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LOCAL MATCHING INDICATORS FOR TRANSPORT PROBLEMS WITH CONCAVE COSTS

JULIE DELON, JULIEN SALOMON, AND ANDREĀ SOBOLEVSKIĀ

ABSTRACT. In this paper, we introduce a class of local indicators that enable to compute efficiently optimal transport plans associated to arbitrary weighted distributions of N demands and M supplies in \mathbb{R} in the case where the cost function is concave. Indeed, whereas this problem can be solved linearly when the cost is a convex function of the distance on the line (or more generally when the cost matrix between points is a Monge matrix), to the best of our knowledge, no simple solution has been proposed for concave costs, which are more realistic in many applications, especially in economic situations. The problem we consider may be unbalanced, in the sense that the weight of all the supplies might be larger than the weight of all the demands. The local indicators, which can be used hierarchically to solve the transportation problem for concave costs on the line, also reveal the “hidden convexity” of this problem.

1. INTRODUCTION

The origins of optimal transportation go back to the late eighteen century, when Monge [16] published his *Mémoire sur la théorie des déblais et des remblais* (1781). The problem, which was rediscovered and further studied by Kantorovich in the 1940’s, can be described in the following way. Given two probability distributions μ and ν on X and c a measurable cost function on $X \times X$, find a joint probability measure π on $X \times X$ with marginals μ and ν and which minimizes the transportation cost

$$(1) \quad \int \int_{X \times X} c(x, y) d\pi(x, y).$$

Probability measures π with marginals μ and ν are called *transport plans*. A transport plan that minimizes the cost (1) is said to be *optimal*.

When the measures μ and ν are discrete (linear combinations of Dirac masses), the problem can be recast as finite linear programming. For $N \geq 1$, consider two discrete distributions of mass, or *histograms*, given on \mathbb{R}^N : $\{(p_i, s_i)\}$, which represents “supplies” at locations p_i with weights s_i and $\{(q_j, d_j)\}$, which represents “demands” at locations q_j with weights d_j (notation from [1]) and assume that all values of s_i and d_j are positive reals with $S := \sum_i s_i$ and $D := \sum_j d_j$. The problem consists in minimizing the transport cost

$$(2) \quad \sum_{i,j} c(p_i, q_j) \gamma_{ij},$$

where γ_{ij} is the amount of mass going from p_i to q_j , subject to the conditions

$$(3) \quad \gamma_{ij} \geq 0, \quad \sum_j \gamma_{ij} \leq s_i, \quad \sum_i \gamma_{ij} \leq d_j, \quad \sum_{i,j} \gamma_{ij} = \min(S, D).$$

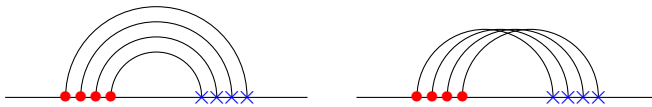


FIGURE 1. On the left: optimal plan associated to a concave cost. On the right: optimal plan associated to a convex cost. Supplies are represented by red points and demands by blue crosses.

The matrix of values $\gamma = \{\gamma_{ij}\}$ is still called *transport plan*. When $S = D$, the problem is said to be *balanced* and is only a reformulation of (1) for discrete measures. When $S \neq D$, the problem is said to be *unbalanced*. The cases $S < D$ and $S > D$ can be treated in the same way. This paper deals with balanced problems and unbalanced problems of the form $S > D$.

In the *unitary case*, *i.e.* when all the masses s_i and d_j are equal to a single value v , it turns out that if γ is optimal, for all i, j , $\gamma_{ij} \in \{0, v\}$ and for all j there exists only one i such that $\gamma_{ij} = v$ (each demand receives all the mass from one supply). In the balanced case, the matrix γ is thus a permutation matrix up to the factor v . In the unbalanced case, the permutation matrix is padded with some zero rows. As a consequence, the balanced case boils down to an *assignment problem*, known as the *linear sum assignment problem*. Such problems have been thoroughly studied by the combinatorial optimization community [6].

Optimal transportation problems appear in many fields, such as economy or physics for instance, see e.g. [4, 9, 13]. In economic examples optimal transport is often related to the field of logistic where supplies are furnished by producers at specific places p_i and in specific quantities d_i , while demands corresponds to consumers locations and needs. Depending on the application, various cost functions c can be used. For instance, concave functions of the distance appear as more realistic cost functions in many economic situations. Indeed, as underlined by McCann [15], a concave cost “*translates into an economy of scale for longer trips and may encourage cross-hauling.*”

During the last decades, many authors have taken interest in the study of existence, uniqueness and properties of optimal plans [2, 11, 14], with a specific interest for convex costs, *i.e.* costs c that can be written as convex functions of the distance on the line. Detailed descriptions of these results can be found in the books [24, 25]. One case of particular interest is the one-dimensional case, which, when c is a convex function of the distance on the line, has been completely understood [22] both for continuous and discrete settings. Indeed, this problem has an explicit solution that does not depend on c (provided that it is convex) and consists in a monotone rearrangement (see Chapter 2.2 of [24]). In the unitary case, this property can also be seen as a consequence of another interesting result, true for any dimension N , which says that the *linear sum assignment problem* is solved by the identical permutation, provided that the cost matrix $(c(p_i, q_j))_{i,j}$ is a Monge matrix¹ [6]. Several approaches have been proposed to generalize the convex one-dimensional result to the case of the circle, where the starting point for the monotone rearrangement is not known, and its choice and hence the optimal plan itself, unlike in the

¹A matrix C is said to be a Monge matrix if it satisfies $c_{ij} + c_{kl} \leq c_{il} + c_{kj}$ when $i < k$ and $j < l$.

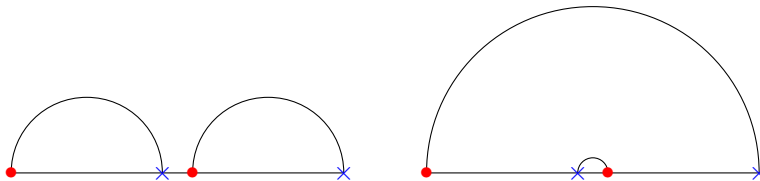


FIGURE 2. On the left: solutions associated to the concave cost $c(x, y) = |x - y|^{0.9}$, and on the right to the cost $c(x, y) = |x - y|^{0.5}$. Supplies are represented by red points and demands by blue crosses.

case of an interval, do depend on the cost function c . Most of these approaches concern either the unitary case [12, 27, 26, 7, 8, 23] or the more general discrete case 2 [17, 19, 20, 18, 21]. Recently an efficient method has been introduced to tackle this issue in a continuous setting [10]. Unfortunately, these results on the line and the circle do not extend to non-convex costs, in particular to concave costs (see Figure 1 for an example). Although it is of broad interest for many applications, few works treat this case (see however the important paper [15]) and computing solutions is far from obvious in general. Indeed, contrary to the convex case on the line, optimal plans strongly depends on the choice of the function c . Consider the case of two unitary supplies at positions $p_1 = 0$ and $p_2 = 1.2$ and two unitary demands at positions $q_1 = 1$ and $q_2 = 2.2$ on the line, as drawn on Figure 2. If the cost function is $c(x, y) = |x - y|^{0.9}$, the left solution will be optimal, whereas the other one will be chosen for $c(x, y) = |x - y|^{0.5}$. For a convex cost, the left solution would always be chosen.

In practice, when no analytic solution is given (*i.e.* most of the time), finding optimal plans can be a tedious task. As underlined before, in a discrete setting, the problem can be written as a linear programming problem, and optimal plans can be constructed numerically by using for instance the simplex method or specialized methods such as the auction algorithms [3] and various algorithms for the assignment problem (see [6] for details). However these methods do not take into account essential geometric features of the problem, such as the fact that it is one-dimensional or that the cost function is concave.

The goal of this paper is to introduce a class of functions that reveals the local structure of optimal transport plans in the one-dimensional case, when the cost c is a concave function of the distance. As a by-product, we build an algorithm that permits to obtain optimal transport plans in the unitary case in less than $O(N^2)$ operations in both balanced and unbalanced cases, where N is the number of points under consideration. Once generalized to the non unitary case, the complexity of this algorithm becomes $O(N^3)$ in the worst case. However, let us insist that our aim is not to compete with recent linear assignment algorithms, which may be more interesting in practice, at least for balanced problems, but rather to achieve a more complete understanding of the “hidden convexity” of the assignment problem for concave costs on the line (*cf* discussion in [5]). Observe that our algorithm complements the method suggested by McCann [15], although the approach we follow here is closer to the purely combinatorial approach of [1]. The results of this last work, in which the cost $c(x, y) = |x - y|$ was considered, are extended here

to the general framework of strictly concave cost functions. (Note that the very special case considered in [1] may be also regarded as convex, which allows to apply the sorting algorithm on the line or results of [10] on the circle.)

The paper is organized as follows. In Section 2, we present the main result of the paper, which states that consecutive matching points in the optimal plan can be found thanks to local indicators, independently of other points on the line. Section 3 is devoted to different technical results, necessary to the proof of this result, which is itself presented in Section 4. Thanks to the low number of evaluations of the cost function required to apply the indicators, we derive in Section 5 an algorithm that finds an optimal transport plan in $O(N^2)$ operations in the worst case. We briefly conclude with some remarks on further improvements in Section 6.

2. SETTING OF THE PROBLEM AND MAIN RESULT

2.1. The optimal transport problem. This paper deals with the problem of finding an optimal transport plan in the case where the problem contains possibly more supplies than demands and the transport cost is strictly concave: the larger the distance to cover is, the less the transport costs per unit distance, while the marginal cost (the derivative of the cost function) decreases monotonically.

Consider two integers M, N and two sets of points $P = \{p_i : i = 1, \dots, M\}$ and $Q = \{q_i : i = 1, \dots, N\}$ in \mathbb{R} that represent respectively the supply and demand locations. Let $s_i > 0$ be the capacity of i th supply and $d_j > 0$ the capacity of j th demand. We suppose that $S := \sum_i s_i \geq D := \sum_j d_j$, *i.e.* that the problem may be unbalanced.

