

Euclidean random matching in 2D for non-constant densities

Dario Benedetto · Emanuele Caglioti

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Abstract We consider the two-dimensional random matching problem in \mathbb{R}^2 . In a challenging paper, Caracciolo et al. [11], on the basis of a subtle linearization of the Monge-Ampère equation, conjectured that the expected value of the square of the Wasserstein distance, with exponent 2, between two samples of N uniformly distributed points in the unit square is $\log N/2\pi N$ plus corrections, while the expected value of the square of the Wasserstein distance between one sample of N uniformly distributed points and the uniform measure on the square is $\log N/4\pi N$. These conjectures have been proved by Ambrosio et al. [3].

Here we consider the case in which the points are sampled from a non-uniform density. For first we give formal arguments leading to the conjecture that if the density is regular and positive in a regular, bounded and connected domain Λ in the plane, then the leading term of the expected values of the Wasserstein distances are exactly the same as in the case of uniform density, but for the multiplicative factor equal to the measure of Λ .

We do not prove these results but, in the case in which the domain is a square, we prove estimates from above that coincides with the conjectured result.

Keywords Euclidean matching · Optimal transport · Monge-Ampère equation · Empirical measures

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D. Benedetto
Dipartimento di Matematica, SAPIENZA Università di Roma, Piazzale Aldo Moro 5, 00185 Rome, Italy
E-mail: benedetto@mat.uniroma1.it

E. Caglioti
Dipartimento di Matematica, SAPIENZA Università di Roma, Piazzale Aldo Moro 5, 00185 Rome, Italy
E-mail: benedetto@mat.uniroma1.it

1 Introduction

Let μ be a probability distribution defined on the unit square $Q = [0, 1]^2$. Let us consider two sets $\underline{x}^N = \{x_i\}_{i=1}^N$ and $\underline{y}^N = \{y_i\}_{i=1}^N$ of N points independently sampled from the distribution μ . The Euclidean Matching problem with exponent 2 consists in finding the matching $i \rightarrow \pi_i$, i.e. the permutation π of $\{1, \dots, N\}$ which minimizes the sum of the squares of the distances between x_i and y_{π_i} , that is

$$C_N(\underline{x}^N, \underline{y}^N) = \min_{\pi} \sum_{i=1}^N |x_i - y_{\pi_i}|^2. \quad (1.1)$$

The cost defined above can be seen, but for a constant factor N , as the square of the 2-Wasserstein distance between two probability measures. In fact, the p -Wasserstein distance $W_p(\nu_1, \nu_2)$, with exponent $p \geq 1$, between two probability measures ν_1 and ν_2 , is defined by

$$W_p^p(\nu_1, \nu_2) = \inf_{J_{\nu_1, \nu_2}} \int J_{\nu_1, \nu_2}(\mathrm{d}x, \mathrm{d}y) |x - y|^p,$$

where the infimum is taken on all the joint probability distributions $J_{\nu_1, \nu_2}(\mathrm{d}x, \mathrm{d}y)$ with marginals with respect to $\mathrm{d}x$ and $\mathrm{d}y$ given by $\nu_1(\mathrm{d}x)$ and $\nu_2(\mathrm{d}y)$, respectively. Defining the empirical measures

$$X^N(\mathrm{d}x) = \frac{1}{N} \sum_{i=1}^N \delta_{x_i}(x) \mathrm{d}x, \quad Y^N(\mathrm{d}x) = \frac{1}{N} \sum_{i=1}^N \delta_{y_i}(x) \mathrm{d}x,$$

it is possible to show that

$$C_N(\underline{x}^N, \underline{y}^N) = N W_2^2(X^N, Y^N),$$

(see for instance [8]). In the sequel we will shorten $C_N = C_N(\underline{x}^N, \underline{y}^N)$.

In the challenging paper [11], at first for particles in the torus of measure one, then also in the case of the square, see [14], Caracciolo et al. conjectured that when x_i and y_i are sampled independently with uniform density on Q , then

$$\mathbb{E}_{\sigma}[C_N] \sim \frac{\log N}{2\pi}, \quad (1.2)$$

where with \mathbb{E}_{σ} we denoted the expected value with respect to the uniform distribution $\sigma(\mathrm{d}x) = \mathrm{d}x$ of the points $\{x_i\}$ and $\{y_i\}$, and where we say that $f \sim g$ if $\lim_{N \rightarrow +\infty} f(N)/g(N) = 1$. In terms of W_2^2 the conjecture is equivalent to

$$\mathbb{E}_{\sigma}[W_2^2(X^N, Y^N)] \sim \frac{\log N}{2\pi N}. \quad (1.3)$$

Moreover, in [11] it is conjectured that asymptotic of the expected value of $W_2^2(X^N, \sigma)$ between the empirical density X^N and the uniform probability measure $\sigma(\mathrm{d}x)$ on Q is given by

$$\mathbb{E}_{\sigma}[W_2^2(X^N, \sigma)] \sim \frac{\log N}{4\pi N}. \quad (1.4)$$

A first general results showing that in the case of the unit square $\mathbb{E}_\sigma[W_2^2(X^N, Y^N)]$ behaves as $\frac{\log N}{N}$ has been obtained in [4]. The conjectures above has been proved by Ambrosio et al. [3]. In [1] finer estimates are given and it is proved that the result can be extended to the case when the particles are sampled from the volume measure on a two-dimensional Riemannian compact manifold. In [2] it is shown that the properties of the optimal transport map for $W_2(X^N, \sigma)$ are in agreement with the result in [11].

