

ON THE COMPUTATION OF KANTOROVICH-WASSERSTEIN DISTANCES BETWEEN 2D-HISTOGRAMS BY UNCAPACITATED MINIMUM COST FLOWS

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Abstract. In this work, we present a method to compute the Kantorovich-Wasserstein distance of order one between a pair of two-dimensional histograms. Recent works in Computer Vision and Machine Learning have shown the benefits of measuring Wasserstein distances of order one between histograms with n bins, by solving a classical transportation problem on very large complete bipartite graphs with n nodes and n^2 edges. The main contribution of our work is to approximate the original transportation problem by an uncapacitated min cost flow problem on a reduced flow network of size $O(n)$ that exploits the geometric structure of the cost function. More precisely, when the distance among the bin centers is measured with the 1-norm or the ∞ -norm, our approach provides an optimal solution. When the distance among bins is measured with the 2-norm: (i) we derive a quantitative estimate on the error between optimal and approximate solution; (ii) given the error, we construct a reduced flow network of size $O(n)$. We numerically show the benefits of our approach by computing Wasserstein distances of order one on a set of grey scale images used as benchmark in the literature. We show how our approach scales with the size of the images with 1-norm, 2-norm and ∞ -norm ground distances, and we compare it with other two methods which are largely used in the literature.

Key words. Kantorovich metric, Wasserstein distance, Transportation Problem, Network Simplex, Uncapacitated Minimum Cost Flow Problem

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1. Introduction. The Transportation Problem, also called the Hitchcock-Koopmans transportation problem [17], is a historical problem for the mathematical programming community [42]. Indeed, the Transportation Problem is a particular case in the discrete setting of the more general Monge-Kantorovich Transportation Problem, largely studied in the functional analysis community (e.g., see [49, 3]), since the pioneering work of the French mathematician Gaspard Monge in 1781 [31], and later the fundamental work of L.V. Kantorovich on the theory of Linear Programming duality [48]. In the discrete setting, the Transportation Problem played a fundamental role in the development of the (Network) Simplex algorithm and of all the related network flows problems [42, 20, 1]. In the continuous setting, the Transportation Problem has recently gathered a renewed interest in computer science and applied mathematics, as an efficient method to compute distances between probability measures. We just mention here the attention gathered from the Machine Learning community in the use of the Wasserstein distances within Generative Adversarial Networks (GAN) [4], which was possible thanks to recent developments of very efficient numerical algorithms based on entropic regularization [13, 44, 11, 2].

In this paper, we focus on the Kantorovich metric, i.e. the Wasserstein (Vaserstein) distance of order 1, between two-dimensional histograms. By exploiting the geometric cost structure of the problem, we reduce the computation of Kantorovich distances to the problem of solving an uncapacitated minimum cost flow problem [34] on a graph with a prescribed topology. We consider three types of transportation costs among locations, induced by the p -norms with $p = 1$, $p = 2$, and $p = \infty$. For each norm, we build a flow network with a prescribed topology and given costs: our

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aim is to keep the size of the flow network as small as possible in order to accelerate the computation of Kantorovich distances, while limiting the use of computer memory. In addition, for the 2-norm, we provide a flow network that permits to find an approximate solution, and we derive a quantitative estimate on the error between optimal and approximate solution.

We stress the importance of having fast methods to compute exact and approximate Kantorovich distances. As discussed next, these distances are used as subproblems of more general tasks, and they are usually (re)computed again, and again, and again. Having a strongly polynomial algorithm of worst-case complexity $O(N^3 \log N)$ (e.g., [20]), where N is the number of locations of the transportation problem, it is definitely not enough. In addition, the size of Transportation Problems that must be solved is so large, that we need new numerical methods with strong mathematical foundations to solve such problems in practice. The contribution of our paper tackles exactly this numerical challenge.

Related Works. In mathematical programming, the Hitchcock-Koopmans transportation problem is considered a well-solved problem, since it can be solved with strongly polynomial algorithms or with Network Simplex algorithms [1, 20]. Recent work focused on the structure of the Transportation polytope [5, 9], on variations of the problem with nonlinear variables [47], or on mixed production transportation problems with concave costs [23]. However, our paper follows a different (numerical) line of research, which aims at solving very large instances of structured Hitchcock-Koopmans problems.

Our work is closely related to what, in the computer vision and image retrieval community, is known as the *Earth Mover's Distance (EMD)* [38, 36]. In this context, the Kantorovich metric is used to compute the distance between images by precomputing so-called SIFT descriptors (special type of histograms, see [30]) and then by computing distances between such descriptors. The advantages of using a more computationally demanding metric instead of other simpler metrics is empirically demonstrated by the quality of the results, and in addition is elegantly supported by the mathematical theory that lays the foundation of the Kantorovich metric. Remarkable results were also obtained in the context of cell biology for comparing flow cytometry diagrams [8, 35] and in radiation therapy to improve the comparison of histograms related to tumor shape [25].

In statistics and probability, the Kantorovich distance is known as the Mallow's distance [28]. It has been used for the assessment of goodness of fit between distributions [32, 46] as well as an alternative to the usual g -divergences as cost function in minimum distance point estimation problems [6, 7]. It was used to compare 2D histograms, but only considering the 1-norm as a cost structure of the underlying Transportation Problem [29]. Another interesting application is the computation of the mean of a set of empirical probability measures based on the Kantorovich metric [14]. In machine learning, the use of Kantorovich distances is increasingly spreading in different contexts. Apart from the GAN networks [4], it has been used in unsupervised domain adaptation [12], in semi-supervised learning [45], and as a Loss Function for learning probability distributions [18]. For the theoretical foundations of the Monge-Kantorovich Transportation Problem, we refer the interested reader to [39, 49], while for a survey on recent applications of Optimal Transportation to [43].

Outline. In [section 2](#) we review the Kantorovich distance (i.e., the Wasserstein distance of order 1) in the discrete setting and we show its connection with Linear Programming ([subsection 2.2](#)) and with uncapacitated minimum cost flow problems ([subsection 2.3](#) and [subsection 2.4](#)). In [subsection 2.5](#), we discuss how to reduce

the time complexity of evaluating the Kantorovich distance by approximating the transportation problem with a flow problem on a specific reduced network, we define the relative approximation error which is incurred upon by introducing a reduced flow network, and we provide a bound upon it.

Our main contributions are presented in [section 3](#), where we exploit the reduced flow networks to efficiently compute Kantorovich distances while using the 1-norm, the 2-norm, and the ∞ -norm as ground distances. In addition, for the 2-norm, we derive a quantitative estimate on the error between the optimal solution and an approximate solution on a reduced flow network ([Theorem 3.4](#)).

In [section 4](#), we give all the details of the results presented in [subsection 2.3-subsection 2.5](#). Precisely, in [subsection 4.1](#), we recall the classical Strong Duality Theorem, which we use in [subsection 4.2](#) in order to establish a relation between the minimum of the cost flow problem and the infimum of Kantorovich's transportation problem. The equivalence of these two problems is well known ([Proposition 4.1](#)), but we choose to give a proof here, as we were not able to find one in any reference. In [Proposition 4.3](#) we state and prove the bound on the relative approximation error $\mathcal{E}_G(b)$ introduced in [\(2.12\)](#). This is key in the proof of the error estimate [\(3.2\)](#) in [Theorem 3.4](#).

Finally, in [section 5](#) we conclude by reporting our extensive numerical experiments.

2. Background. In this section, we review the basic notions and we fix the notation used in this paper. Moreover, in [subsection 2.5](#) we state under which conditions Optimal Transportation and minimum cost flow problems yield the same optimal solutions, and we state a universal upper bound on the relative approximation error.

2.1. Kantorovich distance in the discrete setting. Let $X = \{x_1, \dots, x_{n_1}\}$ and $Y = \{y_1, \dots, y_{n_2}\}$ be two discrete spaces. Given two probability vectors on X and Y , denoted $\mu = (\mu(x_1), \dots, \mu(x_{n_1}))$ and $\nu = (\nu(y_1), \dots, \nu(y_{n_2}))$, and a cost $c : X \times Y \rightarrow \mathbb{R}_+$, the *Kantorovich-Rubinshtein functional* between μ and ν is defined as

$$(2.1) \quad \mathcal{W}_c(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \sum_{(x, y) \in X \times Y} c(x, y) \pi(x, y)$$

where $\Pi(\mu, \nu)$ is the set of all the probability measures on $X \times Y$ with marginals μ and ν , i.e., of the probability measures π such that

$$\sum_{y \in Y} \pi(x, y) = \mu(x) \quad \text{and} \quad \sum_{x \in X} \pi(x, y) = \nu(y)$$

for every (x, y) in $X \times Y$. Such probability measures are sometimes called transportation plans or couplings for μ and ν . An important special case is when $X = Y$ and the cost function c is a distance on X . In this case, which is our main interest in this article, \mathcal{W}_c is a distance on the simplex of probability vectors on X , also known as *Wasserstein distance* of order 1. It is worth mentioning that a Wasserstein distance of order p can be defined, more in general, for arbitrary probability measures on a metric space (X, d) by

$$(2.2) \quad W_p(\mu, \nu) := \left(\inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times X} d^p(x, y) \pi(dxdy) \right)^{\min(1/p, 1)},$$

where now $\Pi(\mu, \nu)$ is the set of all probability measures on the Borel sets of $X \times X$ that have marginals μ and ν , see, e.g., [3]. The infimum in (2.2) is attained and any probability π which realizes the minimum is called an *optimal transportation plan*.

2.2. Linear Programming and Earth Mover's Distance. The Kantorovich-Rubinshtein transportation problem in the discrete setting can be seen as a special case of the following Linear Programming problem, where we assume now that μ and ν are generic vectors of dimension n_1 and n_2 , with positive components,

$$(2.3) \quad (P) \quad \min \quad \sum_{x \in X} \sum_{y \in Y} c(x, y) \pi(x, y)$$

$$(2.4) \quad \text{s.t.} \quad \sum_{y \in Y} \pi(x, y) \leq \mu(x) \quad \forall x \in X$$

$$(2.5) \quad \sum_{x \in X} \pi(x, y) \geq \nu(y) \quad \forall y \in Y$$

$$(2.6) \quad \pi(x, y) \geq 0.$$

Note that the maximum flow quantity is equal to

$$\sum_{x \in X} \sum_{y \in Y} \pi(x, y) = \min \left\{ \sum_{x \in X} \mu(x), \sum_{y \in Y} \nu(y) \right\}.$$

If $\sum_x \mu(x) = \sum_y \nu(y)$ we have the so-called *balanced* transportation problem, otherwise the transportation problem is said to be *unbalanced*. For balanced optimal transportation problems, constraints (2.4) and (2.5) must be satisfied with equality, and the problem reduces to the Kantorovich transportation problem (up to normalization of the vectors μ and ν). Problem (P) is also related to the so-called *Earth Mover's distance*. In this case, $X, Y \subset \mathbb{R}^d$ and x_i (y_j , respectively) is the center of the data cluster i (j , respectively). Moreover, $\mu(x_i)$ ($\nu(y_j)$, respectively) is the number of points in the cluster i (j , respectively) and, finally, $c(x_i, y_j)$ is some measure of dissimilarity between x_i and y_j . Once the optimal transportation π^* is determined, the Earth Mover's distance between the *signatures* $(x_i, \mu(x_i))_i$ and $(y_j, \nu(y_j))_j$ is defined as

$$EMD(\mu, \nu) = \frac{\sum_{x \in X} \sum_{y \in Y} c(x, y) \pi^*(x, y)}{\sum_{x \in X} \sum_{y \in Y} \pi^*(x, y)}.$$

The Earth Mover's distance (EMD) was first introduced by Rubner et al. for color and texture images in [37] and [38].