We deal with minimizing the cost

$$(4) \quad C(\gamma) = \sum_{i,j} c(p_i, q_j) \gamma_{ij},$$

where $c(p_i, q_j) \in \mathbb{R}^+$ is the cost resulting from transport of a unit mass between p_i and q_j . The quantity γ_{ij} is the amount of mass going from p_i to q_j , subject for all i, j to the conditions

$$(5) \quad \gamma_{ij} \geq 0, \quad \sum_j \gamma_{ij} \leq s_i, \quad \sum_i \gamma_{ij} = d_j$$

(observe that since $D \leq S$, these conditions are equivalent to (3)). We call the case $S = D$ *balanced* and the case $S > D$ *unbalanced*. Observe that in the latter case the total supply is larger than the total demand, and therefore some of the supplies may remain *underused* ($\sum_j \gamma_{ij} < s_i$).

We focus on the case where the function c involves a strictly concave function as stated in the next definition.

Definition 1. *The cost function c in (7) is said to be concave if it is defined by $c(p, q) = g(|p - q|)$ with $p, q \in \mathbb{R}$, where $g: \mathbb{R}^+ \rightarrow \mathbb{R}$ is a strictly concave non-decreasing function such that $g(0) := \lim_{x \rightarrow 0} g(x) \geq -\infty$.*

Note that strict concavity of g implies its *strict* monotonicity. Some examples of such costs are given by $g(x) = \log x$ with $g(0) = -\infty$ and $g(x) = \sqrt{x}$ with $g(0) = 0$. If $g(0) > -\infty$, we assume without loss of generality that $g(0) = 0$ (this changes the value of (4) by an amount $Dg(0)$ independent of the transport plan).

In what follows, we denote by γ^* a given optimal transport plan between P and Q : $C(\gamma^*) \leq C(\gamma)$ for all γ satisfying (5). Observe that if two points p_i and q_j have

the same position, then there exists an optimal transport plan γ^* between P and Q such that $\gamma_{ij}^* = \min\{s_i, d_j\}$, *i.e.* that all mass shared by the two marginal measures stays in place [24]. Indeed, suppose that a supply p and a demand q located at the same point are not matched together but to some other demand and supply p' and q' located at distances x and y respectively. Irrespective of whether $g(0) = 0$ or $g(0) = -\infty$, as soon as g is strictly concave, one has

$$g(0) + g(x + y) < g(x) + g(y)$$

for all x, y , which implies that matching p and q is cheaper. Therefore a common point of P and Q with unequal values s_i and d_j may be replaced with a single supply of capacity $s_i - d_j$, if this quantity is positive, or with a single demand of capacity $d_j - s_i$. In the following, we will therefore assume that common points do not exist, *i.e.* that the sets P and Q are disjoint.

2.2. The non-crossing rule. One significant feature of concave costs is that trajectories of mass elements under an optimal transport plan do not cross each other, as described by the following lemma.

Lemma 2. *Consider two pairs of points (p_i, q_j) and $(p_{i'}, q_{j'})$ such that*

$$(6) \quad c(p_i, q_j) + c(p_{i'}, q_{j'}) \leq c(p_{i'}, q_j) + c(p_i, q_{j'}).$$

Then, the open intervals

$$I = (\min(p_i, q_j), \max(p_i, q_j)), \quad I' = (\min(p_{i'}, q_{j'}), \max(p_{i'}, q_{j'}))$$

are nested, in the sense that the following alternative holds:

- (1) *either $I \cap I'$ is empty,*
- (2) *or one of these intervals is a subset of the other.*

This result directly follows from the concavity of the cost function and is often referred to as the “non-crossing rule” [1, 15]. The proof is based on the same ideas as used in [15]. Essentially, the case $p_i < q_{j'} < q_j < p_{i'}$ and the similar case with p 's and q 's interchanged are ruled out in view of (6) by monotonicity of g , whereas the case $p_i < p_{i'} < q_j < q_{j'}$ and the symmetrical one are ruled out by the strict concavity of g .

In the unbalanced case, some supplies may lie outside all nested segments.

Definition 3. *A point $r \in P \cup Q$ is said to be exposed in the transport plan γ if $r \notin (\min(p_i, q_j), \max(p_i, q_j))$ whenever $\gamma_{ij} > 0$.*

Lemma 4. *In the unbalanced case all underused supplies are exposed in the optimal transport plan.*

Indeed, should an underused supply p_i belong to the interval between p_{i_0} and q_{j_0} such that $\gamma_{i_0 j_0} > 0$, the amount of mass equal to $\min\{\gamma_{i_0 j_0}, s_i - \sum_j \gamma_{ij}\}$ could be remapped to go to q_{j_0} from p_i rather than p_{i_0} , thus reducing the total cost of transport because of the strict monotonicity of the function g .

A first consequence of these rules is usually called the *local balance of supplies and demands*: in the unitary case, there are as many supplies as demands between any two matched points p_{i_0} and q_{j_0} , whereas for general real supplies and demands, the total supply and the total demand within the interval corresponding to p_{i_0} and q_{j_0} with $\gamma_{i_0 j_0} > 0$ may differ but balance can always be achieved by including suitable shares of s_{i_0} and d_{j_0} (for details see subsection 2.4). This consequence

permits to conclude that the search for optimal transport plans can be restricted to *chains* defined in the following two subsections.

2.3. Chains in the unitary case. We start with the *unitary* case, when $s_i = d_j = 1$ for all i, j and therefore $S = M$ and $D = N \leq M$. It is well known that if γ minimizes the cost (4) under conditions (5), then without loss of generality one can assume that $\gamma_{ij} \in \{0, 1\}$ for all i, j , so that the problem can be reformulated as finding the minimum of the quantity

$$(7) \quad C(\sigma) = \sum_{1 \leq j \leq N} c(p_{\sigma^{-1}(j)}, q_j).$$

over all partial maps $\sigma: \{1, \dots, M\} \rightarrow \{1, \dots, N\}$ whose inverse σ^{-1} is injective and defined for all $1 \leq j \leq N$: namely $j = \sigma(i)$ and $i = \sigma^{-1}(j)$ iff $\gamma_{ij} = 1$. We denote by σ^* the map for which this minimum is attained.

We now proceed to the definition of chains. Given a supply point p_i , define its *left neighbor* q'_i as the nearest demand point on the left of p_i such that the numbers of supplies and demands in the interval (q'_i, p_i) are equal; define the *right neighbor* q''_i of p_i in a similar way. Furthermore define left and right neighbors of a demand point q_j to be the supply points that have q_j as respectively their right and left neighbor. Iterating this procedure, one obtains a subset that is preserved by σ^* because of the local balance property.

Definition 5 (unitary case). *A chain is a maximal alternating sequence of supplies and demands of one of the forms*

- (1) $(p_{i_1}, q_{j_1}, \dots, p_{i_k}, q_{j_k})$,
- (2) $(q_{j_1}, p_{i_1}, \dots, q_{j_k}, p_{i_k})$,
- (3) $(p_{i_1}, q_{j_1}, \dots, q_{j_{k-1}}, p_{i_k})$,

with $k \geq 1$ and such that each pair of consecutive points in the sequence is made of a point and its right neighbor.

Examples of chains are shown in Figure 3. Observe that because of Case (3), some chains can be composed of only one (unmatched) supply, and no demand.

The importance of chains for transport optimization stems from the fact that, according to the non-crossing rule, matching in an optimal plan can occur only between points that belong to the same chain. Indeed, an extension of the proof of Lemma 3 of [1] shows that the family of chains forms a partition of $P \cup Q$. In particular, if a chain is composed of a single supply, it cannot be matched in any optimal transport plan and can thus be dismissed from the problem.

Note finally that the construction of the set of chains only depends on relative positions of supplies and demands and does not involve any evaluation of the cost function. The exact construction is not described here because it is subsumed by the algorithm presented in subsection 2.5.

2.4. Chains in real-valued histograms. In this case the notions of right and left neighbors should be defined for *infinitesimal elements* of supply and demand. The corresponding definition may be given in purely intrinsic terms, but the following graphical representation makes it more evident.

Consider the signed measure $\sum_i s_i \delta_{p_i} - \sum_j d_j \delta_{q_j}$ on the real line, where δ_x is a unit Dirac mass at x . Plot its cumulative distribution function F , whose graph has an upward jump at each p_i and a downward jumps at each q_j , and augment it with

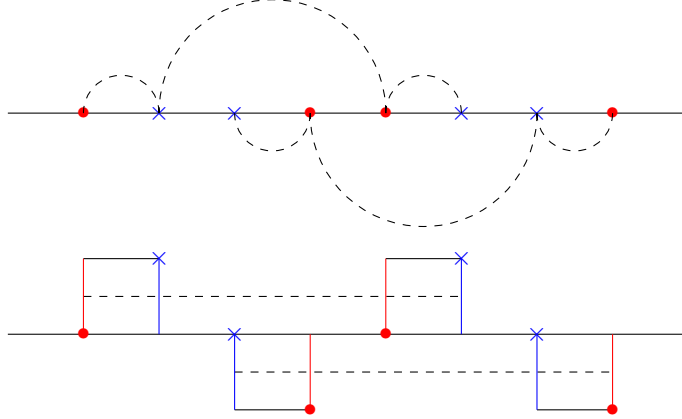


FIGURE 3. Example of a problem containing two chains. Top: chains represented as collections of dashed arcs. Bottom: chains represented as dashed lines connecting elements of mass that are left and right neighbors.

vertical segments to make the graph into a continuous curve (Figure 4). Thus, e.g., the segment corresponding to a supply point p_i connects the points of the graph with coordinates $(p_i, F(p_i))$ and $(p_i, F(p_i+0) = F(p_i) + s_i)$ (assuming left continuity of F). Here and below in figures similar to Figure 4 vertical segments corresponding to supply points are plotted in red and those corresponding to demand points in blue (color online).

Infinitesimal elements of supply and demand are pairs of the form (p_i, y') with $F(p_i) \leq y' \leq F(p_i + 0)$ and (q_j, y'') with $F(q_j + 0) \leq y'' \leq F(q_j)$. Geometrically a supply element (p_i, y') (demand element (q_j, y'')) corresponds to the point (p_i, y') (respectively, (q_j, y'')) in the vertical segment corresponding to the supply p_i (demand q_j) in the graph of the cumulative distribution function F (see Figure 4).

For an infinitesimal element of supply (p_i, y) define

$$\begin{aligned} r(p_i, y) &= \min\{q_j \in Q : q_j > p_i, F(q_j + 0) \leq y \leq F(q_j)\}, \\ \ell(p_i, y) &= \max\{q_j \in Q : q_j < p_i, F(q_j + 0) \leq y \leq F(q_j)\} \end{aligned}$$

(with the usual convention $\min \emptyset = \infty$, $\max \emptyset = -\infty$) and call the mass elements $(r(p_i, y), y)$ and $(\ell(p_i, y), y)$ respectively the *right neighbor* and the *left neighbor* of (p_i, y) if $r(p_i, y)$ and $\ell(p_i, y)$ are finite. The definition of right and left neighbors is then extended to elements of demand by defining $r(q_j, y) = p_i$ whenever $q_j = \ell(p_i, y) > -\infty$ and $\ell(q_j, y) = p_i$ whenever $q_j = r(p_i, y) < \infty$. Inspection of Figure 4 should make these definitions clear.