We notice that if we consider square (or manifold) of measure $|Q| \neq 1$, the cost has to be multiplied by $|Q|$. Namely, if we extract $\{x_i\}$ uniformly in Q , then the points $\{\gamma x_i\}$, with $\gamma > 0$, are uniformly distributed in γQ , and $C_N(\underline{x}^N, \underline{y}^N) = \gamma^{-2} C_N(\gamma \underline{x}^N, \gamma \underline{y}^N)$. By imposing that $|\gamma Q| = 1$, i.e. $\gamma^{-2} = |Q|$, we obtain that the expectation of the cost $C_N(\gamma \underline{x}^N, \gamma \underline{y}^N)$ verifies the asymptotic estimate (1.2).

In this paper we consider the case of non-uniform measure $\mu(dx) = \rho(x) dx$ with ρ strictly positive and regular.

In particular in Section 2 we study the asymptotic behavior of the expected value of the cost when ρ is a density on Q , piecewise constant on a grid of sub-squares. On the basis of the analysis of this case, in Conjecture 1 we guess that, in the case of regular and strictly positive density, the asymptotic behavior is still described by the right-hand-sides of eq.s (1.3) and (1.4). In the case of a density defined on a regular connected bounded set Λ in the plane, we expect that the asymptotic behavior changes only for the multiplicative factor $|\Lambda|$ (see Conjecture 2).

In Section 3 we face the random Euclidean matching problem with the strategy presented in [11, 14], showing that the results conjectured in 2 can be formally justified on the basis of that approach.

We do not fully prove the conjectures, but in section 4 we prove that (1.3) and (1.4) give exact estimates from above of the cost, in the case of strictly positive and Lipschitz continuous density on Q .

Although this work concerns the two-dimensional case for cost and Wasserstein distance with exponent 2, we briefly review here what is known in the other cases, up to our knowledge.

In dimension 2, for $p \geq 1$, $p \neq 2$, in [4] it has been proved that the expected cost per particle $\mathbb{E}[C_N]/N$ is $O(N^{-p/2})$ as $N \rightarrow \infty$. The value of the limit as $N \rightarrow +\infty$ of $N^{p/2} \mathbb{E}[C_N]/N$ is not known.

In dimension 1 the random Euclidean matching problem in a segment is almost completely characterized, for any $p \geq 1$. This is due to the fact that the best matching between two set of points on a line is monotone. When the density is uniform on the segment $[0, 1]$ and $p = 2$, one gets $\mathbb{E}[C_N] \rightarrow 1/3$ as $N \rightarrow \infty$. In this case, it is well known that it is possible to compute explicitly $\mathbb{E}[C_N]$ for any N , in fact $\mathbb{E}[C_N] = N/3(N+1)$. Moreover, for any $p \geq 1$, $\mathbb{E}[C_N]/N \sim c_p N^{-p/2}$, where c_p is known, see [13]. Very recently, an expression for C_N , for any N and for any value of $p \geq 1$, has been determined, see [12]. The different behavior in the case in which the density vanishes in some point or in a segment has been analyzed in [9] (see the Remark 3 at the end of Section 2). A general discussion on the one-dimensional, also for the case of non-constant densities and of densities defined on all the line, can be found in [7].

In dimension $d \geq 3$, it has been proved that $\mathbb{E}[C_N]/N \sim cN^{-p/d}$, for any $p \geq 1$ (see [19], [15] for $p = 1$, and [16] for $p \geq 1$).

2 Some conjectures for non-constant densities

Let us consider the case $\mu(dx) = \rho(x) dx$ with $\rho(x)$ is piecewise constant with respect to a regular grid of sub-squares of Q . For sake of simplicity we consider the case in which the grid is made by four sub-squares: $[0, 1/2)^2$, $[0, 1/2) \times [1/2, 1]$, $[1/2, 1] \times [0, 1/2)$, $[1/2, 1]^2$ (see fig. 1).

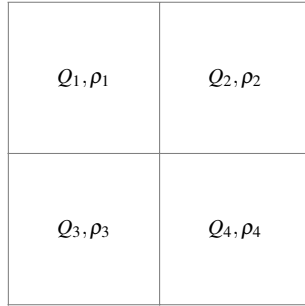


Fig. 1 Grid of 2×2 squares.

Let us denote by $Q_k : i = 1, \dots, 4$, the four squares and by $\rho_k > 0$, $k = 1, \dots, 4$ the corresponding constant densities. Now, let $\{x_i\}_{i=1}^N$ and $\{y_i\}_{i=1}^N$ be two samples of N independent points from the distribution μ , and let us denote with R_k and S_k the number of points x_i and y_i in Q_k , respectively. Then, both R_k and S_k will be equal to $N_k = \rho_k N/4$ plus terms of the order of \sqrt{N} .

Now we make two ansatzes.

1. Up to a correction $o(\log N)$, we can calculate $\mathbb{E}_\mu[C_N]$ by restricting ourselves to the case in which both R_k and S_k are equal to $N_k = \rho_k N/4$ (rounded to integer numbers in such a way that the sum of the N_k is N).
2. Given the samples with $R_k = S_k = N_k$, the optimal cost, with the constraint that x_i and y_{π_i} are in the same square, is C_N plus an error $o(\log N)$.

Under these assumptions we get that, but for terms of order 1, the expected value of the cost of the optimal matching will be given by the sum of the expected value of the cost of the optimal couplings in the four squares.

Now let us notice that, by eq. (1.3), if we sample N_k particles uniformly and independently in a square of size $|Q_k|$, then the expected value of the cost is simply given by $|Q_k|^{\frac{\log N}{2\pi}}$, as follows by the scaling argument shown in the previous section.

