A Data Dependent Algorithm for Querying Earth Mover’s Distance with Low Doubling Dimension

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Abstract

In this paper, we consider the following query problem: given two weighted point sets \(A\) and \(B\) in the Euclidean space \(\mathbb{R}^d\), we want to quickly determine that whether their earth mover’s distance (EMD) is larger or smaller than a pre-specified threshold \(T \geq 0\). The problem finds a number of important applications in the fields of machine learning and data mining. In particular, we assume that the dimensionality \(d\) is not fixed and the sizes \(|A|\) and \(|B|\) are large. Therefore, most of existing EMD algorithms are not quite efficient to solve this problem.

Here, we consider the problem under the assumption that \(A\) and \(B\) have low doubling dimension, which is common for high-dimensional data in real world. Inspired by the geometric method \textit{net tree}, we propose a novel “data-dependent” algorithm to solve this problem efficiently. We also study the performance of our method on real datasets, and the experimental results suggest that our method can save a large amount of running time comparing with existing EMD algorithms.

1 Introduction

Given two weighted point sets \(A\) and \(B\) in the Euclidean space \(\mathbb{R}^d\), the weight of each point in \(A\) represents its supply, and the weight of each point in \(B\) represents its demand. The \textit{Earth Mover’s Distance (EMD)} is the minimum transportation cost from \(A\) to \(B\). We can build a complete bipartite graph \(A \times B\) where each pair of points \((a_i, b_j) \in A \times B\) is connected by an edge with the weight equal to their Euclidean distance (or some other specified distance); so the EMD between \(A\) and \(B\) can be obtained by computing the minimum cost flow [Ahuja et al., 1993] in the bipartite graph. Actually, the transportation problem is a discrete version of the well-known \textit{Monge-Kantorovich} problem that has been extensively studied in Mathematics [Villani, 2008]. EMD has many applications in real world. In particular, it has been widely used for computing the similarity between two patterns in pattern recognition and image retrieval problems [Rubner et al., 2000]. Most of these applications consider the EMD in terms of low dimensional patterns, such as 2D images and 3D shapes. In recent years, several important applications of EMD in high-dimensional Euclidean space have been studied in the fields of machine learning and data mining. Below, we introduce two examples briefly.

1. Computing similarity between different datasets. Crowdsourcing is an emerging topic in the big data era [Li et al., 2015]. We often receive different datasets from various sources and want to quickly estimate their values. For example, we can perform evaluation or classification on the received datasets by comparing them with our own reliable datasets. In practice, a dataset (e.g., image dataset) is often represented as a set of high-dimensional vectors, and therefore the task can be modeled as computing the similarity between two point sets in a high-dimensional Euclidean space.

2. Domain adaptation. In supervised learning, our task usually is to learn the knowledge from a given labeled training dataset and the performance heavily depends on the quality of the labels. However, in many scenarios, labeled data could be very limited. We can generate the labels for an unlabeled dataset by exploiting an existing annotated dataset, that is, transfer the knowledge from a source domain to a target domain, and thus the problem is called “domain adaptation” in the area of transfer learning [Pan and Yang, 2010]. Due to its importance to many machine learning applications, the problem has received a great amount of attention in the past few years. Recently, [Courty et al., 2017] modeled the domain adaptation problem as a transportation problem of computing the EMD between the source and target domains. Similar to the first application, the datasets are often represented as high-dimensional point sets and therefore we need to compute their EMD in high dimension.

In some practical scenarios, we may only need to quickly answer the question that whether the EMD between the given point sets is larger or smaller than a threshold, instead of returning the exact EMD value or the EMD induced map. For example, given two large-scale datasets, we may just want to know that whether they are similar enough and do not care about the detailed map of the data items; for the domain adaptation problem, we may want to quickly determine that whether the given annotated dataset is a suitable source for the unlabeled dataset before conducting the expensive computation for the transportation problem. Thus, it is critical to design a fast algorithm to query the EMD for these applications. However, existing methods for computing or es-
imating EMD in high dimensions often suffer from the issues like high complexity or high distortion (a detailed discussion on existing methods is given in Section 1.1).

In this paper, we study the problem of querying EMD particularly for the data having low doubling dimension (we will provide the formal definition of doubling dimension in Section 1.2). Roughly speaking, the doubling dimension measures the intrinsic dimension of data [Chan et al., 2016]. The reason of considering the problem with low doubling dimension is that real-world high-dimensional data often reveals small intrinsic dimension. For example, a given image set could be represented as a set of very high-dimensional vectors, while the vectors may be distributed nearby a low-dimensional manifold, and thus their intrinsic dimension could be much smaller than the dimension of the Euclidean space [Belkin, 2003].