Definition 6 (real-valued case). *A chain is a sequence of elements of mass that has one of the forms*

- (1) $((p_{i_1}, y), (q_{j_1}, y), \dots, (p_{i_k}, y), (q_{j_k}, y))$ with $\ell(p_{i_1}, y) = -\infty$, $r(q_{j_k}, y) = \infty$;
- (2) $((q_{j_0}, y), (p_{i_1}, y), \dots, (q_{j_{k-1}}, y), (p_{i_k}, y))$ with $\ell(q_{j_0}, y) = -\infty$, $r(p_{i_k}, y) = \infty$;
- (3) $((p_{i_1}, y), (q_{j_1}, y), \dots, (q_{j_{k-1}}, y), (p_{i_k}, y))$ with $\ell(p_{i_1}, y) = -\infty$, $r(p_{i_k}, y) = \infty$.

Here $k \geq 1$ and $q_{j_{m-1}} = \ell(p_{i_m}, y) > -\infty$, $q_{j_m} = r(p_{i_m}, y) < \infty$ for all m between 1 and k except the cases specified above.

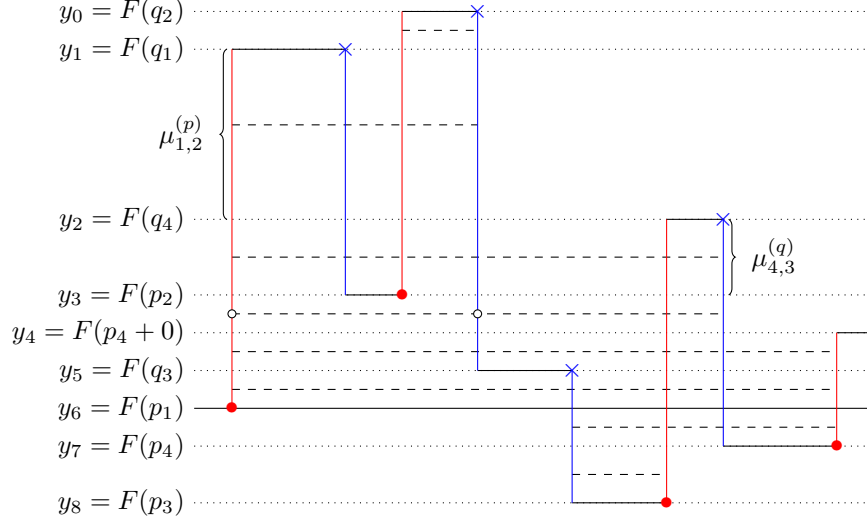


FIGURE 4. Example of construction of chains for a problem with general masses (color online). Red points and blue crosses mark the values of the cumulative distribution function F at supply points p_i and demand points q_j according to the convention of left continuity. Small white circles represent a pair of neighboring demand and supply elements. Chains connecting some neighboring mass elements are shown with dashed lines. All chains have the same structure in each horizontal stratum delimited with dotted lines. Capacity $m_k := y_{k-1} - y_k$ of stratum k measures the amount of mass exchanged in that stratum. For example, the subsegment denoted $\mu_{1,2}^{(p)}$ (resp. $\mu_{4,3}^{(q)}$) represents the share of supply located at p_1 (resp. of demand located at q_4) that participates in the mass exchange in stratum 2 (resp. 3). Detailed explanations are given in the text. Observe that the problem is unbalanced, and chains in strata 5 and 6 have three supplies and two demands.

Note that chains have similar structure inside *strata* defined in the above graphical representation as bands separated by horizontal lines corresponding to ordinates from the set $\{F(p_1 \pm 0), \dots, F(p_M \pm 0), F(q_1 \pm 0), \dots, F(q_N \pm 0)\}$: within each stratum all left and right neighbors are the same and only the y parameters differ.

2.5. Data structure and algorithm for computing chains. We now describe how to efficiently compute and store the structure of chains and strata for a given histogram. This discussion applies both for the real and unitary case (the latter is degenerate in that all elements of each supply and demand point belong to a single stratum, *cf* Figures 3 and 4). Our construction is an adaptation of that of Aggarwal et al [1, Section 3] with somewhat different terminology and notation.

The basic storage structure can be described as follows. Observe that for a supply point p_i the function $r(p_i, \cdot)$ is piecewise constant and right continuous on the segment $[F(p_i), F(p_i + 0)]$. For each p_i build a list consisting of triples $(p_i, y'_{i,m}, r(p_i, y'_{i,m}))$ in the increasing order of $m \geq 0$, where $y'_{i,0} = F(p_i)$ and $y'_{i,m}$

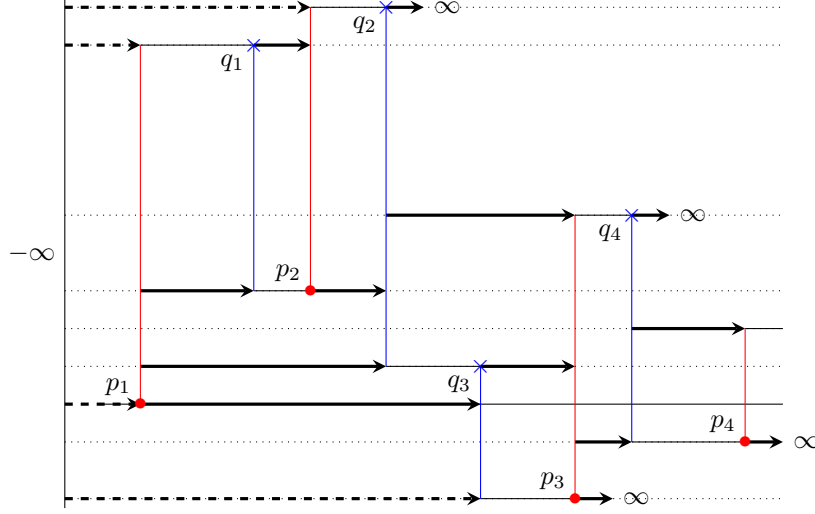


FIGURE 5. Lists \mathcal{L} (solid arrows) and \mathcal{L}_0 (dashed arrows) encoding the structure of the histogram from Figure 4. See explanations in the text.

corresponds to m th jump of $r(p_i, \cdot)$ as the second argument increases. For a demand point (q_j, d_j) build a similar list of triples $(q_j, y''_{j,m}, r(q_j, y''_{j,m}))$ where $y''_{j,0} = F(q_j)$ and $y''_{j,m}$ decreases with m . Finally build a list \mathcal{L} as concatenation of these lists for all supply and demand points in $P \cup Q$ in the increasing order of the abscissa. In Figure 5, which features the same histogram as Figure 4, the elements of the combined list \mathcal{L} are represented with thick solid arrows. Their order corresponds to traversing the p_i 's and q_j 's left to right and for each of these points, to listing the right neighbors in the increasing order of y for p_i and in the decreasing order of y for q_j : in short, to traversing the continuous broken line formed by the graph of F together with the red and blue vertical segments.

Note that all elements in \mathcal{L} that start with p_i have one of the two following forms: $(p_i, F(p_i), q_j)$ with $q_j = r(p_i, F(p_i))$ or $(p_i, F(q_j + 0), q_j)$ with $p_i = \ell(q_j, F(q_j + 0))$. Similarly, elements starting with q_j have either the form $(q_j, F(q_j), p_i)$ with $p_i = r(q_j, F(q_j))$ or $(q_j, F(p_i + 0), p_i)$ with $q_j = \ell(p_i, F(p_i + 0))$. Therefore all elements of \mathcal{L} involve one of the values $F(p_i \pm 0)$ or $F(q_j \pm 0)$ and hence \mathcal{L} has at most $2(M + N)$ elements. To see this refer to Figure 5 and observe, e.g., that the function $r(p_i, \cdot)$ has a jump at y only when, during the upward scan of the vertical segment corresponding to supply p_i , one encounters on the right the bottom end of a vertical segment corresponding to $q_j = r(p_i, y)$ (i.e., the point with $y = F(q_j + 0)$). A similar observation holds for downward scan of segments corresponding to demand elements.

The list \mathcal{L} can be regarded as a “dictionary” that allows to look up the right neighbor of any supply element (p, y) or demand element (q, y) . To do this, e.g., for (p, y) , locate in \mathcal{L} an element (\bar{p}, \bar{y}) immediately preceding (p, y) and return the element $(r(\bar{p}, \bar{y}), y)$. Again, inspection of Figure 5 should convince the reader that this procedure is correct. Note that the search operation in an ordered list of length $O(M + N)$ requires an $O(\log(M + N))$ number of comparisons.

The list \mathcal{L} can be built in a linear number of operations $O(M + N)$ using the following algorithm. Here $\mathcal{S}_p, \mathcal{S}_q$ are stacks storing pairs of the form (r, X) where $r \in P \cup Q$ and $X \in \mathbb{R}$.

Algorithm 1.

- Set $\mathcal{S}_p \leftarrow \emptyset, \mathcal{S}_q \leftarrow \emptyset, \text{list } \mathcal{L} \leftarrow \emptyset, f \leftarrow S - D, p \leftarrow \max P, q \leftarrow \max Q;$
- loop A:
 - if $p = -\infty$ and $q = -\infty$ then break loop A;
 - else if $p > q$ then
 - * set $s \leftarrow$ supply value of $p, P \leftarrow P \setminus \{p\};$
 - * loop B:
 - if $\mathcal{S}_q = \emptyset$ then prepend $(p, f - s, \infty)$ to \mathcal{L} and break loop B;
 - pop the pair (q', f') from stack $\mathcal{S}_q;$
 - if $f' \leq f - s$ then prepend $(p, f - s, q')$ to \mathcal{L} , push the pair (q', f') on stack \mathcal{S}_q if $f' < f - s$, and break loop B;
 - else prepend (p, f', q') to $\mathcal{L};$
 - * repeat loop B;
 - * push the pair (p, f) on stack \mathcal{S}_p and set $f \leftarrow f - s, p \leftarrow \max P;$
 - else if $p < q$ then
 - * set $d \leftarrow$ demand value of $q, Q \leftarrow Q \setminus \{q\};$
 - * loop C:
 - if $\mathcal{S}_p = \emptyset$ then prepend $(q, f + d, \infty)$ to \mathcal{L} and break loop C;
 - pop the pair (p', f') from stack $\mathcal{S}_p;$
 - if $f' \geq f + d$ then prepend $(q, f + d, p')$ to \mathcal{L} , push (p', f') on stack \mathcal{S}_p if $f' > f + d$, and break loop C;
 - else prepend (q, f', p') to $\mathcal{L};$
 - * repeat loop C;
 - * push the pair (q, f) on stack \mathcal{S}_q and set $f \leftarrow f + d, q \leftarrow \max Q;$
 - end if;
- repeat loop A;
- stop.