As noted in [38], the EMD is a true metric on distributions, and it is exactly the same as the Wasserstein distance, also known as Mallows distance. For more details on this, see e.g. [28] and the references therein. The cost function used in the EMD is typically a true distance, in general an L_p distance.

2.3. Uncapacitated minimum cost flow problem on a graph. As we shall see in subsection 2.4, a standard way to solve problem (P) is to recast it as an uncapacitated minimum cost flow problem. For this reason, we briefly recall the definition of *minimum cost flow problem* on a directed graph.

Let $G = (V, E)$ be a directed network with no self-loops, where V is the vertex set and E the set of edges. Consider a cost function $c : E \rightarrow [0, +\infty)$ and a function

$b : V \rightarrow \mathbb{R}$ such that $\sum_{v \in V} b(v) = 0$. A flow (or b -flow) on G is any function $f : E \rightarrow [0, +\infty)$ such that

$$(2.7) \quad \sum_{v:(u,v) \in E} f(u,v) - \sum_{v:(v,u) \in E} f(v,u) = b(u) \quad \forall u \in V.$$

In the following, we denote by $\mathcal{F}(G, b)$ the class of all the b -flows on G . The (*uncapacitated*) *minimum cost flow problem* associated to (G, c, b) consists in finding a b -flow f which minimizes the cost

$$\sum_{(u,v) \in E} c(u,v) f(u,v).$$

See, e.g., [1] or Chapter 9 in [26]. In what follows, we set

$$(2.8) \quad F_{G,c}(b) := \min_{f \in \mathcal{F}(G,b)} \sum_{(u,v) \in E} c(u,v) f(u,v).$$

It is easy to see that if G is a subgraph of G' , then

$$(2.9) \quad F_{G,c}(b) \geq F_{G',c}(b).$$

2.4. Wasserstein distance of order one as a minimum cost flow problem.

It is easy to re-write $\mathcal{W}_c(\mu, \nu)$ as a minimum cost flow problem. Consider the bipartite graph

$$G_{X \rightarrow Y} = (X \cup Y, E_{X \rightarrow Y})$$

with $E_{X \rightarrow Y} = \{(x, y) : x \in X, y \in Y\}$, and define

$$b(u) := \begin{cases} \mu(u) & \text{if } u \in X, \\ -\nu(u) & \text{if } u \in Y. \end{cases}$$

It is plain to check that

$$(2.10) \quad F_{G_{X \rightarrow Y}, c}(b) = \mathcal{W}_c(\mu, \nu).$$

Incidentally, an uncapacitated minimum cost flow problem of this kind is known as *Hitchcock problem* [17].

In general, given a network $G = (V, E)$ with $n = |V|$ nodes and $k = |E|$ arcs, Orlin's algorithm [34] solves the uncapacitated minimum cost flow problem $F_{G,c}(b)$ for integer supplies/demands b in $O(n \log(\min\{n, D\})S(n, k))$, where $D := \max_{v \in V} \{|b(v)|\}$ and $S(n, k)$ is the complexity of finding a shortest path in G . Using Dijkstra's [16] algorithm $S(n, k) = O(n \log n + k)$. This gives, for general supplies/demands, the cost $O(n \log(n)(n \log n + k))$. Combining (2.10) with the previous observations, one obtains that $\mathcal{W}_c(\mu, \nu)$ can be computed exactly with a time complexity $O((n_1 + n_2)^3 \log(n_1 + n_2))$.

When $X = Y$, with $|X| = |Y| =: n$, and c is a distance, one can show that the flow problem associated with $\mathcal{W}_c(\mu, \nu)$ can be formulated on an auxiliary network, which is smaller than the bipartite graph $G_{X \rightarrow X}$. More precisely, set $b = \mu - \nu$ and let K_n be the complete (directed) graph on X (without self-loops). If c is a distance, then

$$(2.11) \quad \mathcal{W}_c(\mu, \nu) = F_{K_n, c}(b).$$

A detailed proof of this fact is given in [Proposition 4.1](#) in [section 4](#).

Although K_n is smaller than $G_{X \rightarrow X}$, the problem of determining $F_{K_n, c}(b)$ is computationally demanding for relatively small n . Using the previous considerations on the computational cost of a minimum flow problem, it is easy to see that the time complexity of computing $F_{K_n, c}(b)$ is $O(n^3 \log(n))$ and hence it is of the same order of the complexity of computing $F_{G_{X \rightarrow X}, c}(b)$.

Even if (2.11) is not satisfactory by itself, it is the starting point of our further developments. In section 3 we shall exploit the cost structure (for some special costs) to reduce the number of edges in the graph on which the flow problem is formulated, and to largely simplify the complexity of the problem when X is the space of base points of a 2D histogram.

2.5. Relaxation and Error bounds: main ideas. Before moving to our main results concerning the computation of the \mathcal{W}_c distance between 2D-histograms, let us briefly outline our main ideas in a more general setting. All the details are postponed to section 4.

Let $G = (V, E) \subset K_n$ be a directed graph and consider the corresponding flow problem as an approximation of the original flow problem on the complete graph K_n . One has that $F_{G, c}(b) \geq F_{K_n, c}(b)$, which means that the relative error of approximation between the original minimum and its relaxation $F_{G, c}$ satisfies

$$(2.12) \quad \mathcal{E}_G(b) := \frac{F_{G, c}(b) - F_{K_n, c}(b)}{F_{G, c}(b)} \in [0, 1].$$

If one is able to find a subgraph $G \subset K_n$ for which $\mathcal{E}_G(b) = 0$, one can reduce the problem of computing $F_{K_n, c}(b)$ to a simpler minimum flow problem, i.e. to the evaluation of $F_{G, c}(b)$. Even if this is not possible, one can still use a subgraph G to approximate $F_{K_n, c}(b)$ and control the relative error of approximation $\mathcal{E}_G(b)$.

This last goal is obtained by deriving a universal upper bound on $\mathcal{E}_G(b)$. To this end define

$$(2.13) \quad c_G(x, y) := \min_{\gamma \in \Gamma(x, y)} \sum_{k=0}^{|\gamma|-1} c(\gamma_k, \gamma_{k+1})$$

where $\Gamma(x, y)$ is the set of directed paths in G from vertex x to vertex y and $|\gamma|$ is the length of the path γ , composed of edges γ_k , and set

$$\Gamma_{G, c} := \max \left\{ 1 - \frac{c(x, y)}{c_G(x, y)} : (x, y) \in X^2, x \neq y \right\}.$$

In Proposition 4.3 (section 4) we prove that, if c is a distance,

$$(2.14) \quad 0 \leq \mathcal{E}_G(b) \leq \Gamma_{G, c}$$

for any vector b . Hence, combining (2.11) and (2.14) we get

$$(1 - \Gamma_{G, c})F_{G, c}(\mu - \nu) \leq \mathcal{W}_c(\mu, \nu) \leq F_{G, c}(\mu - \nu)$$

for any couple of measures (μ, ν) and any distance c . In the light of these considerations, the key-point is to find a small graph $G \subset K_n$ for which $\Gamma_{G, c}$ is easy to compute and/or zero.

3. Efficient Computation of \mathcal{W}_c distance between 2D-Histograms. Histograms can be seen as discrete measures on a finite set of points in \mathbb{R}^d . Here we are interested in the case in which $d = 2$. To represent a two-dimensional histogram with $N \times N$ equally spaced bins, we take without loss of generality

$$X = \mathcal{L}_N := \{\mathbf{i} = (i_1, i_2) : i_1 = 0, 1, \dots, N-1, i_2 = 0, 1, \dots, N-1\}.$$

One can think of each point (i_1, i_2) as the center of a bin.

In this case, $\#\mathcal{L}_N = N^2$ and the complete directed graph $K = K_{N^2}$ has $N^2(N^2 - 1) = O(N^4)$ edges. Note that, according to last section's notation, we are considering a set of $n = N^2$ points. To simplify notation, we write $K = K_{N^2}$.

Following the idea sketched in [subsection 2.5](#), the goal is to approximate \mathcal{W}_c (or equivalently $F_{K,c}$), with $F_{G,c}$ for a suitable small graph $G \subset K$.

When the distance among the bins is measured with the 1-norm L_1 or the infinity-norm L_∞ , we provide an optimal solution using a graph G with $O(N^2)$ edges. When the distance between bins is measured with the L_2 -norm: (i) we show that an optimal solution can be obtained using a reduced network with around half the size of the complete bipartite graph, (ii) given an error, we provide an approximate solution using a reduced network of size $O(N^2)$.

In order to describe the subgraphs G , we use the following notation. Given $\mathbf{i} = (i_1, i_2) \in \mathbb{Z} \times \mathbb{Z}$, $\mathbf{j} = (j_1, j_2) \in \mathbb{Z} \times \mathbb{Z}$, define $\mathbf{i} + \mathbf{j} = (i_1 + j_1, i_2 + j_2)$. If $G = (V, E)$ is a graph and $\mathbf{i}, \mathbf{j} \in V$, we denote the directed edge connecting \mathbf{i} to \mathbf{j} by $(\mathbf{i}, \mathbf{j}) \in E$. Let $\mathbb{N}_0 := \mathbb{N} \setminus \{0\}$, $\mathbb{Z}_0 := \mathbb{Z} \setminus \{0\}$. For $L \in \mathbb{N}_0$, we define the following sets of vertices

$$\begin{aligned} V_0 &:= \{(1, 0), (0, 1), (-1, 0), (0, -1)\}, \\ V_L &:= V_0 \cup \{(i_1, i_2) \in \mathbb{Z}_0 \times \mathbb{Z}_0 : |i_1| \leq L, |i_2| \leq L, \\ &\quad \text{and } |i_1| \text{ and } |i_2| \text{ are coprime}\}. \end{aligned}$$

The condition on the divisors of $|i_1|$ and $|i_2|$ implies that any point of coordinates $\mathbf{i} \in V_L$ is “visible” from the origin $(0,0)$, in the sense that there is no point with integer coordinates on the line segment between the origin and \mathbf{i} .