Therefore,

$$\begin{aligned}\mathbb{E}_\mu[C_N] &= \sum_{k=1}^4 |Q_k| \frac{\log(\rho_k N/4)}{2\pi} + o(\log N) \\ &= \sum_{k=1}^4 |Q_k| \frac{\log N}{2\pi} + \sum_{k=1}^4 |Q_k| \frac{\log(\rho_k/4)}{2\pi} + o(\log N) \\ &= \frac{\log N}{2\pi} \left(\sum_{k=1}^4 |Q_k| \right) + o(\log N) = \frac{\log N}{2\pi} + o(\log N),\end{aligned}$$

where we used that $\sum |Q_k| = 1$. We can notice that the dependence of $\mathbb{E}_\mu[C_N]$ on the values of the densities ρ_k does not affect the leading term, that only depends on the measure of the set.

This analysis can be extended when we consider a regular grid of m^2 squares. Therefore, by noticing that it is possible to approximate a continuous density ρ as well as we want in L_∞ with a piecewise constant density, we are led to the following conjectures.

Conjecture 1 *Let $\mu(dx) = \rho(x) dx$ a probability measure defined on Q where ρ is a smooth positive density on Q . Let $\{x_i\}_{i=1}^N$ and $\{y_i\}_{i=1}^N$ be two samples of points independently distributed with μ . Then*

$$\mathbb{E}_\mu[C_N] \sim \frac{\log N}{2\pi}. \quad (2.1)$$

Reasoning in the same way, we can conjecture that the asymptotic behavior of the 2–Wasserstein distance between the empirical measure X^N and the measure μ itself verifies

$$\mathbb{E}_\mu[W_2^2(X^N, \mu)] \sim \frac{\log N}{4\pi N}. \quad (2.2)$$

Let us notice that the two ansatzes above are far from been obvious. Nevertheless, in the next section we will prove that the right-hand-sides of eq.s (2.1) and (2.2) give exact estimates from above of the expected values.

Let us now consider a bounded connected set Λ in \mathbb{R}^2 with regular boundary, and consider a partition of Λ with squares of sides $1/m$, as in fig. 2. Let us suppose that the probability measure μ has a smooth and positive density in Λ , and define $\Lambda_k = Q_k \cap \Lambda$.

Then with the same reasoning made for the case of the square Q , formally we get

$$\begin{aligned}\mathbb{E}_\mu[C_N] &\sim \sum_{k:Q_k \subset \Lambda} |Q_k| \frac{\log(\rho_k N/|Q_k|)}{2\pi} \\ &= \frac{\log N}{2\pi} \sum_{k:Q_k \subset \Lambda} |Q_k| + O(1) \sim |\Lambda| \frac{\log N}{2\pi},\end{aligned}$$

where ρ_k is the average of ρ on Λ_k . In fact, we expect that any of the square Q_k in Λ contributes to $\mathbb{E}[C_N]$ with a term $\sim \frac{|Q_k|}{2\pi} \log N$. We have also neglected the contribution of the squares close to the boundary.

Therefore, we are led to the following conjecture.

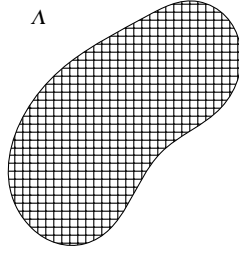


Fig. 2 Set A covered with squares.

Conjecture 2 Let $\mu(dx) = \rho(x) dx$, a probability measure defined on Λ where ρ is a smooth positive density. Let $\{x_i\}_{i=1}^N$ and $\{y_i\}_{i=1}^N$ two samples of N points independently distributed with μ .

$$\mathbb{E}_\mu[C_N] \sim |\Lambda| \frac{\log N}{2\pi} \quad \text{and} \quad \mathbb{E}_\mu[W_2^2(X^N, \mu)] \sim |\Lambda| \frac{\log N}{4\pi N}.$$

Remark 1 If the measure of the support of μ is infinite (for instance if the support is all \mathbb{R}^2), we expect that

$$\lim_{N \rightarrow \infty} \frac{\mathbb{E}_\mu[C_N]}{\log N} = +\infty.$$

This is in agreement with the fact, proved by Talagrand in [20], that when the density is the Gaussian, i.e. $\rho = \frac{1}{2\pi} e^{-|x|^2/2}$, the average of the cost satisfies for large N

$$(\log N)^2 \leq \mathbb{E}_\mu[C_N] \leq C(\log N)^2.$$

Notice that an estimate from above proportional to $(\log N)^2$ was previously proved by Ledoux in [16]. Moreover, in [20] the author says that a similar estimate can be obtained for densities $\rho \propto e^{-|x|^\alpha}$ obtaining a bound from below for the cost proportional to $(\log N)^{1+2/\alpha}$, and therefore much larger than $\log N$.

Remark 2 In the above conjectures we require that ρ is positive, but we can reformulate the conjectures using the measure of the support of ρ instead of the measure of Λ . The condition which really can change the asymptotic behavior of the cost is the connection of the support of ρ . Namely, if this condition is not satisfied, the result may be false. In particular if ρ is constant in two squares whose distance is positive, we get that the expected value of cost is $O(\sqrt{N}) \gg O(\log N)$. To get an idea of what happens, consider

$$\mu(dx) = \frac{1}{2} (\delta_{z_1}(x) + \delta_{z_2}(x)) dx.$$

Then

$$\begin{aligned} X^N(dx) &= \left(\frac{R}{N} \delta_{z_1}(x) + \frac{N-R}{N} \delta_{z_2}(x) \right) dx, \\ Y^N(dx) &= \left(\frac{S}{N} \delta_{z_1}(x) + \frac{N-S}{N} \delta_{z_2}(x) \right) dx, \end{aligned}$$

where R and S are independent binomial variables of mean $N/2$ and variance $N/4$. It is easy to show that

$$C_N = L^2 |R - S|$$

where $L = |z_1 - z_2|$. Then, by noticing that $R - S$ has variance $N/2$, by the Central Limit Theorem we get that the leading term of the expected value of the cost is $L^2 \sqrt{N/\pi}$. This behavior is independent of the dimension. The reader can find in the paper [9] the exact asymptotic value in the one-dimensional case of two disjoint intervals of the same length and with constant density.