Observe that if f is initialized with $S - D = F(\infty)$, then at the exit of loop A it will contain $F(-\infty) = 0$. However it is possible to initialize f with any other value, e.g. 0, in which case its exit value will be smaller exactly by the amount $S - D$. It is therefore not necessary to compute this quantity beforehand.

To find leftmost mass elements of chains we also need a list \mathcal{L}_0 of a similar format that stores “right neighbors of $-\infty$.” To build this list, a variant of the above procedure is used. While the list \mathcal{L} was built by “prepending” elements, i.e., adding them in front of the list, the following algorithm uses both prepending and appending, i.e. adding new elements at the end of the list. The stacks $\mathcal{S}_p, \mathcal{S}_q$ and the variable f are assumed to be in the same state as at the end of loop A, in particular the stacks contain exactly those p and q points whose corresponding vertical segments are “visible from $-\infty$.”

Algorithm 2.

- Set lists $\mathcal{L}_0 \leftarrow \emptyset, \mathcal{L}' \leftarrow \emptyset, \mathcal{L}'' \leftarrow \emptyset;$
- repeat until $\mathcal{S}_q \neq \emptyset:$
 - pop the pair (q', f') from stack \mathcal{S}_q and append $(-\infty, f', q')$ to $\mathcal{L}'';$
- repeat until $\mathcal{S}_p \neq \emptyset:$

- pop the pair (p', f') from stack \mathcal{S}_p and prepend $(-\infty, f', p')$ to \mathcal{L}' ;
- if $\mathcal{L}' = \emptyset$ then
 - set $(-\infty, q', f') \leftarrow$ the first element of \mathcal{L}'' and append $(-\infty, f, q')$ to \mathcal{L}_0 ;
- else
 - set $(-\infty, p', f') \leftarrow$ the last element of \mathcal{L}' ;
 - if $\mathcal{L}'' = \emptyset$ then append $(-\infty, f, p')$ to \mathcal{L}_0 ;
 - else
 - * set $(-\infty, q', f') \leftarrow$ the first element of \mathcal{L}'' ;
 - * append $(-\infty, f, \min\{p', q'\})$ to \mathcal{L}_0 ;
 - end if;
- end if;
- set $\mathcal{L}_0 \leftarrow$ concatenation of \mathcal{L}' , \mathcal{L}_0 and \mathcal{L}'' .

Finally the list \mathcal{L} is scanned and the values $F(p_i \pm 0)$, $F(q_j \pm 0)$, which appear as second elements of its constituent triples and define locations of the dotted lines separating strata, are sorted in decreasing order to give the sequence

$$y_0 > y_1 > \cdots > y_K,$$

where K is the number of strata, k -th stratum by definition lies between y_{k-1} and y_k , and $1 \leq K \leq M + N$ ($K = M + N = 8$ in the example of Figures 4, 5). This is the only stage in the process of building the data structure that requires a superlinear number of operations, namely $O((M + N) \log(M + N))$.

2.6. Chain decomposition of transport optimization. Observe that the initial transport optimization problem can be replaced with a problem of transporting the Lebesgue measure supported on “red” vertical segments (representing supply) to the Lebesgue measure supported on their “blue” counterparts (representing demand). The cost function \bar{c} in the new problem is defined for all points of these vertical segments, i.e., mass elements, but depends only on their horizontal coordinates: $\bar{c}(p_i, y', q_j, y'') = c(p_i, q_j)$.

Define the *capacity* of k -th stratum as $m_k = y_{k-1} - y_k$ and the *share of supply* p_i (*demand* q_j) *in stratum* k as $\mu_{i,k}^{(p)} = m_k$ if $F(p_i) \leq y_k < y_{k-1} \leq F(p_i + 0)$ (respectively, $\mu_{j,k}^{(q)} = m_k$ if $F(q_i) \geq y_{k-1} > y_k \geq F(q_i + 0)$) and 0 otherwise. For the vertical segments representing supply and demand graphically, shares are equal to the lengths of their pieces contained between the dotted lines (Figure 4); we will use notation $\mu_{i,k}^{(p)}$, $\mu_{j,k}^{(q)}$ for these subsegments as well. Note that $\sum_k \mu_{i,k}^{(p)} = s_i$ (respectively, $\sum_k \mu_{j,k}^{(q)} = d_j$).

Definition 7. For a given histogram with supplies (p_i, s_i) and demands (q_j, d_j) define a stratified transport plan as the set of nonnegative values $(\gamma_{i,k;j,\ell})$, where $1 \leq i \leq M$, $1 \leq j \leq N$, and $1 \leq k, \ell \leq K$, such that the following conditions are satisfied:

$$(8) \quad \sum_{i,k} \gamma_{i,k;j,\ell} = \mu_{j,\ell}^{(q)} \text{ for all } j, \ell, \quad \sum_{j,\ell} \gamma_{i,k;j,\ell} \leq \mu_{i,k}^{(p)} \text{ for all } i, k.$$

Note that the numbers

$$(9) \quad \gamma_{ij} = \sum_{k,\ell} \gamma_{i,k;j,\ell}$$

form an admissible transport plan (i.e., all conditions (3) are satisfied). We will call this plan the *projection* of the stratified plan in question. The cost of a stratified transport plan is defined as $\sum_{i,k,j,\ell} c(p_i, q_j) \gamma_{i,k;j,\ell}$; of course it coincides with the cost of its projection.

Conversely, let $\gamma = (\gamma_{ij})$, $1 \leq i \leq M$, $1 \leq j \leq N$ be an admissible transport plan; we call a stratified transport plan that satisfies (9) a *stratification* of γ . Any admissible transport plan admits a non-empty set of stratifications. Indeed, it is easy to check that e.g. for $\gamma_{i,k;j,\ell} = \gamma_{ij} \mu_{i,k}^{(p)} \mu_{j,\ell}^{(q)} / s_i d_j$ all conditions (8)–(9) are satisfied.

We now prove that any optimal transport plan in the initial problem can be “lifted” to a bundle of disjoint transport plans operating in individual strata. Therefore to solve the transport optimization problem for histograms with general real values of supply and demand, it suffices to split the problem into transportation problems inside strata, where they reduce to the unitary case because the mass exchanged in each stratum equals its capacity, and solve these problems one by one.

Lemma 8. *An optimal transport plan $\bar{\gamma}$ admits a stratification $(\bar{\gamma}_{i,k;j,\ell})$ that satisfies $\bar{\gamma}_{i,k;j,\ell} = 0$ whenever $\ell \neq k$*

Proof. Indeed, let $(\gamma_{i,k;j,\ell})$ be any stratification of $\bar{\gamma}$ and suppose that $\gamma_{i_0,k_0;j_0,\ell_0} > 0$ with $\ell_0 \neq k_0$. Without loss of generality we restrict the argument to the case $p_{i_0} < q_{j_0}$.

Suppose first that $\ell_0 > k_0$, i.e., that the demand subsegment $\mu_{j_0,\ell_0}^{(q)}$ occupies a lower stratum than the supply subsegment $\mu_{i_0,k_0}^{(p)}$. The total supply located *between* these subsegments, i.e., the sum of all $\mu_{i_0,k}^{(p)}$ with $k < k_0$ and $\mu_{i,k}^{(p)}$ with $p_{i_0} < p_i < q_{j_0}$, is then smaller than the total demand between these subsegments, i.e., the sum of all $\mu_{j,\ell}^{(q)}$ with $p_{i_0} < q_j < q_{j_0}$ and all $\mu_{j_0,\ell}^{(q)}$ with $\ell < \ell_0$. (From inspection of Figure 4 it should be easy to see that their difference is equal to $\sum_{k_0 \leq s < \ell_0} m_s$, although we will not need this quantity here.) Since the first condition (8) must be fulfilled for all j, ℓ , it follows that some demand share $\mu_{j',\ell'}^{(q)}$ located between $\mu_{i_0,k_0}^{(p)}$ and $\mu_{j_0,\ell_0}^{(q)}$ in just defined sense must be satisfied with supplies located outside. But this leads to crossing of the corresponding trajectories (*cf* Lemma 2), which implies that the total cost of the plan $(\gamma_{i,k;j,\ell})$ can be at least preserved, or even reduced, by a suitable rescheduling of mass elements.

Now suppose that $\ell_0 < k_0$. This implies the existence of extra supply $\mu_{i',k'}^{(p)}$ between $\mu_{i_0,k_0}^{(p)}$ and $\mu_{j_0,\ell_0}^{(q)}$. If this supply share is matched, it has to feed some demand located outside, which again leads to crossing and can be ruled out just as above. If this supply share is not matched (which may happen in an unbalanced problem), then it can be matched to the nearest demand share located between $\mu_{i_0,k_0}^{(p)}$ and $\mu_{j_0,\ell_0}^{(q)}$, thus reducing the total cost. Here the “nearest” demand share is defined as $\mu_{j,\ell}^{(q)}$ with either the smallest $q_j > p_{i'}$ and the smallest ℓ such that $\mu_{j,\ell}^{(q)} > 0$, or the largest $q_j < p_{i'}$ and the largest ℓ such that $\mu_{j,\ell}^{(q)} > 0$, depending on which q_j is closer to $p_{i'}$. In all cases we have a contradiction with the original assumption. \square

Most of the rest of the paper deals with the research of optimal transport plans in the case of chains: we focus in the sequel on the cases where P and Q satisfy $M = N$ (*balanced case*) and

$$(10) \quad p_1 < q_1 < \dots < p_i < q_i < p_{i+1} < q_{i+1} < \dots < p_N < q_N,$$

or $M = N + 1$ (*unbalanced case*) and

$$(11) \quad p_1 < q_1 < \dots < p_i < q_i < p_{i+1} < q_{i+1} < \dots < p_N < q_N < p_{N+1}.$$

In these cases the set $P \cup Q$ is called *balanced chain* and *unbalanced chain* respectively.