3.1. L_1 ground distance. In this section we recover, as a special case of our approach, the method proposed in [\[29\]](#) to efficiently compute the L_1 -EMD by solving a flow problem on a graph with $O(N^2)$ edges. Let us consider as ground distance the L_1 distance on \mathcal{L}_N , i.e. $c = d_1$, where

$$d_1(\mathbf{i}, \mathbf{j}) = |i_1 - j_1| + |i_2 - j_2|.$$

In this case, as a subgraph of K we choose

$$G_0 := (\mathcal{L}_N, E_0) \quad \text{where} \quad E_0 := \{(\mathbf{i}, \mathbf{i} + \mathbf{j}) : \mathbf{i} \in \mathcal{L}_N, \mathbf{j} \in V_0, \mathbf{i} + \mathbf{j} \in \mathcal{L}_N\},$$

see [Figure 1](#). Note that the set of (directed) edges of G_0 has cardinality $2(N-1)N = O(N^2)$.

It is a simple exercise to see that in this case $\Gamma_{G_0, d_1} = 0$ for every N . This means that one can compute the distance $\mathcal{W}_{d_1}(\mu, \nu)$ between two normalized histograms μ and ν without any error, by solving a minimum cost flow problem on the graph G_0 which has N^2 nodes and $O(N^2)$ edges. We summarize the previous statements, recalling that $F_{G,c}(b)$ was defined in [\(2.8\)](#), in the next

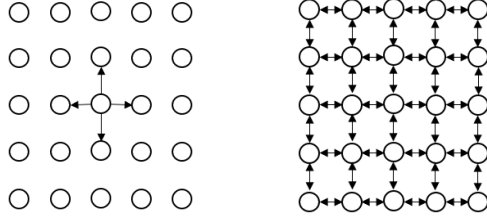


FIG. 1. The edges connecting the middle node \mathbf{i} to the four nodes $\mathbf{i} + \mathbf{j}$, with $\mathbf{j} \in V_0$ (left). Iterating for all $\mathbf{i} \in \mathcal{L}_5$ we obtain G_0 (right). The resulting geometry is also known as taxicab or Manhattan geometry.

PROPOSITION 3.1. Under the previous assumptions, $\Gamma_{G_0, d_1} = 0$ and hence

$$F_{G_0, d_1}(b) = F_{K, d_1}(b).$$

In particular,

$$\mathcal{W}_{d_1}(\mu, \nu) = F_{G_0, d_1}(\mu - \nu)$$

for every couple of probability measures μ and ν on \mathcal{L}_N .

3.2. L_∞ ground distance. In this section, we specialize our approach to deal with the L_∞ ground distance. If $c = d_\infty$, where $d_\infty(\mathbf{i}, \mathbf{j}) = \max(|i_1 - j_1|, |i_2 - j_2|)$, we consider the graph (see [Figure 2](#))

$$G_1 := (\mathcal{L}_N, E_1) \quad \text{where} \quad E_1 := \{(\mathbf{i}, \mathbf{i} + \mathbf{j}) : \mathbf{i} \in \mathcal{L}_N, \mathbf{j} \in V_1, \mathbf{i} + \mathbf{j} \in \mathcal{L}_N\}.$$

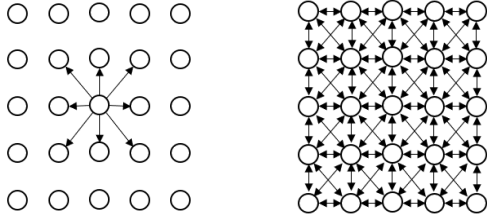


FIG. 2. The edges connecting the middle node \mathbf{i} to the eight nodes $\mathbf{i} + \mathbf{j}$, with $\mathbf{j} \in V_1$ (left), and the graph G_1 (right). With respect to [Figure 1](#), four edges are added to each inner node.

Also in this case it is easy to see that $\Gamma_{G_1, d_\infty} = 0$ and the number of edges in G_1 is again $O(N^2)$, more precisely $2(N-1)(2N-1)$.

PROPOSITION 3.2. One has $\Gamma_{G_1, d_\infty} = 0$ and hence $F_{G_1, d_\infty}(b) = F_{K, d_\infty}(b)$. In particular,

$$\mathcal{W}_{d_\infty}(\mu, \nu) = F_{G_1, d_\infty}(\mu - \nu)$$

for every couple of probability measures μ and ν on \mathcal{L}_N .

3.3. L_2 ground distance. Here we face the challenging problem of efficiently computing the Wasserstein distance of order 1 between 2D-histograms using the euclidean L_2 norm as ground distance. Let us consider $c = d_2$, where

$$d_2(\mathbf{i}, \mathbf{j}) = \sqrt{|i_1 - j_1|^2 + |i_2 - j_2|^2}.$$

In order to build a suitable subgraph of K , we further consider the vertices sets V_L defined above. For $1 \leq L \leq N - 1$, we define the graph

$$(3.1) \quad G_L := (\mathcal{L}_N, E_L) \quad \text{with} \quad E_L := \{(\mathbf{i}, \mathbf{i} + \mathbf{j}) : \mathbf{i} \in \mathcal{L}_N, \mathbf{j} \in V_L, \mathbf{i} + \mathbf{j} \in \mathcal{L}_N\},$$

(we say that G_L is the graph induced by V_L). See [Figure 3](#).

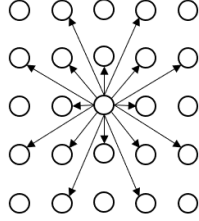


FIG. 3. The set of edges $\{(\mathbf{i}, \mathbf{i} + \mathbf{j})\}$, where \mathbf{i} is the middle node and $\mathbf{j} \in V_2$. The graph G_2 is now too crowded to be clearly visualized.

Our results concerning the L_2 ground distance are the following: in [Proposition 3.3](#) we show that when $L = N - 1$ (i.e., the induced subgraph is G_{N-1}) the approximation error is zero. Again, this means that one can compute $\mathcal{W}_{d_2}(\mu, \nu)$ by solving a minimum cost flow problem on a graph which is strictly contained in the complete graph K . Unfortunately, in this case, the number of required edges is of order N^4 ([Proposition 3.3](#)). To conclude, in [Theorem 3.4](#), we provide a sharp estimate on the error due to the approximation of K with G_L , for $L < N - 1$.

PROPOSITION 3.3. *With the previous notation, if $c = d_2$, then $c_{G_{N-1}} = d_2$, hence $\Gamma_{G_{N-1}, d_2} = 0$ and*

$$\mathcal{W}_{d_2}(\mu, \nu) = F_{G_{N-1}, d_2}(\mu - \nu)$$

for every couple of probability measures μ, ν on \mathcal{L}_N . Moreover, if E_{N-1} denotes the set of edges of G_{N-1} , then

$$\lim_{N \rightarrow +\infty} \frac{\#E_{N-1}}{N^4} = \frac{6}{\pi^2}.$$

The next result, in combination with [\(2.14\)](#), shows that one can approximate the true value $\mathcal{W}_{d_2}(\mu, \nu)$ by computing $F_{G_L, d_2}(\mu - \nu)$ with $L < N - 1$ and obtain an explicit bound on the relative error.

THEOREM 3.4. *Let $c = d_2$, then for every $1 \leq L < N - 1$*

$$(3.2) \quad 1 - \frac{\sqrt{1 + 4L^2}}{L + \sqrt{1 + L^2}} \leq \Gamma_{G_L, d_2} \leq c(L) \left(1 - \frac{L}{\sqrt{1 + L^2}} \right),$$

where $0.25 < c(L) < 0.26$ and $c(L)$ is monotone decreasing. Asymptotically,

$$(3.3) \quad \Gamma_{G_L, d_2} = \frac{1}{8L^2} - \frac{11}{128L^4} + O\left(\frac{1}{L^6}\right) \quad \text{for } L \rightarrow +\infty.$$

3.4. Proofs of [subsection 3.3](#). Define the set

$$\tilde{V}_L := \{(i_1, i_2) \in V_L : i_1 \geq i_2 \geq 0\}.$$

By restricting to \tilde{V}_L , we consider only directions characterized by angles α ranging between 0 and $\pi/4$; all other directions may be obtained from \tilde{V}_L by rotations of $k\pi/4$, for $k = 1, \dots, 7$. To every element $\mathbf{i} \in \tilde{V}_L$ we associate the slope

$$t_{\mathbf{i}} := \frac{i_2}{i_1}.$$

The collection of these slopes, for $L \geq 1$, forms the so-called Farey sequence \mathfrak{F}_L , see e.g. Section 4.5 in [21] or Chapter 6 in [33]. For example, for $L = 1, 2, 3$, we have

$$\mathfrak{F}_1 = \left\{ \frac{0}{1}, \frac{1}{1} \right\}, \quad \mathfrak{F}_2 = \left\{ \frac{0}{1}, \frac{1}{2}, \frac{1}{1} \right\}, \quad \mathfrak{F}_3 = \left\{ \frac{0}{1}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, \frac{1}{1} \right\}.$$

Since the elements in V_L are pairwise coprime, the mapping

$$t : \tilde{V}_L \rightarrow \mathfrak{F}_L, \quad \mathbf{i} \mapsto \frac{i_2}{i_1}$$

is one-to-one, i.e., there is a bijection between \tilde{V}_L and \mathfrak{F}_L . We will therefore use some known properties of the Farey sequence to prove an estimate on the graph induced by V_L . Before proving [Proposition 3.3](#), we need the following remark.

LEMMA 3.5. *Each point \mathbf{j} in the square lattice \mathcal{L}_L can be written as*

$$\mathbf{j} = m\mathbf{i}$$

where m is an integer and \mathbf{i} is in V_{L-1} .

Proof. Let $\mathbf{j} = (j_1, j_2) \in \mathcal{L}_L$. By definition of \mathcal{L}_L , $0 \leq j_1, j_2 \leq L-1$. If j_1 and j_2 are coprime, then $\mathbf{j} \in V_{L-1}$ (i.e., we can choose $m = 1$, $\mathbf{i} = \mathbf{j}$). If they are not coprime, then there exists $m \in \mathbb{N}$ and $\mathbf{i} \in V_{L-1}$ such that $(j_1, j_2) = (mi_1, mi_2)$. \square

We will also use known results on the asymptotic density of coprime numbers. Given a compact convex set D in \mathbb{R}^2 containing the origin, the number of primitive lattice points in the “blow up” set $\sqrt{x}D$, i.e. the number of coprime numbers in $\sqrt{x}D$, diverges as x goes to $+\infty$ as $6xa(D)/\pi^2$, where $a(D)$ is the area of D . Under suitable regularity assumptions on D , one can derive precise estimates on the remainder, see e.g. [24].