Remark 3 Non-constant densities have been previously addressed in [14], in which the authors present a general expression which also allows the explicit calculation of the asymptotic value of the cost in the one dimensional case. Again on the one-dimensional case, in [9] the authors consider also a matching problem as in eq. (1.1) but where the distance appears with the power $p \geq 1$, not necessarily 2. The expected value of the cost per particle $\mathbb{E}[C_N]/N$ goes as $cN^{-p/2}$, but interestingly c can diverge if the density approaches zero at some point.

3 A formal proof

It is possible to extend the method by Caracciolo et al. [11] to a generic (positive) density. In particular in [14] a formula for $\mathbb{E}_\mu[C_N]$ and for its fluctuations is presented, in the general case. The formula for $\mathbb{E}_\mu[C_N]$ is computed in the case of the uniform density σ in the square, recovering the results in [11]. Here we follow the approach presented in the papers above, considering the general case of a smooth and positive density and deriving formally eq. (2.1) of Conjecture 1 (eq. (2.2) can be derived essentially in the same way).

In the framework of this approach, the main argument we use to derive eq. (2.1) consists in noticing that the singular part of the Green function of the linearized Monge-Ampère equation, that in the case of a generic density is an elliptic operator in divergence form, has a very simple expression.

3.1 Constant density

The strategy proposed in [11] to compute the expected value of C_N consists in linearizing the Monge-Ampère equation (which is the Euler Lagrange equation for the Monge-Kantorovich problem) and then to put a suitable cut-off on the expression founded. For first, we here report the argument in [11] for the case of constant density, and we refer to [11, 14] for the justification of the approach and further details.

By linearizing the Monge-Ampère equation around the uniform probability measure $\sigma(dx) = dx$, the Wasserstein distance between two regular measures is approximated by

$$\int_Q |\nabla \psi|^2 = - \int_Q \psi \Delta \psi \quad (3.1)$$

where ψ solves

$$\Delta \psi = -\delta\rho, \quad (3.2)$$

with Neumann boundary conditions, and where $\delta\rho$ is the difference of the densities of the two measures. We use formally (3.1) in the case of singular measures, introducing later a suitable cut-off that make finite the cost. In the bipartite case

$$\delta\rho(x) dx = X^N(dx) - Y^N(dx) \quad (3.3)$$

and the cost is N times the Wasserstein distance, that is

$$C_N \sim N \int_Q |\nabla \psi|^2 = N \int_Q \psi \delta\rho.$$

It is convenient to introduce the Green function ϕ_z for the Laplace problem on Q , which is the solution, with zero average, of

$$\Delta \phi_z(x) = -\delta_z(x) + 1,$$

with Neumann boundary conditions. Since ψ solves eq. (3.2) with $\delta\rho$ given in eq. (3.3), from the definition of $\phi_z(x)$ we get

$$\psi(x) = \Delta^{-1} \delta\rho(x) = \frac{1}{N} \left(\sum_{i=1}^N \phi_{x_i}(x) - \sum_{j=1}^N \phi_{y_j}(x) \right)$$

and then

$$C_N \sim \frac{1}{N} \int_Q \left(\sum_{i=1}^N \phi_{x_i} - \sum_{j=1}^N \phi_{y_j} \right) \left(\sum_{i=1}^N \delta_{x_i} - \sum_{j=1}^N \delta_{y_j} \right).$$

Taking the expectation in the location of the delta functions, and using that the Green function has zero average, we get

$$\begin{aligned} \mathbb{E}_\sigma[C_N] &\sim \frac{1}{N} \mathbb{E}_\sigma \int_Q \left[\left(\sum_{i=1}^N \phi_{x_i} - \sum_{j=1}^N \phi_{y_j} \right) \left(\sum_{i=1}^N \delta_{x_i} - \sum_{j=1}^N \delta_{y_j} \right) \right] \\ &= \frac{1}{N} \mathbb{E}_\sigma \sum_{i=1}^N \int_Q (\phi_{x_i} \delta_{x_i} + \phi_{y_i} \delta_{y_i}) = 2 \int_Q dz \int_Q dx |\nabla \phi_z(x)|^2 \\ &= 2 \int_Q dx |\nabla \phi_0(x)|^2, \end{aligned}$$

(the integral in x does not depend on the position of z , then we can fix it in $z = 0$). By Parseval's Lemma, the right-hand-side can be written in Fourier series, with respect to the base of cosines, as

$$\frac{2}{\pi^2} \sum_{k \in \mathbb{N}^2 \setminus \{0\}} \frac{1}{|k|^2}.$$

This series is not summable but a natural cut-off can be imposed by summing up to k as large as $\frac{1}{\lambda}$ where $\lambda = \frac{1}{\sqrt{N}}$ is the characteristic length of the system, i.e. the typical distance between a point x and its closest point y . In this way one gets $\mathbb{E}_\sigma[C_N] \sim \frac{1}{2\pi} \log N + O(1)$. It is important to notice that if the cut-off is chosen to be $\lambda = \alpha/\sqrt{N}$

then the leading term of does not depend on the constant α , which only affects the $O(1)$ term.