2.7. Main result. Thanks to the non-crossing rule, one knows that in any optimal transport plan there exist at least two consecutive points (p_i, q_i) or (q_i, p_{i+1}) that are matched. Starting from this remark, we take advantage of the structure of a chain to introduce a class of indicators that enable to detect a priori such pairs of points.

Definition 9 (Local Matching Indicators of order k). *Given $k > 0$, consider $2k + 2$ consecutive points in a chain. If the first point is a supply p_i , define*

$$I_k^p(i) = c(p_i, q_{i+k}) + \sum_{\ell=0}^{k-1} c(p_{i+\ell+1}, q_{i+\ell}) - \sum_{\ell=0}^k c(p_{i+\ell}, q_{i+\ell}),$$

else denote the first point q_i and define

$$I_k^q(i) = c(p_{i+k+1}, q_i) + \sum_{\ell=1}^k c(p_{i+\ell}, q_{i+\ell}) - \sum_{\ell=0}^k c(p_{i+\ell+1}, q_{i+\ell}).$$

This definition is schematically depicted in Figure 6 in the case $k = 2$.



FIGURE 6. Schematic representation of an indicator of order 2.

Note that in the first alternative of this definition, we have necessarily $1 \leq k \leq N - 1$, $1 \leq i \leq N - k$. In the second alternative, we have necessarily $1 \leq k \leq N - 2$ and $1 \leq i \leq N - k - 1$ in the balanced case and $1 \leq k \leq N - 1$ and $1 \leq i \leq N - k$ in the unbalanced case. The interest of these functions lies in the next result.

Theorem 10 (Negative Local Matching Indicators of order k). *Let $k_0 \in \mathbb{N}$ with $1 \leq k_0 \leq N - 1$ and $i_0 \in \mathbb{N}$, such that $1 \leq i_0 \leq N - k_0$. In the unbalanced case, suppose in addition that g is strictly monotone.*

Assume that

- (1) $I_k^p(i) \geq 0$ for $k = 1, \dots, k_0 - 1$, $i_0 \leq i \leq i_0 + k_0 - k$,
- (2) $I_k^q(i') \geq 0$ for $k = 1, \dots, k_0 - 1$, $i_0 \leq i' \leq i_0 + k_0 - k - 1$, (resp. $1 \leq i' \leq i_0 + k_0 - k$ in the unbalanced case)
- (3) $I_{k_0}^p(i_0) < 0$.

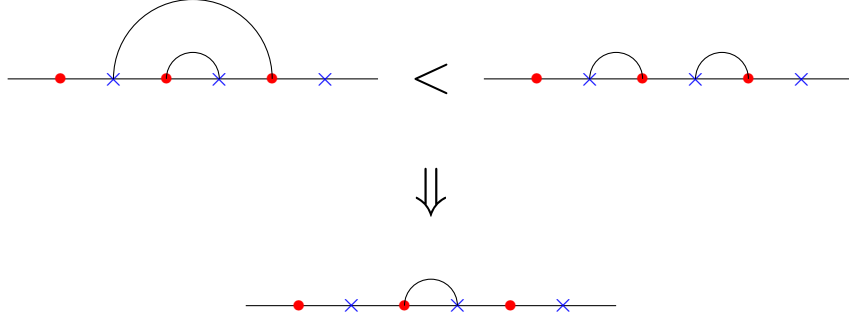


FIGURE 7. Schematic representation of the result of Theorem 10 in the case $k_0 = 1$.

Then any permutation σ associated to an optimal transport plan satisfies $\sigma(i) = i - 1$ for $i = i_0 + 1, \dots, i_0 + k_0$.

If the third condition is replaced by $I_{k_0}^q(i_0) < 0$ (with the same bounds on k_0 and i_0 in the unbalanced case, and with $1 \leq k_0 \leq N - 2$ and $1 \leq i_0 \leq N - k_0 - 1$ in the balanced case), then any permutation σ associated to an optimal transport plan satisfies $\sigma(i) = i$ for $i = i_0 + 1, \dots, i_0 + k_0$.

This result is represented in broad outline in Figure 7. For practical purposes, these indicators allow to find pairs of neighbors that are matched in an optimal transport plan.

3. TECHNICAL RESULTS

This section aims at introducing technical results that are required to prove Theorem 10. We keep the notations introduced therein. We start with a basic result that plays a significant role in the proof of Theorem 10. As for the non-crossing rule, the concavity of the cost function is an essential assumption of this lemma.

Lemma 11. *We keep the previous notations. For $x, y \in \mathbb{R}^+$, define*

$$\varphi_{k,i}^p(x, y) = g(x + y + q_{i+k} - p_i) + \sum_{\ell=0}^{k-1} c(p_{i+\ell+1}, q_{i+\ell}) - g(x) - g(y) - \sum_{\ell=1}^{k-1} c(p_{i+\ell}, q_{i+\ell}),$$

for $k, i \in \mathbb{N}$, such that $1 \leq k \leq N - 1$ and $1 \leq i \leq N - k$, and

$$\varphi_{k,i}^q(x, y) = g(x + y + p_{i+k+1} - q_i) + \sum_{\ell=1}^k c(p_{i+\ell}, q_{i+\ell}) - g(x) - g(y) - \sum_{\ell=1}^{k-1} c(p_{i+\ell+1}, q_{i+\ell}),$$

for $k, i \in \mathbb{N}$, such that $1 \leq k \leq N - 2$ and $1 \leq i \leq N - k - 1$ in the balanced case and $1 \leq k \leq N - 1$ and $1 \leq i \leq N - k$ in the unbalanced case. Both functions $\varphi_{k,i}^p(x, y)$ and $\varphi_{k,i}^q(x, y)$ are decreasing with respect to each of their two variables.

This lemma is a direct consequence of the concavity of the function g . To deal with unbalanced chains, we need two additional lemmas, one of them requiring that g is strictly monotone. The first result is a simple extension of a lemma usually referred as “The rule of three” in the literature [15].

Lemma 12 (“rule of three”). *Suppose that g is strictly monotone. Under the assumptions (1–3) of Theorem 10, the following inequalities are satisfied*

$$|q_j - p_{j+1}| < \min(|p_{i_0} - q_j|, |p_{j+1} - q_{i_0+k_0}|), \quad \forall j \in \{i_0, \dots, i_0 + k_0 - 1\}.$$

If $I_{k_0}^q(i'_0) < 0$ instead of $I_{k_0}^p(i_0) < 0$, the inequalities become

$$|p_j - q_j| < \min(|q_{i_0} - p_j|, |q_j - p_{i_0+k_0+1}|), \quad \forall j \in \{i_0 + 1, \dots, i_0 + k_0\}.$$

Proof: Assumption (3) of Theorem 10 implies that

$$c(q_j, p_{j+1}) + c(p_{i_0}, q_{i_0+k_0}) < \sum_{i=i_0}^{i_0+k_0} c(p_i, q_i) - \sum_{i=i_0}^{i_0+k_0-1} c(p_{i+1}, q_i) + c(q_j, p_{j+1}).$$

Now, because of Assumption (1), we have $I_{j-i_0}^p(i_0) \geq 0$ and $I_{i_0+k_0-j-1}^p(j+1) \geq 0$, which means that

$$\sum_{i=i_0}^j c(p_i, q_i) \leq c(p_{i_0}, q_j) + \sum_{i=i_0}^{j-1} c(p_{i+1}, q_i)$$

and

$$\sum_{i=j+1}^{i_0+k_0} c(p_i, q_i) \leq c(p_{j+1}, q_{i_0+k_0}) + \sum_{i=j+1}^{i_0+k_0-1} c(p_{i+1}, q_i).$$

Thus,

$$c(q_j, p_{j+1}) + c(p_{i_0}, q_{i_0+k_0}) < c(p_{i_0}, q_j) + c(p_{j+1}, q_{i_0+k_0}).$$

Since g is strictly increasing and since $|p_{i_0} - q_{i_0+k_0}| \geq \max(|p_{i_0} - q_j|, |p_{j+1} - q_{i_0+k_0}|)$, this implies that $|p_{j+1} - q_j| < \min(|p_{i_0} - q_j|, |p_{j+1} - q_{i_0+k_0}|)$. The result in the case $I_{k_0}^q(i'_0) < 0$ can be deduced by symmetry. \square

Note that in this proof, only the fact that the cost is an strictly increasing function of the distance is necessary. In particular the result also holds in the case where the cost function is increasing and convex.

Lemma 13 (“partial sums”). *Under the assumptions of Theorem 10, for any ℓ in $\{i_0 + 1, \dots, i_0 + k_0\}$ and ℓ' in $\{i_0, \dots, i_0 + k_0 - 1\}$, the following inequalities are satisfied:*

$$(12) \quad \sum_{i=i_0}^{\ell-1} c(p_i, q_i) > \sum_{i=i_0}^{\ell-1} c(p_{i+1}, q_i),$$

and

$$(13) \quad \sum_{i=\ell'+1}^{i_0+k_0} c(p_i, q_i) > \sum_{i=\ell'}^{i_0+k_0-1} c(p_{i+1}, q_i).$$

Proof: In order to prove inequality (12), remark that since $I_{i_0}^p(k_0) < 0$

$$\begin{aligned} \sum_{i=i_0}^{\ell-1} c(p_i, q_i) &= \sum_{i=i_0}^{i_0+k_0} c(p_i, q_i) - \sum_{i=\ell}^{i_0+k_0} c(p_i, q_i) \\ &> c(p_{i_0}, q_{i_0+k_0}) + \sum_{i=i_0}^{i_0+k_0-1} c(p_{i+1}, q_i) - \sum_{i=\ell}^{i_0+k_0} c(p_i, q_i), \end{aligned}$$

for ℓ such that $i_0 + 1 \leq \ell \leq i_0 + k_0$. Moreover, since $I_{i_0+k_0-\ell}^p(\ell) \geq 0$ and g is increasing,

$$\sum_{i=i_0}^{\ell-1} c(p_i, q_i) > c(p_{i_0}, q_{i_0+k_0}) + \sum_{i=i_0}^{i_0+k_0-1} c(p_{i+1}, q_i) - c(p_\ell, q_{i_0+k_0}) - \sum_{i=\ell}^{i_0+k_0-1} c(p_{i+1}, q_i),$$

which leads to the inequality (12). The proof of Equation (13) follows the same path. \square

On the contrary to the previous results, the next lemma will not be used in the proofs of this paper. We state it since it permits to detect isolated point, hence, it can be used to save computational time.