LEMMA 3.6. *Let \mathcal{D} be the set of squares in \mathbb{R}^2 containing $(0, 0)$ with side of length 1. For any $D \in \mathcal{D}$ and $x > 0$ set $B_D(x) = \#\{z = (z_1, z_2) \in Z_0^2 : z/\sqrt{x} \in D : \gcd(z_1, z_2) = 1\}$. Then, there is a constant C such that for every $x \geq 1$*

$$\sup_{D \in \mathcal{D}} \left| B_D(x) - \frac{6x}{\pi^2} \right| \leq C\sqrt{x}[1 + \log(\sqrt{x})].$$

Proof. One can write $B_D(x) = \#\{z \in Z_0^2 : Q(z) \leq x, \gcd(z_1, z_2) = 1\}$ where

$$Q(z) = \left(\inf\{t > 0 : z/t \in D\} \right)^2.$$

Set also $A_D(x) = \#\{z \in Z_0^2 : Q(z) \leq x\}$. Combining these definitions with well-known properties of the Möbius function μ , one can prove that

$$B_D(x) = \sum_{m \in \mathbb{N}} A_D\left(\frac{x}{m^2}\right) \mu(m).$$

See e.g. [24] or Lemma 4 in [50]. Since D is a square of length 1 containing the origin, then $A_D\left(\frac{x}{m^2}\right) = 0$ whenever $m > \sqrt{x}$. Moreover,

$$\left|A_D(x) - x\right| \leq 4\sqrt{x}.$$

Combining these facts,

$$B_D(x) = x \sum_{m \leq \sqrt{x}} \frac{\mu(m)}{m^2} + R(x)$$

where, recalling also that $|\mu(m)| \leq 1$,

$$|R(x)| \leq \sum_{m \leq \sqrt{x}} \left| \left(A_D\left(\frac{x}{m^2}\right) - \frac{x}{m^2} \right) \mu(m) \right| \leq 4\sqrt{x} \sum_{m \leq \sqrt{x}} \frac{1}{m}.$$

To conclude recall that $\sum_{m \geq 1} \frac{\mu(m)}{m^2} = 6/\pi^2$ to write, for $x \geq 1$,

$$\left| B_D(x) - \frac{6x}{\pi^2} \right| \leq 4\sqrt{x} \sum_{m \leq \sqrt{x}} \frac{1}{m} + x \sum_{m > \sqrt{x}} \frac{1}{m^2} \leq C[\sqrt{x}(1 + \log \sqrt{x})]. \quad \square$$

Proof. (Proof of [Proposition 3.3](#)) Let us start by proving that

$$\mathcal{W}_{d_2}(\mu, \nu) = F_{G_{N-1}, d_2}(\mu - \nu).$$

By definition [\(3.1\)](#),

$$G_{N-1} = (\mathcal{L}_N, E_{N-1}), \quad E_{N-1} := \{(\mathbf{i}, \mathbf{i} + \mathbf{j}) : \mathbf{i} \in \mathcal{L}_N, \mathbf{j} \in V_{N-1}, \mathbf{i} + \mathbf{j} \in \mathcal{L}_N\}.$$

Given $\mathbf{i}, \mathbf{j} \in \mathcal{L}_N$, an admissible path γ connecting \mathbf{i} to \mathbf{j} in G_{N-1} is a collection of edges $\gamma_m = (\mathbf{x}_m, \mathbf{y}_m) \in E_{N-1}$, $m = 1, \dots, M$ such that $\mathbf{x}_1 = \mathbf{i}$, $\mathbf{y}_m = \mathbf{x}_{m+1}$, and $\mathbf{y}_M = \mathbf{j}$. The length of a path $\gamma = \{\gamma_1, \dots, \gamma_M\}$ is the sum of the lengths of its edges, that is

$$|\gamma| = \sum_{\gamma_m \in \gamma} |\gamma_m| = \sum_{m=1}^M d_2(\mathbf{x}_m, \mathbf{y}_m).$$

We denote by $\Gamma(\mathbf{i}, \mathbf{j})$ the set of all admissible paths connecting \mathbf{i} to \mathbf{j} . We want to prove that

$$d_2(\mathbf{i}, \mathbf{j}) = c_{G_{N-1}}(\mathbf{i}, \mathbf{j}) \quad \forall \mathbf{i}, \mathbf{j} \in \mathcal{L}_N,$$

that is, according to definition [\(2.13\)](#), that for every $\mathbf{i}, \mathbf{j} \in \mathcal{L}_N$ there exists $\gamma \in \Gamma(\mathbf{i}, \mathbf{j})$ such that $d_2(\mathbf{i}, \mathbf{j}) = |\gamma|$. Let $\mathbf{i}, \mathbf{j} \in \mathcal{L}_N$, since

$$\max\{|j_1 - i_1|, |j_2 - i_2|\} \leq N - 1,$$

then the vertex $(|j_1 - i_1|, |j_2 - i_2|)$ belongs to \mathcal{L}_N . By Lemma [Lemma 3.5](#) there exists $\mathbf{v} \in V_{N-1}$ such that $\mathbf{j} - \mathbf{i} = m\mathbf{v}$ (the coordinates in V_L are not restricted to positive integers). Choosing as admissible path

$$\gamma = \{(\mathbf{i}, \mathbf{i} + \mathbf{v}), (\mathbf{i} + \mathbf{v}, \mathbf{i} + 2\mathbf{v}), \dots, (\mathbf{i} + (m-1)\mathbf{v}, \mathbf{i} + m\mathbf{v})\},$$

we compute

$$\begin{aligned} c_{G_{N-1}}(\mathbf{i}, \mathbf{j}) &\leq |\gamma| = \sum_{k=0}^{m-1} d_2(\mathbf{i} + k\mathbf{v}, \mathbf{i} + (k+1)\mathbf{v}) \\ &= md_2(\mathbf{0}, \mathbf{v}) = d_2(\mathbf{0}, m\mathbf{v}) = d_2(\mathbf{i}, \mathbf{j}). \end{aligned}$$

Since $c_{G_{N-1}}(\mathbf{i}, \mathbf{j}) \geq d_2(\mathbf{i}, \mathbf{j})$ for all $\mathbf{i}, \mathbf{j} \in \mathcal{L}_N$, we proved $c_{G_{N-1}} = d_2$. Now we prove the second part of the statement. Let $D_{ij,N} = \{(y_1, y_2) \in \mathbb{R}^2 : -i \leq y_1 \leq N-1-i, -j \leq y_2 \leq N-1-j\}$. The number of coprime integers in $D_{ij,N}$ is $B_{D_{ij,N}}(1)$, moreover $B_{D_{ij,N}}(1) = B_{D_{ij,N}^*}((N-1)^2)$, where $D_{ij,N}^* = \{(y_1, y_2) \in \mathbb{R}^2 : -i/(N-1) \leq y_1 \leq 1-i/(N-1), -j/(N-1) \leq y_2 \leq 1-j/(N-1)\}$ belongs to \mathcal{D} . Hence, using [Lemma 3.6](#),

$$B_{D_{ij,N}^*}((N-1)^2) = \frac{6(N-1)^2}{\pi^2} + \epsilon_{ij,N}$$

with $|\epsilon_{ij,N}| \leq CN[1 + \log(N)]$ for every i and j . Hence,

$$\frac{\#E_{N-1}}{N^4} = \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} B_{D_{ij,N}}(1) = \frac{6(N-1)^2}{\pi^2} \frac{1}{N^2} + \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \frac{\epsilon_{ij,N}}{N^4}$$

and

$$\left| \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \frac{\epsilon_{ij,N}}{N^4} \right| \leq C \frac{1 + \log(N)}{N},$$

so that

$$\lim_N \frac{\#E_{N-1}}{N^4} = \frac{6}{\pi^2}. \quad \square$$

In order to prove [Theorem 3.4](#) we need some preliminary results. Let \mathbf{i} and \mathbf{j} be two vectors in \tilde{V}_L with $t_i < t_j$. We say that \mathbf{i} and \mathbf{j} are *adjacent* if

$$\{\mathbf{k} \in \tilde{V}_L : t_i < t_{\mathbf{k}} < t_j\} = \emptyset.$$

We say that a vertex $\mathbf{k} = (k_1, k_2) \in \mathcal{L}_N$ lies *inside the convex cone* defined by \mathbf{i} and \mathbf{j} if

$$(3.4) \quad t_i \leq \frac{k_2}{k_1} \leq t_j.$$

LEMMA 3.7. *Let $L \leq N$. Given two adjacent vectors \mathbf{i} and \mathbf{j} in \tilde{V}_L and a vector \mathbf{k} in \mathcal{L}_N that lies inside the convex cone defined by \mathbf{i} and \mathbf{j} , there are non-negative integers A and B such that*

$$\mathbf{k} = A\mathbf{i} + B\mathbf{j}.$$

Proof. Let $t_i = i_2/i_1 < j_2/j_1 = t_j$. Since t_i and t_j are consecutive in the Farey set \mathfrak{F}_L , by [\[33, Thm. 6.1\]](#) we have

$$(3.5) \quad i_1 j_2 - i_2 j_1 = 1.$$

The equation of the line r that is parallel to \mathbf{i} and passes through $\mathbf{k} = (k_1, k_2)$ is

$$y - k_2 = \frac{i_2}{i_1}(x - k_1).$$

The point (x_0, y_0) where r intersects $y = xj_2/j_1$ is

$$x_0 = \frac{i_1k_2 - i_2k_1}{i_1j_2 - i_2j_1}j_1, \quad y_0 = \frac{i_1k_2 - i_2k_1}{i_1j_2 - i_2j_1}j_2.$$

Let $B := \frac{i_1k_2 - i_2k_1}{i_1j_2 - i_2j_1}$. By (3.4) and (3.5) B is integer and nonnegative. In the same way, the intersection between the line that is parallel to \mathbf{j} and passes by \mathbf{k} , and the line $y = xi_2/i_1$, is a point

$$(x_1, y_1) = A(i_1, i_2), \quad \text{where } A = \frac{j_2k_1 - j_1k_2}{i_1j_2 - i_2j_1} \in \mathbb{N}.$$

We conclude that $\mathbf{k} = (x_1, y_1) + (x_0, y_0) = A\mathbf{i} + B\mathbf{j}$, with $A, B \in \mathbb{N}$. \square

LEMMA 3.8. *Let $L \in \mathbb{N}$ be fixed. Let*

$$\beta_k \text{ be the angle between } \mathbf{u}_k = \left(1, \frac{k}{L}\right) \text{ and } \mathbf{u}_{k+1} = \left(1, \frac{k+1}{L}\right),$$

for $k = 0, \dots, L-1$. Then

$$(3.6) \quad \cos(\beta_k) < \cos(\beta_{k+1}) \quad \text{for } k = 0, \dots, L-1.$$

Proof. A straightforward computation shows that

$$\cos(\beta_k) = \frac{\mathbf{u}_k \cdot \mathbf{u}_{k+1}}{\|\mathbf{u}_k\| \|\mathbf{u}_{k+1}\|} = \frac{L^2 + k(k+1)}{(L^2 + k^2)^{1/2}(L^2 + (k+1)^2)^{1/2}}.$$

Since $\frac{d}{dk} \cos(\beta_k) > 0$, we conclude that $\cos(\beta_k)$ is monotone increasing. \square