In order to face the case of a non-constant density, it is convenient to make the previous computation in the position space, in which the cut-off can be obtained by smoothing the delta-function evolving it, with the heat semigroup, for a time $t = 1/N$. We recall that the Green function can be written as

$$\phi_z(x) = -\frac{1}{2\pi} \log|x-z| + \gamma(x,z),$$

where γ is a regular function. We indicate with f^t the evolution of a function f with the heat semigroup until the time t , and with $G_t(x)$ the heat kernel in the whole space \mathbb{R}^2 . We get again

$$\begin{aligned} \mathbb{E}_\sigma[C_N] &\sim 2 \int_Q \phi'_0(x) \delta'_0(x) dx = 2 \int_Q \phi_0(x) \delta_0^{2t}(x) dx \\ &= -2 \frac{1}{2\pi} \int_{\mathbb{R}} \log|x| G_{2t}(x) dx + O(1) = -\frac{1}{\pi} \log \sqrt{t} + O(1) \quad (3.4) \\ &= \frac{1}{2\pi} \log N + O(1). \end{aligned}$$

3.2 Non-constant density

Now let us consider the case of a probability measure μ of positive and regular density ρ . The main difference from the case of a constant density is that the linearized Monge-Ampère equation reads as

$$\nabla \cdot (\rho \nabla \psi) = -\delta \rho. \quad (3.5)$$

(see for instance [18] and references therein). Also in this case

$$C_N \sim N \int_Q \rho |\nabla \psi|^2 = N \int_Q \psi \delta \rho$$

where ψ satisfies (3.5). We then introduce the Green function $\phi_z(x)$ which is the solution of

$$\nabla \cdot (\rho \nabla \phi_z) = -(\delta_z - \rho) \text{ with } \int_Q \phi_z(x) \rho(x) dx = 0, \quad (3.6)$$

getting

$$\psi = \frac{1}{N} \sum_{i=1}^N \phi_{x_i} - \frac{1}{N} \sum_{j=1}^N \phi_{y_j}$$

and

$$C_N \sim \frac{1}{N} \int_Q \left(\sum_{i=1}^N \phi_{x_i} - \sum_{j=1}^N \phi_{y_j} \right) \left(\sum_{i=1}^N \delta_{x_i} - \sum_{j=1}^N \delta_{y_j} \right).$$

Taking the expectation in the location of the delta functions, that are distributed with density ρ , we get

$$\begin{aligned}\mathbb{E}_\mu[C_N] &\sim \frac{1}{N} \mathbb{E}_\mu \int_Q \left(\sum_{i=1}^N \phi_{x_i} - \sum_{j=1}^N \phi_{y_j} \right) \left(\sum_{i=1}^N \delta_{x_i} - \sum_{j=1}^N \delta_{y_j} \right) \\ &= \frac{1}{N} \mathbb{E}_\mu \int_Q \sum_{i=1}^N (\phi_{x_i} \delta_{x_i} + \phi_{y_i} \delta_{y_i}) = 2 \int_Q dz \rho(z) \int_Q dx \phi_z(x) \delta_z(x).\end{aligned}$$

The key observation we make here consists in noticing that in the equation (3.6), that we rewrite as

$$\rho \Delta \phi_z + \nabla \rho \cdot \nabla \phi_z = -\delta_z + \rho,$$

the term $\nabla \rho \cdot \nabla \phi_z$ is less singular than the δ function, therefore

$$\phi_z(x) = -\frac{1}{2\pi\rho(z)} \log|x-z| + O(1) \quad (3.7)$$

as $x \rightarrow z$ (see the Remark 4 at the end of this section). Finally, we apply the cut-off by evolving δ_z until the time $t = 1/N$ with the heat semigroup. Proceeding as in eq. (3.4)

$$\begin{aligned}\mathbb{E}_\mu[C_N] &\sim -\frac{1}{\pi} \int_Q dz \rho(z) \int_Q dx \frac{1}{\rho(z)} \log|x-z| G_{2t}(x-z) + O(1) \\ &= \frac{1}{2\pi} \log N \left(\int_Q dz \right) + O(1) = \frac{1}{2\pi} \log N + O(1),\end{aligned}$$

that is in agreement with our conjecture.

The argument can be generalized to any regular bounded domain Λ in the plane and to the case of the torus. In the latter case, the operator Δ requires periodic boundary conditions.

Indeed, changing the domain or the boundary condition only affects the regular part of the Green function in (3.7).

Remark 4 Denoting with Δ^{-1} the inverse of the Laplacian, we have

$$\phi_z = -\Delta^{-1} \left(\frac{\delta_z - \rho}{\rho} \right) - \Delta^{-1} \frac{\nabla \rho \cdot \nabla \phi_z}{\rho}.$$

This expression suggests that divergent part of ϕ_z is

$$-\frac{1}{2\pi\rho(z)} \log|x-z|,$$

and then that $|\nabla \rho \cdot \nabla \phi_z / \rho|$ is bounded by $\frac{c}{|x-z|}$. It is easy to show that applying Δ^{-1} to this term we obtain a bounded continuous function. A rigorous proof of (3.7) when the domain is all \mathbb{R}^2 can be found, for instance, in [5], and can be extended to the case of the square with minor modifications.

4 Estimate from above

In this section we prove that

Theorem 1 *Let $\mu(dx) = \rho(x) dx$ be a probability measure defined on Q , where ρ is a Lipschitz continuous strictly positive density.*

1. *Let $\{x_i\}_{i=1}^N$ and $\{y_i\}_{i=1}^N$ be two samples of N points chosen independently with distribution μ . Then*

$$\limsup_{N \rightarrow \infty} \frac{2\pi}{\log N} \mathbb{E}_\mu[C_N] \leq 1 \quad (4.1)$$

that is equivalent to

$$\limsup_{N \rightarrow \infty} \frac{2\pi N}{\log N} \mathbb{E}_\mu[W_2^2(X^N, Y^N)] \leq 1 \quad (4.2)$$

2. *Moreover*

$$\limsup_{N \rightarrow \infty} \frac{4\pi N}{\log N} \mathbb{E}_\mu[W_2^2(X^N, \mu)] \leq 1 \quad (4.3)$$

We first prove the second part of the theorem, and then we show that (4.3) implies (4.2).

