2\gamma$ since $\mathsf{d}\big(B(x_1,\varepsilon), B(y_1,\varepsilon)\big) \ge \gamma - 2\varepsilon > 0$, therefore also $\mu + \nu \le \pi$. If we let

$$\tilde{\mu} = \frac{1}{\mu(X^N)} P^1_\# \nu \otimes P^{2,\dots,N}_\# \mu, \qquad \tilde{\nu} = \frac{1}{\mu(X^N)} P^1_\# \mu \otimes P^{2,\dots,N}_\# \nu,$$

then the previous observations tell us that the following probability measure is a valid competitor plan

$$\tilde{\pi} = \pi - (\mu + \nu) + (\tilde{\mu} + \tilde{\nu}) \in \Pi(\rho).$$

The contradiction will be reached if we show that $C(\tilde{\pi}) < C(\pi)$. Notice that for $2 \leq i < j \leq N$ one has $P^{i,j}_{\#}(\mu + \nu) = P^{i,j}_{\#}(\tilde{\mu} + \tilde{\nu})$, therefore

$$\begin{aligned}
C(\pi) - C(\tilde{\pi}) &= C(\mu + \nu) - C(\tilde{\mu} + \tilde{\nu}) \\
&= \sum_{j=2}^{N} \int_{X \times X} c \,\mathrm{d}P^{1,j}_{\#}(\mu + \nu) - \sum_{j=2}^{N} \int_{X \times X} c \,\mathrm{d}P^{1,j}_{\#}(\tilde{\mu} + \tilde{\nu}) \\
&\geq \int_{X \times X} c \,\mathrm{d}P^{1,2}_{\#}\mu - \sum_{j=2}^{N} \int_{X \times X} c \,\mathrm{d}P^{1,j}_{\#}(\tilde{\mu} + \tilde{\nu}) \\
&\geq \|\mu\|_{\mathrm{TV}} m(\alpha + 2\varepsilon) - (\|\mu\|_{\mathrm{TV}} + \|\nu\|_{\mathrm{TV}})(N-1)M(\gamma) \\
&= \|\mu\|_{\mathrm{TV}}[m(\alpha + 2\varepsilon) - 2(N-1)M(\gamma)] > 0
\end{aligned}$$

for $\varepsilon$ small, as $m(\alpha + 2\varepsilon) \to m(\alpha)$ when $\varepsilon \to 0$. □

Putting together the previous results, it is possible to show the continuity of the cost function $\mathscr{C}$ under a more general hypothesis than the one assumed in [BCP16], following the same strategy. Moreover, as Theorem 6.3.2 tells us, the threshold $1/N$ is sharp.

**Theorem 6.3.8** (Continuity of the cost)**.** *Assume that the cost $c$ is continuous outside of the diagonal.*[3] *Let $\rho \in \mathscr{P}(X)$ be such that $a(\rho) < 1/N$ or, equivalently, $\kappa(\rho, r) < 1/N$ for some $r > 0$. Then $\mathscr{C}$ is continuous at $\rho$.*

*Proof.* The proof is exactly the same as the one for [BCP16, Theorem 3.9], just noticing that we have achieved the diagonal bound Theorem 6.3.7 under the less restrictive assumption. A rought sketch follows for completeness.

If $\rho_n \rightharpoonup \rho$, they all satisfy $\kappa(\rho_n, r') < 1/N$ for some $r' > 0$, thanks to Lemma 6.2.4. But then by Theorem 6.3.7 there exists $\alpha > 0$ such that we have $\pi_n(D_\alpha) = 0$ for all optimal plans $\pi_n \in \Pi(\rho_n)$, therefore we can replace the cost $c$ with the bounded one

$$c_\alpha(x_1, \dots, x_n) = \begin{cases} c(x_1, \dots, x_n) & \text{if } x \in D_\alpha^c, \\ \binom{N}{2} M(\alpha) & \text{if } x \in D_\alpha. \end{cases}$$

The corresponding functional $\mathscr{C}_\alpha$ is weakly continuous and coincides with $\mathscr{C}$ along the sequence $\rho_\alpha$ because of the diagonal bound. □

[3] In this case $m$ and $M$ can also be taken to be continuous.

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