Proof. (Proof of Theorem 3.4) In order to prove the upper bound in (3.2), we first draw an estimate on a continuous approximation of Γ_{G_L, d_2} . Let

$$\mathbf{i} = (i_1, i_2), \quad \mathbf{j} = (j_1, j_2), \quad \mathbf{k} = x\mathbf{i} + y\mathbf{j}, \quad \text{with } i_1, i_2, j_1, j_2, x, y \in \mathbb{R}_+$$

and

$$|\mathbf{i}| = \sqrt{i_1^2 + i_2^2} = 1, \quad |\mathbf{j}| = \sqrt{j_1^2 + j_2^2} = 1.$$

A straightforward computation shows

$$\delta(x, y, \theta) := \frac{|\mathbf{k}|}{|x\mathbf{i}| + |y\mathbf{j}|} = \frac{\sqrt{x^2 + y^2 + 2xy\theta}}{x + y},$$

where $\theta := \mathbf{i} \cdot \mathbf{j} = i_1j_1 + i_2j_2$. For fixed x, y ,

the mapping $\theta \mapsto \delta(x, y, \theta)$ is a monotone increasing function

and, since $0 \leq \mathbf{i} \cdot \mathbf{j} \leq 1$, one immediately gets the bound

$$\frac{1}{\sqrt{2}} \leq \inf_{x, y \in \mathbb{R}_+} \frac{\sqrt{x^2 + y^2}}{x + y} = \inf_{x, y \in \mathbb{R}_+} \delta(x, y, 0) \leq \delta(x, y, 1) = 1.$$

On the other hand, for fixed $\theta \in (0, 1)$ we consider

$$f(x, y) = \delta^2(x, y, \theta) = 1 + \frac{2xy}{(x+y)^2}(\theta - 1).$$

Since

$$\nabla f(x, y) = 2 \frac{y-x}{(x+y)^3} (y, -x),$$

the line $y = x$ is a set of stationary points for f . Setting $\mathbf{v} = (-1, 1)/\sqrt{2}$, $P = (x, x)$,

$$f(P + t\mathbf{v}) = 1 + \frac{1-\theta}{2} \left(\frac{t^2}{2x^2} - 1 \right),$$

we see that $y = x$ is the set of global minimum points for f and thus for the mapping $(x, y) \mapsto \delta(x, y, \theta)$, with

$$(3.7) \quad \min_{x, y \in \mathbb{R}_+} \delta(x, y, \theta) = \sqrt{\frac{1+\theta}{2}}.$$

For $1 \leq L \leq N-1$, denote $\tilde{V}_L = \{\mathbf{v}_0, \mathbf{v}_1, \dots, \mathbf{v}_M\}$, indexed in increasing slope order (i.e., so that $t_{\mathbf{v}_0} < t_{\mathbf{v}_1} < \dots < t_{\mathbf{v}_M}$), and let α_k be the angle between \mathbf{v}_k and \mathbf{v}_{k+1} . By [Lemma 3.7](#) for all $\mathbf{k} \in \mathcal{L}_N$ there exist two adjacent vectors $\mathbf{v}_k, \mathbf{v}_{k+1}$ and two integers $A, B \in \mathbb{N}$ such that $\mathbf{k} = A\mathbf{v}_k + B\mathbf{v}_{k+1}$, and therefore, by [\(3.7\)](#)

$$(3.8) \quad \frac{|\mathbf{k}|}{|A\mathbf{v}_k| + |B\mathbf{v}_{k+1}|} \geq \sqrt{\frac{1 + \cos(\alpha_k)}{2}}.$$

We estimate

$$(3.9) \quad \begin{aligned} \Lambda_L &:= \min \left\{ \frac{d_2(\mathbf{i}, \mathbf{j})}{c_{G_L}(\mathbf{i}, \mathbf{j})} : \mathbf{i}, \mathbf{j} \in \mathcal{L}_N, \mathbf{i} \neq \mathbf{j} \right\} \\ &= \min \left\{ \frac{d_2(\mathbf{0}, \mathbf{k})}{c_{G_L}(\mathbf{0}, \mathbf{k})} : \mathbf{k} \in \mathcal{L}_N, \mathbf{k} \neq \mathbf{0} \right\} \\ &= \min_{\mathbf{k} \in \mathcal{L}_N, \mathbf{k} \neq \mathbf{0}} \max \left\{ \frac{|\mathbf{k}|}{|A\mathbf{i}| + |B\mathbf{j}|} : A\mathbf{i} + B\mathbf{j} = \mathbf{k}, \mathbf{i}, \mathbf{j} \in V_L, A, B \in \mathbb{N} \right\} \\ &\stackrel{(3.8)}{\geq} \min_{k=0, \dots, M} \sqrt{\frac{1 + \cos(\alpha_k)}{2}}. \end{aligned}$$

Let

$$\mathbf{U}_L := \left\{ \mathbf{u}_j = \left(1, \frac{j}{L} \right), j = 0, \dots, L-1 \right\}, \quad \mathbf{V}_L := \left\{ \mathbf{v}_k = (1, t_{\mathbf{v}_k}), \mathbf{v}_k \in \tilde{V}_L \right\}.$$

Clearly $\mathbf{U}_L \subseteq \mathbf{V}_L$, since the slopes $t_{\mathbf{v}_k}$ include all elements in the Farey sequences $\mathfrak{F}_1, \dots, \mathfrak{F}_L$. Define the sets of angles

$$\mathcal{A} := \{ \alpha_k = \widehat{\mathbf{v}_k \mathbf{v}_{k+1}} : \mathbf{v}_k \in \mathbf{V}_L \}, \quad \mathcal{B} := \{ \beta_j = \widehat{\mathbf{u}_j \mathbf{u}_{j+1}} : \mathbf{u}_j \in \mathbf{U}_L \}.$$

Since the partitioning of $\pi/4$ induced by \mathbf{V}_L is finer than that of \mathbf{U}_L

$$\max \{ \alpha_k : \alpha_k \in \mathcal{A} \} \leq \max \{ \beta_j : \beta_j \in \mathcal{B} \}.$$

Since the cosine function is monotone decreasing in $[0, \pi/4]$, from [\(3.9\)](#) we obtain

$$\begin{aligned} \Lambda_L &\geq \min_{k=0, \dots, M} \sqrt{\frac{1 + \cos(\alpha_k)}{2}} \geq \min_{j=0, \dots, L-1} \sqrt{\frac{1 + \cos(\beta_j)}{2}} \\ &\stackrel{(3.6)}{=} \sqrt{\frac{1 + \cos(\beta_0)}{2}} = \sqrt{\frac{1}{2} + \frac{L}{2\sqrt{1+L^2}}}, \end{aligned}$$

which thus implies

$$\Gamma_{G_L, d_2} = 1 - \Lambda_L \leq 1 - \sqrt{\frac{1}{2} + \frac{L}{2\sqrt{1+L^2}}}.$$

The upper bound in (3.2) then follows by a simple algebraic manipulation, setting

$$c(L) := \left(2 + \sqrt{2 + \frac{2L}{\sqrt{1+L^2}}} \right)^{-1}.$$

In order to find the lower bound in (3.2), by Proposition 4.3, it is enough to evaluate the error $\mathcal{E}_G(b)$ for a specific choice of $b = \mu - \nu$. We choose as μ a unit mass concentrated in $\mathbf{i} = (L, 0)$, as ν a unit mass concentrated in $\mathbf{j} = (L, 1)$, under the assumption that $N \geq 2L$. A simple computation yields

$$\mathbf{k} := \mathbf{i} + \mathbf{j} = (2L, 1), \quad |\mathbf{k}| = \sqrt{4L^2 + 1}, \quad \frac{|\mathbf{k}|}{|\mathbf{i}| + |\mathbf{j}|} = \frac{\sqrt{4L^2 + 1}}{L + \sqrt{L^2 + 1}},$$

and therefore

$$\mathcal{E}_G(b) = 1 - \frac{\sqrt{4L^2 + 1}}{L + \sqrt{L^2 + 1}}.$$

Finally, in order to estimate the asymptotic behaviour in (3.3), we compute the power expansions

$$\begin{aligned} 1 - \frac{\sqrt{4L^2 + 1}}{L + \sqrt{L^2 + 1}} &= \frac{1}{8L^2} - \frac{11}{128L^4} + \frac{61}{1024L^6} + O\left(\frac{1}{L^8}\right) \quad \text{for } L \rightarrow +\infty, \\ c(L) \left(1 - \frac{L}{\sqrt{1+L^2}}\right) &= \frac{1}{8L^2} - \frac{11}{128L^4} + \frac{69}{1024L^6} + O\left(\frac{1}{L^8}\right) \quad \text{for } L \rightarrow +\infty. \quad \square \end{aligned}$$

Since the expansions are identical up to the $1/L^4$ term, owing to (3.2), we conclude (3.3).

4. Minimum flow on reduced graphs: general theory. In this section we give all the details of the results presented in subsection 2.3-subsection 2.5.

4.1. Dual formulation of a minimum flow problem. In what follows we need some basic results on the dual formulation of the minimum flow problem (2.8). Letting

$$\mathcal{D}(G, b) := \{\varphi : V \rightarrow \mathbb{R} : \varphi(u) - \varphi(v) \leq c(u, v) \forall (u, v) \in E\},$$

the dual problem corresponding to (2.8) is

$$\max_{\varphi \in \mathcal{D}(G, b)} \sum_{u \in V} b(u)\varphi(u).$$

The *Strong Duality theorem* (see e.g. Thm. 9.6 in [1]) states that

$$\max_{\varphi \in \mathcal{D}(G, b)} \sum_{u \in V} b(u)\varphi(u) = \min_{f \in \mathcal{F}(G, b)} \sum_{(u, v) \in E} c(u, v)f(u, v).$$

Moreover, the so-called *Complementary Slackness Optimality Conditions* ensure that if a b -flow is optimal for (G, c) , then there exists a potential φ in $\mathcal{D}(G, b)$ such that $\varphi(u) - \varphi(v) = c(u, v)$ whenever $f(u, v) > 0$. Conversely, if f is a b -flow and there is a potential φ in $\mathcal{D}(G, b)$ such that $\varphi(u) - \varphi(v) = c(u, v)$ whenever $f(u, v) > 0$, and that $f(u, v) = 0$ if $\varphi(u) - \varphi(v) < c(u, v)$, then f and φ are optimal solutions for the primal/dual problem. See e.g. Theorems 9.4 and 9.8 in [1].

4.2. Flows on Reduced Graphs. Assuming that $X = Y$, in place of considering the flow problem on a graph with nodes $X \cup Y$, we start by considering a flow problem for $b = \mu - \nu$ on the “reduced” set of nodes $V = X$. Assuming that $\mu(x) > 0$ and $\nu(x) > 0$ for all $x \in X$, the set of nodes in this problem has cardinality n while in $G_{X \rightarrow Y}$ has cardinality $2n$, where $n = |X|$. For the reduced graph with nodes set X , we choose, as a set of edges, the set of all possible directed links on X , that is $G = K_n$, K_n being the complete (directed) graph on X (without self-loops). Although this choice still considers a large number of edges (more precisely $n(n-1)$) it will be useful in the sequel.

The next proposition summarizes some simple relations between the above defined problems.