Lemma 14 (“isolation rule”). *Suppose that g is strictly monotone. If p_i is an unmatched point in the unbalanced chain (11), then if $i > 1$*

$$c(p_i, q_{i-1}) \geq c(p_{i-1}, q_{i-1})$$

and if $i < N$

$$c(p_i, q_i) \geq c(p_{i+1}, q_i).$$

Proof: Assume for instance that $i > 1$ and $c(p_i, q_{i-1}) < c(p_{i-1}, q_{i-1})$. Thanks to Lemma 4, p_i is isolated, and consequently $\sigma^{-1}(i-1) \leq i-1$. Thus, $c(p_i, q_{i-1}) < c(p_{i-1}, q_{i-1}) \leq c(p_{\sigma^{-1}(i-1)}, q_{i-1})$. It is then cheaper to exclude $p_{\sigma^{-1}(i-1)}$ and match p_i with q_{i-1} , which contradicts the optimality of σ . \square

4. PROOF OF THEOREM 10

We are now in the position to prove our main result. In a first part we focus on the balanced case, and then go to the unbalanced case, which requires more efforts.

4.1. The balanced case. Consider the balanced case, i.e., the situation corresponding to (10). We focus on the case where $I_{k_0}^p(i_0) < 0$. The case $I_{k_0}^q(i'_0) < 0$ can be treated the same way.

The proof consists in proving that Assumptions (1-3) of Theorem 10 imply that neither demand nor supply points located between p_{i_0} and $q_{i_0+k_0}$ can be matched with points located outside this interval, i.e. that the set $\mathcal{S}_{i_0} = \{p_i, i_0 + 1 \leq i \leq i_0 + k_0\} \cup \{q_i, i_0 \leq i \leq i_0 + k_0 - 1\}$ is invariant under an optimal transport plan. In this case, the result follows from Assumption (1-2).

Suppose that \mathcal{S}_{i_0} is not preserved by an optimal transport plan σ^* . Three cases can occur:

- There exists $i_1 \in \mathbb{N}$, such that $1 \leq i_1 \leq i_0$ and $i_0 \leq \sigma^*(i_1) \leq i_0 + k_0 - 1$ and there exists $i'_1 \in \mathbb{N}$, such that $\sigma^*(i_1) + 1 \leq i'_1 \leq i_0 + k_0$ and $i_0 + k_0 \leq \sigma^*(i'_1) \leq N$.
- There exists $i_2 \in \mathbb{N}$, with $i_0 + 1 \leq i_2 \leq i_0 + k_0$ such that $1 \leq \sigma^*(i_2) \leq i_0 - 1$.
- There exists $i_2 \in \mathbb{N}$, with $i_0 + k_0 < i_2 \leq N$ such that $i_0 \leq \sigma^*(i_2) < i_0 + k_0$.

We first prove that Case a) cannot occur.

In Case a), one can assume without loss of generality that $\sigma^*(i_1)$ is the largest index such that $1 \leq i_1 \leq i_0$, $i_0 \leq \sigma^*(i_1) \leq i_0 + k_0 - 1$ and that i'_1 is the smallest index such that $\sigma^*(i_1) + 1 \leq i'_1 \leq i_0 + k_0$, $i_0 + k_0 \leq \sigma^*(i'_1) \leq N$. Assume also that

we are not in Cases b) or c). With such assumptions, the (possibly empty) subset $\{p_i, \sigma^*(i_1) + 1 \leq i \leq i'_1 - 1\} \cup \{q_i, \sigma^*(i_1) + 1 \leq i \leq i'_1 - 1\}$ is stable by σ^* . Because of Assumptions (1–2), no nesting (*i.e.* no pair of nested matchings) can occur in this subset, and $\sigma^*(i) = i$ for $i = \sigma^*(i_1) + 1, \dots, i'_1 - 1$.

On the other hand, since σ^* is optimal, one has:

$$c(p_{i_1}, q_{\sigma^*(i_1)}) + c(p_{i'_1}, q_{\sigma^*(i'_1)}) + \sum_{i=\sigma^*(i_1)+1}^{i'_1-1} c(p_i, q_i) \leq c(p_{i_1}, q_{\sigma^*(i'_1)}) + \sum_{i=\sigma^*(i_1)}^{i'_1-1} c(p_{i+1}, q_i).$$

Thanks to Lemma 11, one deduces from this last inequality that:

$$c(p_{i_0}, q_{\sigma^*(i_1)}) + c(p_{i'_1}, q_{i_0+k_0}) + \sum_{i=\sigma^*(i_1)+1}^{i'_1-1} c(p_i, q_i) \leq c(p_{i_0}, q_{i_0+k_0}) + \sum_{i=\sigma^*(i_1)}^{i'_1-1} c(p_{i+1}, q_i),$$

and then:

$$(14) \quad \begin{aligned} & c(p_{i_0}, q_{\sigma^*(i_1)}) + \sum_{i=i_0}^{\sigma^*(i_1)-1} c(p_{i+1}, q_i) + c(p_{i'_1}, q_{i_0+k_0}) + \sum_{i=i'_1}^{i_0+k_0-1} c(p_{i+1}, q_i) \\ & + \sum_{i=\sigma^*(i_1)+1}^{i'_1-1} c(p_i, q_i) \leq c(p_{i_0}, q_{i_0+k_0}) + \sum_{i=i_0}^{i_0+k_0-1} c(p_{i+1}, q_i). \end{aligned}$$

According to Assumption (1), $I_{\sigma^*(i_1)-i_0}^p(i_0) \geq 0$ and $I_{i_0+k_0-i'_1}^p(i'_1) \geq 0$, so that:

$$\begin{aligned} \sum_{i=i_0}^{\sigma^*(i_1)} c(p_i, q_i) &\leq c(p_{i_0}, q_{\sigma^*(i_1)}) + \sum_{i=i_0}^{\sigma^*(i_1)-1} c(p_{i+1}, q_i) \\ \sum_{i=i'_1}^{i_0+k_0} c(p_i, q_i) &\leq c(p_{i'_1}, q_{i_0+k_0}) + \sum_{i=i'_1}^{i_0+k_0-1} c(p_{i+1}, q_i). \end{aligned}$$

Combining these last inequalities with (14) one finds that:

$$\sum_{i=i_0}^{i_0+k_0} c(p_i, q_i) \leq c(p_{i_0}, q_{i_0+k_0}) + \sum_{i=i_0}^{i_0+k_0-1} c(p_{i+1}, q_i),$$

which contradicts Assumption (3).

Let us now prove that Cases b) and c) contradict the assumptions. As Cases b) and c) can be treated in the same way, we only consider Case b). Without loss of generality, one can assume that i_2 is the smallest index such that $i_0 + 1 \leq i_2 \leq i_0 + k_0$ and $\sigma^*(i_2) \leq i_0 - 1$. Because there are necessarily as many demands as supplies between q_{i_0} and p_{i_2} , there exists one and only one index i'_2 such that $i_0 \leq \sigma^*(i'_2) \leq i_2 - 1$ and $1 \leq i'_2 \leq i_0$. Consequently, the (possibly empty) subsets $\{p_i, i_0 + 1 \leq i \leq \sigma^*(i'_2)\} \cup \{q_i, i_0 \leq i \leq \sigma^*(i'_2) - 1\}$ and $\{p_i, \sigma^*(i'_2) + 1 \leq i \leq i_2 - 1\} \cup \{q_i, \sigma^*(i'_2) + 1 \leq i \leq i_2 - 1\}$ are stable by an optimal transport plan. Because of Assumptions (1–2), no nesting can occur in these subsets, and $\sigma^*(i) = i - 1$ for $i = i_0 + 1, \dots, \sigma^*(i'_2)$ and $\sigma^*(i) = i$ for $i = \sigma^*(i'_2) + 1, \dots, i_2 - 1$.

On the other hand, since σ^* is optimal, one has

$$\begin{aligned} c(p_{i_2}, q_{\sigma^*(i_2)}) + c(p_{i_2'}, q_{\sigma^*(i_2')}) + \sum_{i=i_0+1}^{\sigma^*(i_2')} c(p_i, q_{i-1}) + \sum_{i=\sigma^*(i_2')+1}^{i_2-1} c(p_i, q_i) \\ \leq c(p_{i_2'}, q_{\sigma^*(i_2)}) + \sum_{i=i_0+1}^{i_2} c(p_i, q_{i-1}). \end{aligned}$$

Thanks to Lemma 11, one deduces from this last inequality that:

$$\begin{aligned} c(p_{i_2}, q_{\sigma^*(i_2)}) + c(p_{i_0}, q_{\sigma^*(i_2')}) + \sum_{i=i_0+1}^{\sigma^*(i_2')} c(p_i, q_{i-1}) + \sum_{i=\sigma^*(i_2')+1}^{i_2-1} c(p_i, q_i) \\ (15) \quad \leq c(p_{i_0}, q_{\sigma^*(i_2)}) + \sum_{i=i_0+1}^{i_2} c(p_i, q_{i-1}). \end{aligned}$$

Because the cost is supposed to be increasing with respect to the distance, one finds that $c(p_{i_0}, q_{\sigma^*(i_2)}) \leq c(p_{i_2}, q_{\sigma^*(i_2)})$, so that (15) implies:

$$c(p_{i_0}, q_{\sigma^*(i_2')}) + \sum_{i=i_0+1}^{\sigma^*(i_2')} c(p_i, q_{i-1}) + \sum_{i=\sigma^*(i_2')+1}^{i_2-1} c(p_i, q_i) \leq \sum_{i=i_0+1}^{i_2} c(p_i, q_{i-1}),$$

and then:

$$\begin{aligned} c(p_{i_0}, q_{\sigma^*(i_2')}) + \sum_{i=i_0+1}^{\sigma^*(i_2')} c(p_i, q_{i-1}) + \sum_{i=\sigma^*(i_2')+1}^{i_2-1} c(p_i, q_i) + \sum_{i=i_2+1}^{i_0+k_0} c(p_i, q_{i-1}) \\ (16) \quad \leq \sum_{i=i_0+1}^{i_0+k_0} c(p_i, q_{i-1}). \end{aligned}$$

According to Assumption (1), $I_{\sigma^*(i_2')-i_0}^p(i_0) \geq 0$, so that:

$$\sum_{i=i_0}^{\sigma^*(i_2')} c(p_i, q_i) \leq c(p_{i_0}, q_{\sigma^*(i_2')}) + \sum_{i=i_0}^{\sigma^*(i_2')-1} c(p_{i+1}, q_i).$$

Combining these last inequalities with (16) one finds that:

$$\sum_{i=i_0}^{i_0+k_0} c(p_i, q_i) \leq c(p_{i_0}, q_{i_0+k_0}) + \sum_{i=i_0}^{i_0+k_0-1} c(p_{i+1}, q_i),$$

which contradicts Assumption (3).