The idea of the proof is to divide the square Q into small squares where the density can be considered constant in order to apply the result in eq. (1.4). More precisely, we state the following Lemma.

Lemma 1 *Let $\rho(x)$ be a strictly positive and Lipschitz continuous function defined in $Q^\ell = [0, \ell]^2$, let $\nu(dx) = r(x) dx$ be the probability measure of density $r(x) = \rho(x) / \int_{Q^\ell} \rho$, and let $\sigma^\ell(dx) = \ell^{-2} dx$ be the uniform probability measure on Q^ℓ . Let us denote with $\{x_i\}_{i=1}^R$ a sample of R points independently distributed with ν , and with $\{z_i\}_{i=1}^R$ a sample of R points independently distributed with the uniform probability measure σ^ℓ , and let us indicate with $X^R(dx)$ and $Z^R(dx)$ the corresponding empirical measures.*

Then there exists a constant $c > 0$ such that for sufficiently small ℓ

$$\mathbb{E}_\nu W_2^2(X^R, \nu) \leq (1 + c\ell) \mathbb{E}_{\sigma^\ell} W_2^2(Z^R, \sigma^\ell).$$

Proof Let us denote with L the Lipschitz constant of ρ , and with a a constant such that $\rho(x) \geq a > 0$. The measure ν is approximated by σ^ℓ in the sense that

$$\left| r(x) - \frac{1}{\ell^2} \right| = \frac{1}{\int_{Q^\ell} \rho} \left| \rho(x) - \frac{1}{\ell^2} \int_{Q^\ell} \rho \right| \leq \frac{L}{a\ell}.$$

Moreover,

$$|r(x) - r(y)| \leq \frac{L}{a\ell^2}.$$

Let us define

$$r_2(x_2) = \int_0^\ell r(x'_1, x_2) dx'_1$$

and note that

$$\left| r_2(x_2) - \frac{1}{\ell} \right| \leq \frac{L}{a}.$$

We consider the map

$$\begin{cases} G_1(x_1, x_2) = \ell \frac{1}{r_2(x_2)} \int_0^{x_1} r(x'_1, x_2) dx'_1 \\ G_2(x_1, x_2) = \ell \int_0^{x_2} r_2(x'_2) dx'_2. \end{cases}$$

The map $x = (x_1, x_2) \rightarrow G = (G_1, G_2)$ is continuously differentiable, its Jacobian is $r(x)$, and it is bijective from \mathcal{Q}^ℓ in \mathcal{Q}^ℓ . Then, if x is uniformly distributed on \mathcal{Q}^ℓ , $G(x)$ is distributed with density r . The inverse map Γ of G transports the uniform distribution $\sigma^\ell(dx)$ in the probability measure $\nu(dx)$ of density r . By definition of Γ

$$W_2^2(X^R, \nu) = \inf_J \int J(dx, dy) |\Gamma(x) - \Gamma(y)|^2,$$

where the infimum is taken on the joint probability measures of $Z^n(dx)$ and $\sigma^\ell(dy)$, with $z_i = G(x_i)$. Now we show that

$$\begin{aligned} |\Gamma(x) - \Gamma(y)|^2 &\leq |x - y|^2 \sup_{x \neq y} \frac{|\Gamma(x) - \Gamma(y)|^2}{|x - y|^2} \\ &= |x - y|^2 \sup_{x \neq y} \frac{|x - y|^2}{|G(x) - G(y)|^2} \leq (1 + c\ell) |x - y|^2 \end{aligned}$$

from which the proof follows immediately. Let us define

$$\begin{aligned} \alpha &= \frac{\ell}{x_2 - y_2} \int_{[x_2, y_2]} r_2(x'_2) dx'_2, \\ \beta &= \frac{\ell}{x_1 - y_1} \int_{[x_1, y_1]} \frac{r(x'_1, x_2)}{r_2(x_2)} dx'_1, \\ \gamma &= \frac{\ell}{x_2 - y_2} \int_0^{y_1} \left(\frac{r(x'_1, x_2)}{r_2(x_2)} - \frac{r(x'_1, y_2)}{r_2(y_2)} \right) dx'_1. \end{aligned}$$

Using the estimate on $r - 1/\ell^2$, $r_2 - 1/\ell$ and on the Lipschitz constant of r , we have

$$|\alpha - 1| \leq c\ell, \quad |\beta - 1| \leq c\ell, \quad |\gamma| \leq c\ell.$$

Then

$$\begin{aligned} |G(x) - G(y)|^2 &= (\alpha^2 + \gamma^2)(x_2 - y_2)^2 + \beta^2(x_1 - y_1)^2 + 2\beta\gamma(x_1 - y_1)(x_2 - y_2) \\ &\geq (1 - c\ell)|x - y|^2, \end{aligned}$$

for a suitable constant c and ℓ sufficiently small.

We will also need to bound the 2–Wasserstein distance between two slightly different and positive densities on the square. We can do this with the following Lemma, which is a corollary of Benamou-Brenier formula [6].