PROPOSITION 4.1. *Let μ and ν be two probability vectors on X and $b := \mu - \nu$. (a) If $c(x, x) = 0$ for every $x \in X$, then*

$$\mathcal{W}_c(\mu, \nu) \geq F_{K_n, c}(b).$$

(b) *If, in addition, $c(x, y) \leq c(x, z) + c(z, y)$ for every x, y, z in X , then*

$$\mathcal{W}_c(\mu, \nu) = F_{K_n, c}(b).$$

In order to prove (a) and (b), we introduce an auxiliary bipartite graph with set of nodes $V_b := S_b \cup D_b \subset X$, where $S_b := \{x : b(x) > 0\}$ and $D_b := \{x : b(x) < 0\}$, and set of edges $E_b := \{(x, y) \in S_b \times D_b\}$. Denoting by G_b the bipartite graph (V_b, E_b) , the corresponding minimum cost flow problem can be rewritten as

$$F_{G_b, c}(b) := \min_{f \in \mathcal{F}(G_b, b)} \sum_{x \in S_b, y \in D_b} c(x, y) f(x, y).$$

The cardinality of E_b is $a^+ a^- n^2$, where a^\pm is the fraction of vertexes x with $b(x) > 0$, $b(x) < 0$ respectively, hence $a^+ a^- < 1$, while the set of edges $E_{X \rightarrow X}$ has cardinality n^2 .

The next Lemma specifies the relations between $F_{G_b, c}(b)$, the minimum of the cost flow problem $F_{K_n, c}(b)$, and the inf of Kantorovich’s transportation problem $\mathcal{W}_c(\mu, \nu)$.

LEMMA 4.2. *Let $b : X \rightarrow \mathbb{R}$ be any function.*

(i) *If $c(x, x) = 0$ for every $x \in X$, then $F_{G_b, c}(b) \geq F_{K_n, c}(b)$ and, for $b = \mu - \nu$,*

$$F_{G_b, c}(b) \geq \mathcal{W}_c(\mu, \nu).$$

(ii) *If, in addition, $c(x, y) \leq c(x, z) + c(z, y)$ for every x, y, z in X , then*

$$F_{G_b, c}(b) = F_{K_n, c}(b).$$

Proof. (i) Since $G_b \subset K_n$, (2.9) implies that $F_{G_b, c}(b) \geq F_{K_n, c}(b)$. If $f \in \mathcal{F}(G_b, c)$ with $b = \mu - \nu$, set

$$\pi(x, x) = \min(\mu(x), \nu(x)),$$

and, if $x \in S_b$ and $y \in D_b$,

$$\pi(x, y) = f(x, y).$$

Finally, define $\pi(x, y) = 0$ in all the remaining cases. It is easy to check that such a π belongs to $\Pi(\mu, \nu)$ and again the inequality follows.

(ii) Let \bar{f} be an optimal b -flow for (K_n, c) . For x in S_b and y in D_b let $\Gamma(x, y)$ be the set of directed paths in K_n from x to y with no loops; for any γ in $\Gamma(x, y)$ of

length $|\gamma| = t$ let $\bar{f}(\gamma) = \min\{\bar{f}(\gamma_1), \dots, \bar{f}(\gamma_t)\}$ be the flow through γ from x to y . The total flow from x to y can then be defined by

$$f^*(x, y) := \sum_{\gamma \in \Gamma(x, y)} f(\gamma).$$

Doing this for any (x, y) in E_b , it is easy to see that the resulting f^* is a b -flow in G_b . By the Complementary Slackness Conditions, since \bar{f} is an optimal b -flow for (K_n, c) , then there is φ in $\mathcal{D}_{K_n, b}$ such that $\varphi(u) - \varphi(v) = c(u, v)$ whenever $\bar{f}(u, v) > 0$. Now let x in S_b and y in D_b and γ in $\Gamma(x, y)$ with $\bar{f}(\gamma) > 0$. Since it must be that $\bar{f}(\gamma_i, \gamma_{i+1}) > 0$ for $i = 1, \dots, |\gamma| - 1$, it follows that $\varphi(\gamma_i) - \varphi(\gamma_{i+1}) = c(\gamma_i, \gamma_{i+1})$. Hence,

$$c(x, y) \geq \varphi(x) - \varphi(y) = \sum_{i=1}^{|\gamma|-1} \varphi(\gamma_i) - \varphi(\gamma_{i+1}) = \sum_{i=1}^{|\gamma|-1} c(\gamma_i, \gamma_{i+1}) \geq c(x, y), \quad \square$$

where the last inequality follows by triangle inequality. Summarizing, we have proved that $c(x, y) = \varphi(x) - \varphi(y)$ if $f^*(x, y) > 0$. Conversely, if $c(x, y) > \varphi(x) - \varphi(y)$, then necessarily $f^*(x, y) = 0$. Since clearly φ belongs to $\mathcal{D}(G_b, c)$, then f^* and φ are optimal primal/dual solutions for (G_b, c) by the Slackness Conditions. Using the Strong Duality theorem we conclude that $F_{K_n, c}(b) = \sum_{v \in X} \varphi(v)b(v) = F_{G_b, c}(b)$.

Proof. (Proof of [Proposition 4.1](#).) (a) In order to prove that $\mathcal{W}_c(\mu, \nu) \geq F_{K_n, c}(\mu - \nu)$, note that if $\pi \in \Pi(\mu, \nu)$ then $f(x, y) := \pi(x, y)$ for $x \neq y$ belongs to $\mathcal{F}(K_n, b)$ for $b = \mu - \nu$. Since $c(x, x) = 0$ the inequality follows.

(b) Let $b = \mu - \nu$. By [Lemma 4.2](#)-(i) and part (a), we have that

$$(4.1) \quad F_{G_b, c}(\mu - \nu) \geq \mathcal{W}_c(\mu, \nu) \geq F_{K_n, c}(\mu - \nu).$$

On the other hand, by [Lemma 4.2](#)-(ii),

$$(4.2) \quad F_{G_b, c}(\mu - \nu) = F_{K_n, c}(\mu - \nu).$$

Combining (4.1) and (4.2) immediately yields

$$\mathcal{W}_c(\mu, \nu) = F_{K_n, c}(\mu - \nu). \quad \square$$

The previous result shows that one can compute the EMD between two normalized measures μ and ν (with respect to some ground distance $c = d$) by solving the minimum cost flow problem $F_{G_b, d}(\mu - \nu)$.

Although G_b is smaller than $G_{X \rightarrow X}$, the problem of determining $F_{G_b, d}(b)$ is computationally demanding for relatively small n . Using the previous considerations on the computational cost of a minimum flow problem, it is easy to see that the time complexity of computing $F_{G_b, d}(b)$ is $O(n^3 \log(n))$ and hence it is of the same order of the complexity of computing $F_{G_{X \rightarrow Y}, d}(b)$.

4.3. Error Bounds. In this Section we prove the universal upper bound (2.14), i.e. a bound on $\mathcal{E}_G(b)$ which depends only on the geometry of (G, c) and not on the specific b .

First of all, note that if c is a distance, then c_G (defined in (2.13)) is a distance, and, since $G \subseteq K_n$,

$$(4.3) \quad c_G(x, y) \geq c(x, y) \quad \forall x, y \in V.$$

Denote by $\gamma^{(x,y)}$ any optimal path in G connecting x to y , that is, any path such that

$$\sum_{i=0}^{|\gamma^{(x,y)}|-1} c\left(\gamma_i^{(x,y)}, \gamma_{i+1}^{(x,y)}\right) \leq \sum_{i=0}^{|\gamma|-1} c(\gamma_i, \gamma_{i+1})$$

for any path γ in G from x to y . Then

$$c_G(x, y) = \sum_{i=0}^{|\gamma^{(x,y)}|-1} c\left(\gamma_i^{(x,y)}, \gamma_{i+1}^{(x,y)}\right).$$

Note that clearly $\gamma^{(x,y)}$ need not be unique. The constant

$$\Gamma_{G,c} := \max \left\{ 1 - \frac{c(x, y)}{c_G(x, y)} : (x, y) \in X^2, x \neq y \right\}$$

provides the bound we are looking for.

PROPOSITION 4.3. *If c is a distance, then for every $b : X \rightarrow \mathbb{R}$*

$$0 \leq \mathcal{E}_G(b) \leq \Gamma_{G,c}.$$

Proof. Clearly, it suffices to prove that $F_{G,c}(b) - F_{K_n,c}(b) \leq \Gamma_{G,c}F_{G,c}(b)$, i.e.,

$$(1 - \Gamma_{G,c})F_{G,c}(b) \leq F_{K_n,c}(b).$$

First of all, we notice that by definition of $\Gamma_{G,c}$

$$c_G(x, y) - c(x, y) = \left(1 - \frac{c(x, y)}{c_G(x, y)}\right) c_G(x, y) \leq \Gamma_{G,c} c_G(x, y),$$

and therefore

$$(4.4) \quad (1 - \Gamma_{G,c})c_G(x, y) \leq c(x, y).$$

Let E be the set of edges of G , for every $(x, y) \notin E$, let $\gamma^{(x,y)}$ be an optimal path (with no loops) in G . Now let $f \in \mathcal{F}(K_n, b)$, then

$$\begin{aligned} \sum_{x \neq y} f(x, y)c(x, y) &= \sum_{(\alpha, \beta) \in E} f(\alpha, \beta)c(\alpha, \beta) + \sum_{(x, y) \notin E} f(x, y)c(x, y) \\ &\geq \sum_{(\alpha, \beta) \in E} f(\alpha, \beta)c(\alpha, \beta) \\ &\quad + \sum_{(x, y) \notin E} f(x, y)(1 - \Gamma_{G,c}) \sum_{i=0}^{|\gamma^{(x,y)}|-1} c\left(\gamma_i^{(x,y)}, \gamma_{i+1}^{(x,y)}\right) \\ &= \sum_{(\alpha, \beta) \in E} \left[f(\alpha, \beta) + (1 - \Gamma_{G,c}) \sum_{(x, y) \notin E: (\alpha, \beta) \in \gamma^{(x,y)}} f(x, y) \right] c(\alpha, \beta) \\ &\geq (1 - \Gamma_{G,c}) \sum_{(\alpha, \beta) \in E} \left[f(\alpha, \beta) + \sum_{(x, y) \notin E: (\alpha, \beta) \in \gamma^{(x,y)}} f(x, y) \right] c(\alpha, \beta), \end{aligned}$$

where we used also (4.4) and that, by (4.3), $\Gamma_{G,c} \geq 0$. Letting

$$f'(\alpha, \beta) = \begin{cases} 0 & \text{if } (\alpha, \beta) \notin E \\ f(\alpha, \beta) + \sum_{(x,y) \notin E: (\alpha, \beta) \in \gamma(x,y)} f(x, y) & \text{if } (\alpha, \beta) \in E, \end{cases}$$

one can rewrite the previous inequality as

$$\sum_{x \neq y} f(x, y)c(x, y) \geq (1 - \Gamma_{G,c}) \sum_{(x,y) \in E} f'(x, y)c(x, y).$$

To conclude, one checks that f' belongs to $\mathcal{F}(G, b)$, and hence

$$\sum_{x \neq y} f(x, y)c(x, y) \geq (1 - \Gamma_{G,c})F_{G,c}(b). \quad \square$$

5. Numerical experiments. In this section, we report the results of our numerical experiments. The goal of our experiments is to address the following research questions:

1. Which is the most efficient Minimum Cost Flow algorithm from those available in the literature, considering that our instances of optimal transport have a specific geometric cost function?
2. How fast can we exactly compute the Wasserstein distance of order 1 as a function of the ground distance and as a function of the 2D histogram size?
3. How tight is in practice the bound given in Theorem 3.4 as a function of the parameter L ?
4. How does our approach compare with other state-of-the-art algorithms?