We have then shown that neither demand nor supply points located between p_{i_0} and $q_{i_0+k_0+1}$ can be matched with points located outside this interval. The set \mathcal{S}_{i_0} is then stable by an optimal transport plan. According to Assumption (1-2), no nesting can occur in \mathcal{S}_{i_0} . The result follows. \square

4.2. The unbalanced case. In this section, we show that Theorem 10 still holds in the unbalanced case.

Observe first that none of the points p_j , $i_0 + 1 \leq j \leq i_0 + k_0$ can remain unmatched in an optimal transport plan. Indeed, assume on the contrary that there exists ℓ in $\{i_0 + 1, \dots, i_0 + k_0\}$ such that p_ℓ is unmatched in the optimal transport plan σ^* . According to Lemma 13

$$\sum_{i=i_0}^{\ell-1} c(p_i, q_i) > \sum_{i=i_0}^{\ell-1} c(p_{i+1}, q_i).$$

Therefore we cannot have $\sigma^*(i) = i$ for $i = i_0, \dots, \ell - 1$: otherwise it would be possible to rematch all the points q_i in this interval to their right neighbors and reduce the cost. Hence, as the point p_ℓ is unmatched and isolated, there exists m in $\{i_0, \dots, \ell - 1\}$ such that $(\sigma^*)^{-1}(m) < i_0$. Choose m to be the greatest value of the index with this property and observe that we have $\sigma^*(i) = i$ for all i in the (possibly empty) interval $m + 1 \leq i \leq \ell - 1$. Now, since g is an increasing function,

$$c(p_{(\sigma^*)^{-1}(m)}, q_m) + \sum_{i=m+1}^{\ell-1} c(p_i, q_i) > c(p_{i_0}, q_m) + \sum_{i=i_0}^{\ell-1} c(p_i, q_i) - \sum_{i=i_0}^m c(p_i, q_i)$$

Using again Equation (12) of Lemma 13, one deduces from this last inequality that

$$c(p_{(\sigma^*)^{-1}(m)}, q_m) + \sum_{i=m+1}^{\ell-1} c(p_i, q_i) > c(p_{i_0}, q_m) + \sum_{i=i_0}^{\ell-1} c(p_{i+1}, q_i) - \sum_{i=i_0}^m c(p_i, q_i).$$

It follows from this and from $I_{m-i_0}^p(i_0) \geq 0$ that

$$\begin{aligned} c(p_{(\sigma^*)^{-1}(m)}, q_m) + \sum_{i=m+1}^{\ell-1} c(p_i, q_i) &> c(p_{i_0}, q_m) + \sum_{i=i_0}^{m-1} c(p_{i+1}, q_i) \\ &+ \sum_{i=m}^{\ell-1} c(p_{i+1}, q_i) - \sum_{i=i_0}^m c(p_i, q_i) \\ &\geq \sum_{i=m}^{\ell-1} c(p_{i+1}, q_i). \end{aligned}$$

In other words, it is cheaper to match each q_i , $m \leq i \leq \ell - 1$, with its right neighbor p_{i+1} and to exclude $p_{(\sigma^*)^{-1}(m)}$ than to match each q_i with its neighbor p_i and to exclude p_ℓ . In all cases, the point p_ℓ cannot remain unmatched.

If the point p_{i_0} is matched in the transport plan σ^* , then we can conclude by the already proved first part of Theorem 10 that $\sigma^*(i) = i - 1$ for $i = i_0 + 1, \dots, i_0 + k_0$ (according to Lemma 4 unmatched points are isolated, the existence of an unmatched p_j outside of $[p_{i_0}, q_{i_0+k_0}]$ has no consequence on this result).

Now, assume that p_{i_0} remains unmatched and that there exists m in $i = i_0, \dots, i_0 + k_0 - 1$ such that $(\sigma^*)^{-1}(m) \neq m + 1$. Since p_{i_0} is isolated, and since matched points are either neighbors or separated by more than $2k_0$ points, $(\sigma^*)^{-1}(m) > i_0 + k_0$. One can assume without loss of generality that m is the largest index in $\{i_0, \dots, i_0 + k_0 - 1\}$ satisfying $(\sigma^*)^{-1}(m) > i_0 + k_0$. Now, because of the rule of three, we know that $|p_{i_0+k_0} - q_{i_0+k_0-1}| < |p_{i_0+k_0} - q_{i_0+k_0}|$. Thus $(\sigma^*)^{-1}(i_0 + k_0 - 1) \leq i_0 + k_0$, otherwise there would exist q_j , with $j \geq i_0 + k_0$ such that $|p_{i_0+k_0} - q_j| < |p_{i_0+k_0} - q_{i_0+k_0-1}|$ (again, because of the rule of three),

which contradicts the previous inequality. It follows that $m < i_0 + k_0 - 1$. Two cases can occur: either $(\sigma^*)(i) = i$ for all i in $\{m+1, \dots, i_0 + k_0\}$, or there exists one (and only one) supply p_k in $\{m+1, i_0 + k_0\}$ such that $\sigma^*(k) > i_0 + k_0$. This cannot happen for two different supplies in $\{m+1, i_0 + k_0\}$, otherwise there would be another demand q_ℓ between these supplies such that $(\sigma^*)^{-1}(\ell) > i_0 + k_0$.

In the first case, thanks to equation (13)

$$\begin{aligned} c(q_m, p_{(\sigma^*)^{-1}(m)}) + \sum_{i=m+1}^{i_0+k_0} c(p_i, q_i) &> c(q_m, p_{(\sigma^*)^{-1}(m)}) + \sum_{i=m}^{i_0+k_0-1} c(p_{i+1}, q_i) \\ &> c(q_{i_0+k_0}, p_{(\sigma^*)^{-1}(m)}) + \sum_{i=m}^{i_0+k_0-1} c(p_{i+1}, q_i), \end{aligned}$$

which contradicts the optimality of σ^* .

In the second case, since $I_{k_0}^p(i_0) < 0$,

$$\begin{aligned} c(q_m, p_{(\sigma^*)^{-1}(m)}) + \sum_{i=m+1}^{k-1} c(p_i, q_i) + c(p_k, q_{\sigma^*(k)}) &> c(q_m, p_{(\sigma^*)^{-1}(m)}) + c(p_k, q_{\sigma^*(k)}) \\ + c(p_{i_0}, q_{i_0+k_0}) + \sum_{i=i_0}^{i_0+k_0-1} c(p_{i+1}, q_i) - \sum_{i=i_0}^m c(p_i, q_i) - \sum_{i=k}^{i_0+k_0} c(p_i, q_i). \end{aligned}$$

Now, since $I_{m-i_0}^p(i_0) \geq 0$ and $I_{i_0+k_0-k}^p(k) \geq 0$, this inequality yields

$$\begin{aligned} c(q_m, p_{(\sigma^*)^{-1}(m)}) + \sum_{i=m+1}^{k-1} c(p_i, q_i) + c(p_k, q_{\sigma^*(k)}) &> c(q_m, p_{(\sigma^*)^{-1}(m)}) \\ + c(p_k, q_{\sigma^*(k)}) - c(p_k, q_{i_0+k_0}) + c(p_{i_0}, q_{i_0+k_0}) - c(p_{i_0}, q_m) + \sum_{i=m}^{k-1} c(p_{i+1}, q_i). \end{aligned}$$

The two differences that appear in the right-hand side are positive so that

$$\begin{aligned} c(q_m, p_{(\sigma^*)^{-1}(m)}) + \sum_{i=m+1}^{k-1} c(p_i, q_i) + c(p_k, q_{\sigma^*(k)}) &\geq c(q_{\sigma^*(k)}, p_{(\sigma^*)^{-1}(m)}) \\ &+ \sum_{i=m}^{k-1} c(p_{i+1}, q_i), \end{aligned}$$

which also contradicts the optimality of σ^* .

By symmetry, the theorem remains valid in the case where $I_{k_0}^q(i'_0) < 0$ instead of $I_{k_0}^p(i_0) < 0$. \square

5. ALGORITHM

In this section, we derive from Theorem 10 a simple algorithm to compute the optimal transport plan in the case of chains and give details about its implementation and complexity. For the sake of simplicity, we only consider the balanced case. The unbalanced case can be treated in the same way.

5.1. Computation of optimal transport plans for chains. The recursive use of the local matching indicators defined in Definition 9 is on the basis of the next algorithm.

Algorithm 3.

- Set $\mathcal{P} = \{p_1, \dots, p_N, q_1, \dots, q_N\}$, $\ell^p = (1, \dots, N)$, $\ell^q = (1, \dots, N)$, and $k = 1$;
- while $\mathcal{P} \neq \emptyset$ and $k < N$
 - (1) compute $I_k^p(i)$ and $I_k^q(i')$ for $i = 1, \dots, N - k$ and $i' = 1, \dots, N - k - 1$;
 - (2) define

$$\mathcal{I}_k^p = \{i_0, 1 \leq i_0 \leq N - k, I_k^p(i_0) < 0\},$$

$$\mathcal{I}_k^q = \{i'_0, 1 \leq i'_0 \leq N - k - 1, I_k^q(i'_0) < 0\};$$
 - (3) if $\mathcal{I}_k^p = \emptyset$ and $\mathcal{I}_k^q = \emptyset$, then set $k = k + 1$;
 - (4) else do
 - for all i_0 in \mathcal{I}_k^p and for $i = i_0 + 1, \dots, i_0 + k$, do
 - * define $\sigma^*(\ell_i^p) = \ell_{i-1}^q$,
 - * remove $\{p_{\ell_i^p}, q_{\ell_{i-1}^q}\}$ from \mathcal{P} ,
 - * remove ℓ_i^p and ℓ_{i-1}^q from ℓ^p and ℓ^q respectively;
 - for all i'_0 in \mathcal{I}_k^q and for $i = i'_0 + 1, \dots, i'_0 + k$, do
 - * define $\sigma^*(\ell_i^q) = \ell_i^p$,
 - * remove $\{p_{\ell_i^q}, q_{\ell_i^p}\}$ from \mathcal{P} ,
 - * remove ℓ_i^q and ℓ_i^p from ℓ^p and ℓ^q respectively;
 - set $N = \frac{1}{2}\text{Card}(\mathcal{P})$, and rename the points in \mathcal{P} such that

$$\mathcal{P} = \{p_1, \dots, p_N, q_1, \dots, q_N\},$$

$$p_1 < q_1 < \dots < p_i < q_i < p_{i+1} < q_{i+1} < \dots < p_N < q_N;$$
 - set $k = 1$;
- if $k = N - 1$, for $i = 1, \dots, N$ set $\sigma^*(\ell_i^p) = \ell_i^q$.