Lemma 2 *If ν_1 and ν_2 are two probability measures on a convex domain Λ , absolutely continuous with respect to the Lebesgue measure, with densities bounded from below and from above by finite non-zero constants, then*

$$W_2^2(\nu_1, \nu_2) \leq c \|\nu_1 - \nu_2\|_2^2.$$

Proof The Benamou-Brenier formula allows to estimate the 2–Wasserstein distance between two measures in terms of the \dot{H}^{-1} norm of their difference. More precisely, Theorem 5.34 in [18] says: if ν_1 and ν_2 are two absolutely continuous measures defined on a convex domain Λ , with densities bounded from below and from above by the constants a and b respectively, $0 < a < b$, then

$$\frac{1}{\sqrt{b}} \|\nu_1 - \nu_2\|_{\dot{H}^{-1}(\Lambda)} \leq W_2(\nu_1, \nu_2) \leq \frac{1}{\sqrt{a}} \|\nu_1 - \nu_2\|_{\dot{H}^{-1}(\Lambda)},$$

where the \dot{H}^{-1} norm of a 0–average charge distribution ν is defined by

$$\|\nu\|_{\dot{H}^{-1}(\Lambda)} = \int_{\Lambda} |\nabla \Delta^{-1} \nu|^2,$$

where the inverse of Laplacian is defined with Neumann homogeneous boundary conditions on $\partial\Lambda$. Therefore, by noticing that the \dot{H}^{-1} norm is bounded from above by a positive constant depending only on $|\Lambda|$ times the L_2 norm, we get the result.

We remark that more general results, including the case of non-convex domains, can be found in [17] and references therein. We also remark that this Lemma fails if the supports of the measures are not connected, according to remark 2 at the end of the previous section.

Now we can start to prove Theorem 1. Let m a positive integer and let us cover $Q = [0, 1]^2$ with the m^2 squares $\{Q_k\}_{k=1}^{m^2}$, of sides $1/m$ and of measure $1/m^2$, given by $[i/m, (i+1)/m] \times [j/m, (j+1)/m]$, with $i, j = 0, \dots, m-1$. as in fig. 3.

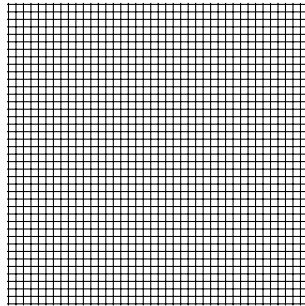


Fig. 3 Regular grid of squares.

We define:

$$\sigma_k(dx) = m^2 dx \text{ the uniform probability measure on } Q_k \quad (4.4)$$

$$p_k = \int_{Q_k} \rho(x) dx \text{ the probability that } x, \text{ extracted with } \mu, \text{ belongs to } Q_k \quad (4.5)$$

$$\mu_k^m(dx) = \frac{1}{p_k} \rho(x) dx \text{ the distribution of } x, \text{ conditioned to } x \in Q_k. \quad (4.6)$$

Let $\{x_i\}_{i=1}^N$ be a sample of N independent points distributed with μ , and let us denote with R_k the number of points x_i in the square Q_k . Let $J_k(dx, dy)$ a joint probability distribution on $Q_k \times Q_k$ with marginals given by

$$\begin{aligned} \int_{Q_k} J_k(dx, \cdot) &= X_k^N(dx) := \frac{1}{R_k} \sum_{j=1}^N \chi\{x_j \in Q_k\} \delta_{x_j}(x) dx \\ \int_{Q_k} J_k(\cdot, dy) &= \mu_k^m(dy). \end{aligned}$$

Then

$$J(dx, dy) = \sum_{k=1}^{m^2} \frac{R_k}{N} J_k(dx, dy)$$

is a joint distribution in $Q \times Q$ with marginals given by

$$\begin{aligned} \int_Q J(dx, \cdot) &= X^N(dx) = \frac{1}{N} \sum_{j=1}^N \delta_{x_j}(x) dx \\ \int_Q J(\cdot, dy) &= \mu^m(dy) := \sum_{k=1}^{m^2} \frac{R_k}{N} \mu_k^m(dy) = \sum_{k=1}^{m^2} \frac{R_k}{p_k N} \rho(y) \chi\{y \in Q_k\} dy. \end{aligned}$$

We will estimate $\mathbb{E}[W_2^2(X^N, \mu)]$ by the triangular inequality, through the estimates of $\mathbb{E}[W_2^2(X^N, \mu^m)]$ and $\mathbb{E}[W_2^2(\mu^m, \mu)]$.

Estimate of $\mathbb{E}[W_2^2(X^N, \mu^m)]$.

By definition

$$W_2^2(X^N, \mu^m) \leq \sum_{i=1}^{m^2} \frac{R_k}{N} W_2^2(X_k^N, \mu_k^m).$$

We first take the expected value conditioned to the variables R_k , which is equivalent to fix $\{R_k\}$ and to extract a sample of R_k particle in Q_k with distribution μ_k^m , as defined in (4.6). Then we will take the expectation in $\{R_k\}$ with respect to μ , which means to extract the multinomial variables $\{R_k\}$ with probability p_k , as defined in (4.5):

$$\mathbb{E}_\mu \left[W_2^2(X^N, \mu^m) \mid \{R_k\}_{k=1}^{m^2} \right] \leq \sum_{i=1}^{m^2} \frac{R_k}{N} \mathbb{E}_{\mu_k^m} W_2^2(X_k^N, \mu_k^m).$$

We estimate $\mathbb{E}_{\mu_k^m} W_2^2(X_k^N, \mu_k^m)$ using Lemma 1, identifying $\ell = 1/m$, Q^ℓ with Q_k , and using the results in Eq. (1.4):

$$\begin{aligned} \mathbb{E}_{\mu_k^m} [W_2^2(X_k^N, \mu_k^m)] &\leq (1+c/m) \mathbb{E}_{\sigma_k} [W_2^2(Z^{R_k}, \sigma_k)] \\ &= (1+c/m) \frac{1}{m^2} \left(\frac{\log R_k}{4\pi R_k} + o(\log R_k/R_k) \right). \end{aligned} \quad (4.7)$$