In order to answer these questions we have run several experiments using the Discrete Optimal Transport Benchmark (DOTmark) [41], which has 10 classes of grey scale images related to randomly generated images, classical images, and real data from microscopy images of mitochondria. In each class there are 10 different grey scale images. Every image is given at the following pixel resolutions: 32×32 , 64×64 , 128×128 , 256×256 , and 512×512 . Table 1 show the *Classical* and the *Microscopy* images, respectively.

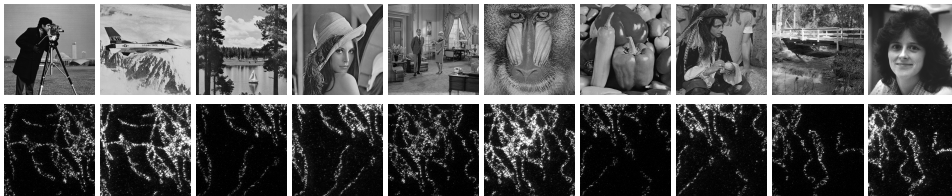


TABLE 1
Classical images and Microscopy images of mitochondria.

Implementation details. We run our experiments using the Network Simplex as implemented in the Lemon C++ graph library¹. The tests were executed on a Dell workstation equipped with an Intel Xeon W-2155 CPU working at 3.3 GHz and with 32 GB of RAM. All the code was compiled with the Microsoft Visual Studio 2017 compiler. Our C++ code is freely available at <https://github.com/stegua/dotlib>.

¹<http://lemon.cs.elte.hu> (last visited on May, 2nd, 2019)

5.1. Comparison of Minimum Cost Flow Algorithms. As a first step, we run a set of experiments to select the fastest min cost flow algorithm for our geometric optimal transportation instances. We considered the following codes:

1. **EMD**: is the exact solver described in [37], based on an implementation (in ANSI-C) of the transportation simplex method, as described in [22].
2. We test three different linear programming algorithms implemented in the commercial solver Gurobi v8.1: **Primal Simplex**, **Dual Simplex**, and **Barrier**. The barrier algorithm is the only parallel algorithms able to exploit the 10 physical cores of our CPU.
3. We test three implementations of Minimum Cost Flow algorithms implemented in the Lemon Graph Library, corresponding to three different combinatorial algorithms: **Cycle Cancelling** [20], **Cost Scaling** [19, 10], and the **Network Simplex** [15]. For a deeper and more general comparison with other implementations among combinatorial algorithms, we refer to [27].

Figure 4 shows the results of our numerical tests. For each method, we compute the distance between any pair of images belonging to the *Classic* class (see Figure 1), with size 32×32 , for a total of 45 problem instances. As ground distance, we use the Euclidean distance, and we solve the corresponding problem defined on a complete bipartite graph, that is the formulation used by the EMD algorithm.

The Network Simplex as implemented in the Lemon Graph library is clearly the fastest exact algorithm, and is able to solve every instance within a small fraction of a second. For this reason, in all our other numerical tests, we use that implementation.

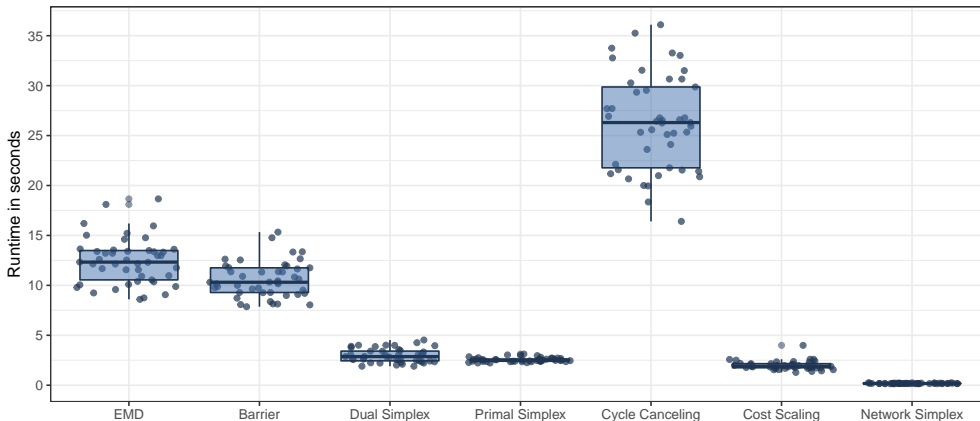


FIG. 4. Comparison of different algorithms for solving the Minimum Cost Flow problem. Each single (jittered) dot gives the running time of computing the distance between a pair of images with the corresponding algorithm.

5.2. Exact distance computations. As second step, we have compared the running times of the flow models proposed in this paper computing the exact Wasserstein distance of order 1 using the d_1 , d_∞ and d_2 ground distances.

First, we compare the running times for solving the models proposed in section 3, with the running times of solving the equivalent problems formulated on bipartite graphs. Both type of problems are solved with the very efficient implementation of the Network Simplex algorithm provided by the Lemon Graph library. Figure 5 shows the boxplots that summarize our results on the classical images of size 64×64 . While

the bipartite graphs are all of the same size, the problems defined with the d_1 distance seem to be simpler, and those with the d_2 distance look slightly harder. By using our reduced network flow models, we get a speedup of two orders of magnitude for d_1 and d_∞ : this is due to the significant reduction of the number of arcs. We recall that the bipartite graphs have $O(n^2)$ arcs, where $n = 64 \times 64$, while our equivalent models have only $O(n)$ arcs. However, for the d_2 distance, the speedup is still present but more modest. In this case, our models have $O(\frac{6}{\pi^2}n^2)$ arcs, against the $O(n^2)$ of the bipartite graphs. In order to get obtain a more significant speedup while controlling the error for the d_2 distance, we have numerically evaluated our approximation scheme, as discussed in the next subsection.

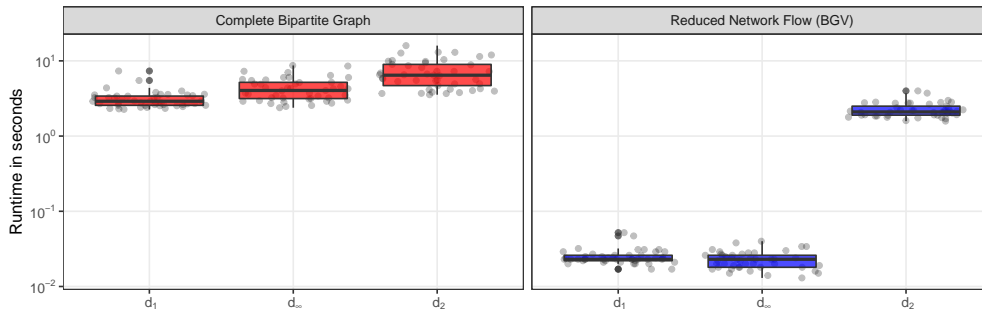


FIG. 5. Running times of solving the same transportation instances on bipartite graphs versus using our reduced flow networks for classical images of size 64×64 .

Once we have completely abandoned the bipartite model, we have run a large set of tests using images of size up to 512×512 with the three different types of ground distances. Table 2 shows aggregate data elaborated from our results. For each combination of image size and ground distance, the table gives the size of the flow network in terms of number of nodes $|V|$ and number of arcs $|A|$. Regarding the running times (in seconds), the same table reports the average, the standard deviation, and the maximum runtime over 450 tests (45 for each of the 10 class of images).

From Table 2, it is clear that the true challenge is to compute the Wasserstein distances using the d_2 ground distance, since with the d_1 and d_∞ ground distances we can solve all the images in at most 1000 seconds (though, in average, it takes 2 or 3 minutes), while with the d_2 ground distance we cannot even solve the instances of size 256×256 , since the code runs out of memory.

5.3. Approximation error \mathcal{W}_{d_2} : Theory vs. Practice. In this section, we present the numerical results on the error obtained in practice when we compute the Wasserstein distance of order 1 with our approximation scheme. The results are presented for the images of size 32×32 , 64×64 and 128×128 , for which we can compute both the exact distance using F_{G_{N-1},d_2} and the approximate distance using F_{G_L,d_2} , with L ranging in the set $\{2, 3, 5, 10\}$.

We measure the relative percentage error, denoted by \mathcal{E}_{G_L} , as the following ratio:

$$\mathcal{E}_{G_L} := \frac{F_{G_L,d_2} - F_{G_{N-1},d_2}}{F_{G_L,d_2}},$$

where F_{G_{N-1},d_2} is equal to the optimal Wasserstein distance, and F_{G_L,d_2} is the value

Image size $N \times N$	Graph size $ V $	Ground distance $ A $	Running times (sec)			
			Average	StdDev	Maximum	
32×32	1024	3968	d_1	0.002	0.001	0.009
		7812	d_∞	0.002	0.001	0.009
		638692	d_2	0.075	0.016	0.154
64×64	4096	16128	d_1	0.023	0.008	0.059
		32004	d_∞	0.024	0.006	0.053
		10205236	d_2	2.011	0.573	4.401
128×128	16384	65024	d_1	0.35	0.13	0.82
		129540	d_∞	0.32	0.08	0.63
		163207372	d_2	57.73	20.17	146.33
256×256	65536	261120	d_1	6.7	3.0	23.7
		521220	d_∞	5.5	1.7	12.9
		<i>out of memory</i>	d_2	-	-	-
512×512	262144	1046528	d_1	182.4	100.5	1056.5
		2091012	d_∞	139.6	58.3	405.0
		<i>out of memory</i>	d_2	-	-	-

TABLE 2

Running times (in seconds) to compute exact Wasserstein distances. Each row gives the average, standard deviation, and maximum time over 450 instances.

of our approximation obtained by solving the uncapacitated min cost flow problem on the network built according to the parameter L . Our goal is to compare the values of \mathcal{E}_{G_L} with the upper bound $\bar{\Gamma}_{G_L}$ predicted by [Theorem 3.4](#), that is

$$\bar{\Gamma}_{G_L} := 1 - \sqrt{\frac{1}{2} + \frac{L}{2\sqrt{1+L^2}}} \geq \mathcal{E}_{G_L}.$$

[Table 3](#) reports the results for the images of size 32×32 , 64×64 and 128×128 . The columns specify, in order, the image size, the value of the parameter L , the cardinality of the arc set E_L , the average runtime in seconds, the upper bound $\bar{\Gamma}_{G_L}$ guaranteed by [Theorem 3.4](#), the empirical average of the errors \mathcal{E}_{G_L} obtained in practice, and the maximum of such errors. Note that while from [Theorem 3.4](#) in order to get an error smaller than 1% we should use at least $L = 5$, in practice, we get on average such small errors already by using $L = 3$. Indeed, we can set the value of parameter L in such a way to achieve the desired trade off between numerical precision in computing the Wasserstein distances and the running time we accept to wait. [Table 4](#) details the maximum error \mathcal{E}_{G_L} obtained for each class of images. This shows that in practice a better trade off between the numerical precision of the distance and the running time can be obtained by considering the type of 2D histograms of interest.