An alternative algorithm consists in testing the sign of each $I_k^p(i)$ and $I_k^q(i')$ as soon as they have been computed and remove the corresponding pairs of points if a negative value is found. What follows also holds for this variant.

5.2. About the implementation and the complexity. The cost of the algorithm can be estimated through the number of additions and evaluations of the cost function that are required to terminate the algorithm. These operations are only carried out in Step 1, when computing the indicators. This section aims at giving details about efficient ways to implement this step and about the complexity of the resulting procedure.

5.2.1. Implementation through a table of indicators. We first define a table that collect the values of indicators and then describe a way to update it. The aim of this structure is to avoid redundant computations. We present it in the balanced case (see (10)).

Consider a table of $N - 1$ lines, where the lines correspond to the values of the indicators of order k . The line k has $2N - 1 - 2k$ entries corresponding to the $N - k$ values of the indicators I_k^p and the $N - k - 1$ values of the indicators I_k^q . At the beginning of the algorithm, the table is empty and Step 1 consists in filling the line k of the table. Let us explain how to modify the table in case a negative indicator has been found.

Following the assumptions of Theorem 10, consider the case where all the indicators that have been computed currently are positive except the last one, denoted by $I_{k_0}^p(i_0) < 0$. According to Step 4, k_0 pairs of supply and demand have to be matched and removed from the current list of points \mathcal{P} . Doing this, the table loses k_0 lines. In each line $k < N - k_0 - 1$ of the new table, only $\min(i_0 - k_0 + k, 2N - 1 - k) - \max(i_0 - k_0 - k, k + 1)$ values are not valid any more since the corresponding indicator involves points that have been modified. Other values are not affected by the withdrawal.

5.2.2. Bounds for the complexity. In the vein of the previous section, we assume up to now that all the numerical values computed during the algorithm are saved. In this framework and as in any assignment problem, the number of evaluations of the cost function cannot exceed $\frac{N(N+1)}{2}$.

The most favorable case consists in finding a negative indicator at each step of the loop. In this case, all points are removed through indicators of order 1. This case requires $O(N)$ additions and evaluations of the cost function.

On the opposite, the worst case corresponds to the case where all the indicators are positive. In such a situation, no pairs are removed until the table is full. All possible transport costs $c(p_i, q_j)$ are computed. Consequently, this case requires $\frac{N(N+1)}{2}$ evaluations of the cost function. The number of additions is also bound by $O(N^2)$ as stated in the next theorem.

Theorem 15. *Denote by $C^+(N)$ the number of additions required to compute an optimal transport plan between N supplies and N demands with the algorithm of Section 5.1. One has:*

$$C^+(N) \leq 3N^2 - 6N.$$

The proof of this result is given in Appendix.

5.2.3. Empirical complexity. In order to estimate the complexity of our algorithm, we have applied it to an increasing number N of pairs of points. For a fixed value of N , 100 samples of points have been chosen randomly in $[0, 1]$, and the mean of the number of additions and evaluations of g has been computed. The results are shown in Figures 8-9. They show that the less concave the cost function is, the more accurate the bound $O(N^2)$ is.

6. POSSIBLE IMPROVEMENTS

The use of Algorithms 1–3 enables to tackle transport problems involving real-valued histograms in $O(N^3)$. Nevertheless, we emphasize that this complexity could be reduced since there is certainly room for improvement in the above algorithmic strategy. As an example, identical indicators may appear in different strata and should not be treated independently to save computational time. The investigation of the interplay between the strata remains for future assessment.

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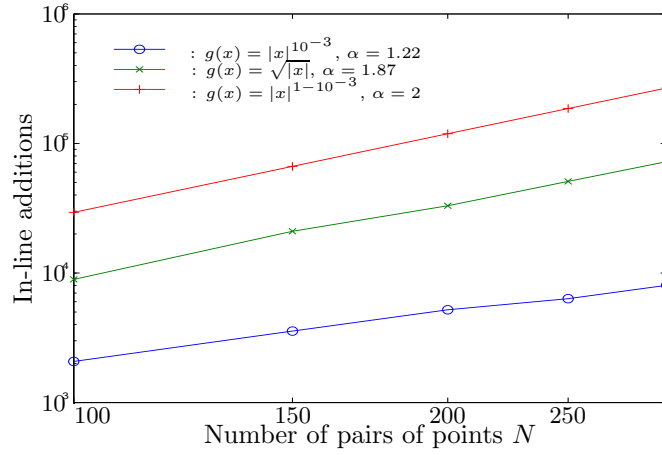


FIGURE 8. Number of in-line additions with respect to the number of pairs, for various cost functions. The number α is the slope of the log-log graphs.

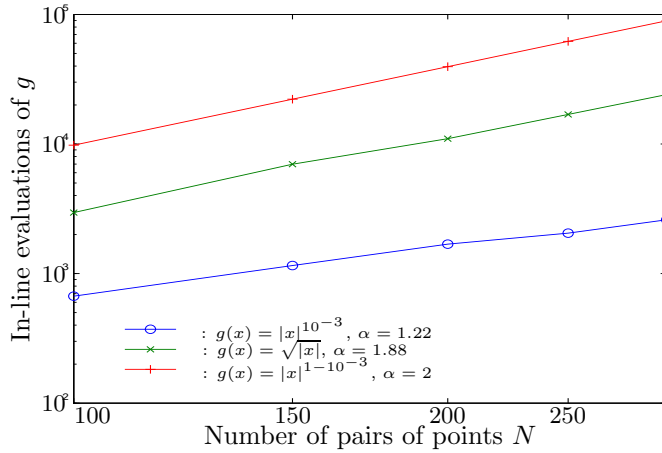


FIGURE 9. Number of in-line evaluations of g with respect to the number of pairs, for various cost functions. The number α is the slope of the log-log graphs.

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APPENDIX : PROOF OF THEOREM 15

Before proving Theorem 15, let us state some intermediate results. In what follows, we denote by $c_k^+(N)$ the number of additions required to achieve Step 1 of the algorithm for an arbitrary value of k .

Lemma 16. *Keeping the previous notations, we have:*

$$(17) \quad c_k^+(N) \leq 3(2(N-k) - 1).$$

Proof: The proof of (17) in the case $k = 1$ is left as exercise for the reader. Suppose that $k > 1$. Consider for example $I_k^p(i)$ and recall that:

$$(18) \quad I_k^p(i) = c(p_i, q_{i+k}) + \sum_{\ell=0}^{k-1} c(p_{i+\ell+1}, q_{i+\ell}) - \sum_{\ell=0}^k c(p_{i+\ell}, q_{i+\ell}).$$

The first term of this formula does not require any addition and most of the other terms have already been computed during the previous steps. Indeed, the first sum has been computed to evaluate $I_{k-1}^q(i)$ and the second one has been computed to evaluate $I_{k-1}^p(i)$. It remains to add $c(p_{i+k}, q_{i+k-1})$ to it to compute the last sum of (18). Since at given order k at most $2(N-k) - 1$ indicators have to be computed, the result follows. \square

We now consider the number of operations required between the beginning of the algorithm and the first occurrence of Step 4.

Lemma 17. *The operations required by the algorithm between its beginning and the first occurrence of Step 4 can be achieved with $\ell_{k_0}^+(N) := 3k_0(2N - k_0 - 2)$ additions, where k_0 denote the current value of k when Step 4 occurs.*

Proof: Between the beginning of the algorithm and the first occurrence of Step 4, only positive indicators have been computed, except for the current value of $k = k_0$. This means that Step 1 has been carried out for $k = 1, \dots, k_0$ since the beginning. The corresponding number of additions is bounded by $\sum_{k=1}^{k_0} c_k^+(N)$. Thanks to Lemma 16, the result follows. \square

Recall now that after Step 4 having been achieved, the parameter k is set to 1. The previous arguments consequently applies to evaluate the number of additions between two occurrences of Step 4, i.e. between two withdrawals. In this way, one finds that this number is bounded by $\ell_{k'_0}^+(N')$, where N' and k'_0 are the current values of N and k at the last occurrence of Step 4. Note that $\ell_{k'_0}^+(N')$ is a coarse upper bound because we are not considering the first occurrence of this step and a part of the indicators has already been computed as explained in Section 5.2.1.

We are now in the position to prove Theorem 15.

Proof (of Theorem 15): Let k_0, k_1, \dots, k_s be the successive orders at which the Step 4 of the algorithm is visited. Observe that some of these numbers can be equal. Assume also that only one negative indicator was found at each of these orders, which is the worst case for complexity. As a consequence, $\sum_{i=0}^s k_i = N$, and the number of additions required for the whole algorithm is lower than

$$C^+ \leq \sum_{i=0}^s \ell_{k_i}^+(N - \sum_{j=0}^{i-1} k_j),$$

where ℓ_k^+ is defined in Lemma 17. Using Lemma 17, we compute

$$\begin{aligned}
C^+ &\leq \sum_{i=0}^s 3k_i(2(N - \sum_{j=0}^{i-1} k_j) - k_i - 2) \\
&= \sum_{i=0}^{s-1} 3k_i(2(N - \sum_{j=0}^{i-1} k_j) - k_i - 2) + 3k_s(2(N - \sum_{j=0}^{s-1} k_j) - k_s - 2) \\
&= \sum_{i=0}^{s-1} 3k_i(2(N - \sum_{j=0}^{i-1} k_j) - k_i - 2) + 3(N - \sum_{j=0}^{s-1} k_j)(N - \sum_{j=0}^{s-1} k_j - 2) \\
&= 3N^2 - 6N - 6 \sum_{i=0}^{s-1} \sum_{j=0}^{i-1} k_i k_j - 3 \sum_{i=0}^{s-1} k_i^2 + 3 \left(\sum_{j=0}^{s-1} k_j \right)^2 \\
&= 3N^2 - 6N.
\end{aligned}$$

□

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