Then, multiplying for R_k/N and summing on k

$$\mathbb{E}_\mu \left[W_2^2(X^N, \mu^m) \mid \{R_k\}_{k=1}^{m^2} \right] \leq (1+c/m) \sum_{k:R_k>0} \left(\frac{1}{m^2} \frac{1}{4\pi N} \log R_k + \frac{1}{m^2} o(\log R_k/N) \right).$$

The expected value of R_k is $N_k = p_k N$, where p_k is of order $1/m^2$. Then we need that N/m^2 diverges with N . For N large, R_k differs from N_k of a term of order \sqrt{N}/m , then

$$\mathbb{E} \left[\sum_{k:R_k>0} \frac{1}{m^2} o(\log R_k/N) \right] = o(\log N/N) + o(\log m/N) = o(\log N/N).$$

Moreover

$$\log R_k = \log(R_k/N_k) + \log p_k + \log N \leq \log(R_k/N_k) + \log N,$$

and since $p_k \leq 1$ and since \log is a convex function

$$\mathbb{E}_\mu [\log R_k] \leq \mathbb{E}_\mu [\log(R_k/N_k)] + \log N \leq \log N.$$

Therefore, we conclude that

$$\mathbb{E}_\mu [W_2^2(X^N, \mu^m)] \leq (1+c/m) \left(\frac{\log N}{4\pi N} + o(\log N/N) \right).$$

Estimate of $\mathbb{E}[W_2^2(\mu^m, \mu)]$.

Here we use Lemma 2:

$$\begin{aligned} W_2^2(\mu^m, \mu) &\leq c \|\mu^m - \mu\|_2^2 = c \sum_{k=1}^{m^2} \left(\frac{R_k}{p_k N} - 1 \right)^2 \int_{Q_k} \rho(x)^2 dx \\ &= c \sum_{k=1}^{m^2} \frac{1}{p_k^2 N^2} (R_k - p_k N)^2 \int_{Q_k} \rho(x)^2 dx. \end{aligned}$$

Taking the expectation

$$\begin{aligned} \mathbb{E}_\mu [W_2^2(\mu^m, \mu)] &\leq c \sum_{k=1}^{m^2} \frac{1}{p_k^2 N^2} N p_k (1-p_k) \int_{Q_k} \rho(x)^2 dx \\ &\leq c \frac{1}{N} \sum_{k=1}^{m^2} \frac{1}{p_k} \int_{Q_k} \rho(x)^2 dx \leq c \|\rho\|_\infty \frac{m^2}{N}. \end{aligned}$$

Proof (Proof of Theorem 1.) Using that $(a+b)^2 \leq (1+\delta)a^2 + (1+1/\delta)b^2$ for any $\delta > 0$, from the triangular inequality for W_2 we have

$$\begin{aligned} \frac{N}{\log N} \mathbb{E}_\mu [W_2^2(X^n, \mu)] &\leq (1+\delta) \frac{N}{\log N} \mathbb{E}_\mu [W_2^2(X^n, \mu^m)] \\ &\quad + (1+1/\delta) \frac{N}{\log N} \mathbb{E}_\mu [W_2^2(\mu^m, \mu)] \\ &\leq (1+\delta)(1+c/m) \left(\frac{1}{4\pi} + o(1) \right) + c(1+1/\delta) \frac{m^2}{\log N}. \end{aligned}$$

We achieve the proof of eq. (4.3) taking the lim sup in N and then passing to the limit $m \rightarrow +\infty$ and $\delta \rightarrow 0$.

To prove estimate (4.1) we use a nice argument introduced in [3, Prop. 2.1]. For first, let us remind that the best coupling between an absolute continue measure μ and X^N can be represented with a measurable map $T_{X^N} : Q \rightarrow Q$ such that T_{X^N} transport $\mu(dx)$ in $X^N(dx)$, and

$$J_T(dx, dy) = \delta(y - T_{X^N}(x)) \rho(x) dx dy$$

is the joint distribution which realize the infimum in the definition of the 2-Wasserstein distance:

$$W_2^2(\mu, X^N) = \int J_T(dx, dy) |x - y|^2 = \int |T_{X^N}(x) - x|^2 \rho(x) dx.$$

Let Y^N another empirical measure obtained extracting N particles with distribution μ , and let T_{Y^N} be the corresponding map which gives the best coupling. Then, since T_{X^N} and T_{Y^N} transport μ in X^N and Y^N respectively,

$$\begin{aligned} W_2^2(X^N, Y^N) &\leq \int |T_{X^N}(x) - T_{Y^N}(x)|^2 \rho(x) dx \\ &= \int |T_{X^N}(x) - x - (T_{Y^N}(x) - x)|^2 \rho(x) dx \\ &= \int |T_{X^N}(x) - x|^2 \rho(x) dx + \int |T_{Y^N}(x) - x|^2 \rho(x) dx + \\ &\quad - 2 \int (T_{X^N}(x) - x) \cdot (T_{Y^N}(x) - x) \rho(x) dx. \end{aligned}$$

Considering that, since X^N and Y^N are independent and identically distributed, also $T_{X^N}(x)$ and $T_{Y^N}(x)$ are independent and identically distributed. Then, taking the expectation,

$$\begin{aligned} \mathbb{E}_\mu [W_2^2(X^N, Y^N)] &\leq 2\mathbb{E}_\mu \int |T_{X^N}(x) - x|^2 \rho(x) dx - 2 \int |\mathbb{E}_\mu [T_{X^N}(x) - x]|^2 \rho(x) dx \\ &\leq 2\mathbb{E}_\mu \int |T_{X^N}(x) - x|^2 \rho(x) dx = \mathbb{E}_\mu W_2^2(X^N, \mu). \end{aligned}$$

Therefore, by (4.3) we get (4.1).

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