Motivated by the results shown in [Table 3](#), we measured how our approximation scheme scales for increasing image sizes, using $L \in \{2, 3, 5, 10\}$ and by restricting our test to the Cauchy images, since they are those with the larger error for $L = 5$ and $L = 10$. For each combination of image size and value of L , [Table 5](#) reports the graph size and the basic statistics on the running time along the same line of the previous tables: average running time along with the respective standard deviations, and maximum running times.

Size	Parameter	$ E_L $	Runtime	$\bar{\Gamma}_{G_L}$	$\text{mean}\{\mathcal{E}_{G_L}\}$	$\text{max}\{\mathcal{E}_{G_L}\}$
128×128	$L = 2$	257 556	0.446	2.675%	1.291%	2.646%
	$L = 3$	510 556	0.748	1.291%	0.463%	1.153%
	$L = 5$	1 254 508	1.153	0.486%	0.121%	0.447%
	$L = 10$	16 117 244	2.424	0.124%	0.019%	0.109%
(exact)	$L = 127$	163 207 372	57.729			

TABLE 3

Bound errors: Theory vs. Practice. Each row gives the averages over 450 instances.

Class	Maximum Bound percentage error \mathcal{E}_{G_L}			
	L=2	L=3	L=5	L=10
CauchyDensity	2.576%	1.147%	0.447%	0.109%
ClassicImages	1.813%	0.716%	0.246%	0.053%
GRFmoderate	2.365%	0.937%	0.348%	0.065%
GRFrough	1.918%	0.780%	0.279%	0.039%
GRFsmooth	2.248%	1.069%	0.338%	0.068%
LogGRF	2.546%	1.019%	0.370%	0.076%
LogitGRF	2.332%	1.104%	0.258%	0.067%
MicroscopyImages	2.069%	0.900%	0.272%	0.045%
Shapes	2.670%	1.168%	0.317%	0.094%
WhiteNoise	0.908%	0.243%	0.043%	0.005%
$\bar{\Gamma}_{G_L}$	2.675%	1.168%	0.447%	0.109%

TABLE 4

Maximum bound errors for each class of images in the benchmark. Each row gives the maximum over 135 instances, for size $N = 32 \times 32, 64 \times 64, 128 \times 128$.

Image size $N \times N$	Param L	Graph size		Running times (sec)		
		$ V $	$ E_L $	Average	StdDev	Maximum
256×256	2	65 536	1 039 380	8.6	2.5	14.8
	3		2 069 596	8.7	2.7	20.9
	5		5 129 836	12.9	1.3	16.8
	10		16 117 244	24.6	4.7	35.3
512×512	2	262 144	4 175 892	170.8	97.2	487.5
	3		8 333 404	148.0	70.6	361.6
	5		20 744 812	171.9	29.7	236.3
	10		65 782 268	471.5	139.4	950.6

TABLE 5

Attacking larger Cauchy images with d_2 ground distance and parameter $L \in \{2, 3, 5, 10\}$. Each row gives the averages over 45 instances.

5.4. Comparison with other approaches. We compare our solution method with other two approaches: the first is the algorithm proposed in [29] for the special case using the Manhattan as ground distance. The second approach is the (heuristic, with no guarantees) improved Sinkhorn’s algorithm [13] as implemented in [40].

Manhattan ground distance [29]. Figure 6 shows the comparison of running time in seconds of our method with the algorithm proposed in [29]. The results refer to the

running time for computing the distances between the 45 possible pairs of classical images, at resolution ranging from 32×32 up to 512×512 . Since both methods are exact, the distance value is always the same (indeed, it is the optimum). Note that apart from the very small case of size 32×32 , our approach is always faster, with the difference increasing for the larger dimensions. While the two methods are using the same network flow model, they are using different solution algorithms: from these results, we can conclude that the Network Simplex implemented in [27] is faster than the implementation of combinatorial algorithm provided by the authors of [29], despite the fact that it has a lower worst-case time complexity.

Sinkhorn’s algorithm [40]. Figure 5 shows the result of comparing the stabilized Sinkhorn’s algorithm described in [40], with our approximation scheme for the Euclidean ground distance described in section 3. We remark that the Sinkhorn’s algorithm, differently from our approach, is a heuristic method and it does not have any guarantee on the optimality gap of the solution it computes. The results refer to the classical images of size 32×32 , 64×64 , and 128×128 . The exact solutions are computed using our approximation scheme with $L = N - 1$. For our approximation approach, we used the values $L \in \{2, 3, 5, 10\}$. As expected, the running time grows with increasing values of L and with increasing size of the images (note the log scale on the vertical axis). Our approach, is not only always faster, but, given the same value of empirical optimality gap, it can be two orders of magnitude faster. In addition, we remark that the Network Simplex runs in a single thread, while the implementation of the Sinkhorn’s algorithm we use runs in parallel on 20 threads.

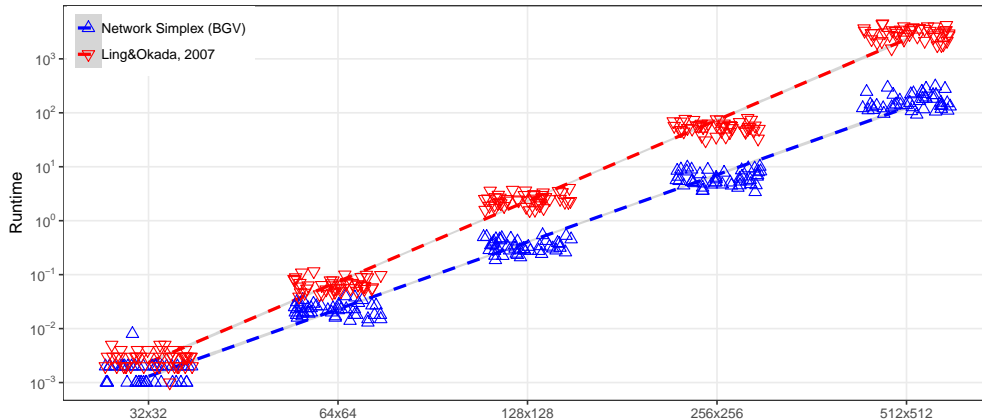


FIG. 6. Comparison of runtime between the algorithm proposed in [29] and our approach based on the Network Simplex algorithm using the Classical images.

6. Conclusion. Comparing two histograms, or establishing which histograms, in a given set, are more alike, is the crucial question in a number of applications with industrial and scientific scope. The staggering availability of data coming, e.g., from the Internet or from biological sampling and imaging, is undoubtedly encouraging the digitalization of data measures (e.g., images), while, at the same time, requiring a computational effort that, as of today, may not be within reach of modern workstations.

Motivated by these considerations, in this article we have addressed the problem of rapidly computing the Kantorovich distance (also known as Wasserstein distance of

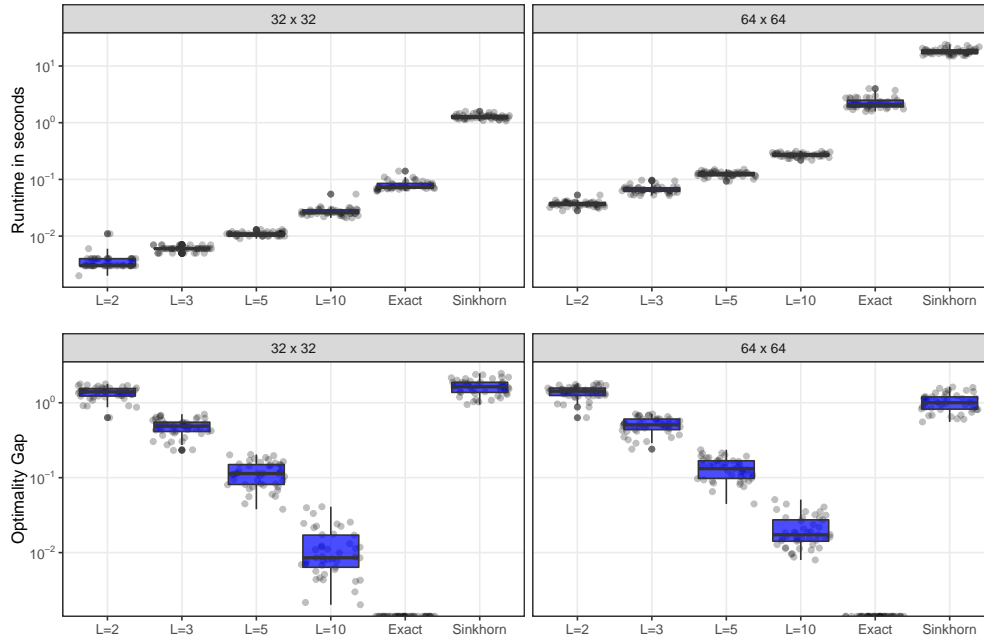


FIG. 7. Comparison of runtime and optimality gap between the Sinkhorn’s algorithm [13] as implemented in [40], and our approximation scheme discussed in section 3, using the Classical images of size 32×32 and 64×64 , with $L \in \{2, 3, 5, 10\}$ (approximate) and $L = N - 1$ (exact).

order 1) between 2D histograms. In our approach, we translate the original discrete optimal transportation problem (2.1) to an uncapacitated minimum cost flow problem on a directed graph (2.7). In section 4 we prove that the two problems are equivalent when the Kantorovich cost c is a distance.

The key observation is that, by reducing the size of the graph in the minimum cost flow, one can approximate the Kantorovich solution at a lower computational cost. Precisely, when the cost c is the *taxicab* or the *maximum* distance, we are able to compute the optimal solution on a reduced flow network of size $O(n)$, where N is number of pixels in the images, i.e., bins of a histogram. When the cost c is the Euclidean distance, the size of the network that yields the exact optimal solution is $O(\frac{6}{\pi^2}n^2)$. Our main contribution, in the Euclidean distance case, is that for any given error $\varepsilon > 0$ we can provide a reduced network of size $O(n)$ that yields an approximate solution, which is at most ε away from the exact one. With our approximation method we were able to compute the distance between 512×512 images, with an error lower than 0.12%, in less than 20 minutes.

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