Our contribution. We develop a “data-dependent” algorithm for solving the EMD query problem: given a value $T \geq 0$, we want to quickly determine that whether the EMD between $A$ and $B$ is larger or smaller than $T$. Our algorithm relies on a hierarchical structure that can be viewed as a simplified net tree in doubling metrics [Har-Peled and Mendel, 2006]. In particular, the height of the structure depends on how close the exact EMD and $T$ are. Specifically, the closer the values, the higher the structure (and the higher the running time). Comparing with the existing EMD methods, our algorithm does not need to build any complicated data structure and is easy to be implemented. Also, our method can be easily modified to handle the case that the doubling dimension of the data is not given in advance.

1.1 Existing Methods for Computing EMD

A number of minimum cost flow algorithms have been developed in the past decades. Suppose $n$ and $m$ are the numbers of vertices and edges in the bipartite graph respectively, and $U$ is the maximum weight. [Orlin, 1988] developed a strongly polynomial algorithm with the time complexity $O(n \log n (m + n \log n))$. [Lee and Sidford, 2014] designed a novel linear solver and one can apply it to solve the minimum cost flow problem in $O(n^{2.5+o(1)} \log(U))$ time. Using the idea of preconditioning, [Sherman, 2017] provided a $(1 + \epsilon)$-approximation algorithm with the running time $O(n^{2+o(1)} \epsilon^{-2})$.

In the community of machine learning, [Cuturi, 2013] proposed a new objective called “Sinkhorn Distance” that smoothes the transportation problem with an entropic regularization term, and it can be solved much faster than computing the exact EMD; [Li et al., 2018] designed a parallel method for computing EMD. Following Cuturi’s work, [Altschuler et al., 2017] provided an additive approximation algorithm for computing EMD with the running time $O(n^2 L^3 (\log n) \epsilon^{-3})$, where $L$ is the maximum edge weight in the bipartite graph.

Since the problem of computing EMD is an instance of the minimum cost flow problem in Euclidean space, a sequence of faster algorithms have been proposed in the community of computational geometry. For example, [Khesin et al., 2019] applied the idea of preconditioning (Sherman, 2017) and designed two randomized $(1 + \epsilon)$-approximation algorithms with the running times $O(ne^{-O(d)} \log(M)^{O(d)} \log n)$ and $O(ne^{-O(d)} \log(U)^{O(d)} \log n)$, respectively ($M$ is the aspect ratio of the given point sets).

Several efficient algorithms also have been developed for estimating the EMD without computing the induced map between the given point sets. For example, [Indyk, 2007] gave a near linear time constant factor approximation algorithm by using the importance sampling technique; [Cabello et al., 2008] showed that it is possible to achieve a $(1 + \epsilon)$-approximation in $O(n^2 \log^2 n)$ time by constructing the geometric spanner; [Andoni et al., 2014] gave a streaming algorithm that can return a $(1 + \epsilon)$-approximation estimate in $O(n^{1+o(1)})$ time. However, most of these algorithms rely on the geometric techniques in low-dimensional space, and their complexities are exponential in the dimensionality $d$. [Li, 2010] generalized the method of [Indyk, 2007] and proposed an $O(\rho)$-approximate estimate of EMD where $\rho$ is the doubling dimension of the given data; however, the algorithm needs a $O(n^{2.5+o(1)} \log(n))$ preprocessing time that could be too high when $n$ is large.

Another natural approach for computing EMD is metric embedding: the two point sets $A$ and $B$ are mapped to two vectors in a normed space (e.g., $l_1$), such that the EMD is approximated by the distance between the two vectors [Andoni et al., 2008; Indyk and Thaper, 2003]. However, this approach often has a large distortion (e.g., $O(\log n \cdot \log d)$) in [Andoni et al., 2008], and thus is not suitable for solving our problem with large $n$ and $d$.

1.2 Preliminaries

We introduce several important definitions in this paper.

**Definition 1** (Earth Mover’s Distance (EMD)). Let $A = \{a_1, a_2, \ldots, a_{n_A}\}$ and $B = \{b_1, b_2, \ldots, b_{n_B}\}$ be two sets of weighted points in $\mathbb{R}^d$ with nonnegative weights $\alpha_i$ and $\beta_j$ for each $a_i \in A$ and $b_j \in B$, and $\sum_{i=1}^{n_A} \alpha_i = \sum_{j=1}^{n_B} \beta_j = W$. The earth mover’s distance between $A$ and $B$ is

$$\mathcal{E}MD(A,B) = \frac{1}{W} \min_F \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} f_{ij} ||a_i - b_j||,$$

where $F = \{f_{ij} \mid 1 \leq i \leq n_A, 1 \leq j \leq n_B\}$ is a feasible flow from $A$ to $B$, i.e., each $f_{ij} \geq 0$, $\sum_{i=1}^{n_A} f_{ij} = \beta_j$, $\sum_{j=1}^{n_B} f_{ij} = \alpha_i$.

**Definition 2** (EMD Query). Given two weighted point sets $A$ and $B$ in $\mathbb{R}^d$ and a value $T \geq 0$, the problem of EMD query is to answer the question that whether $\mathcal{E}MD(A,B) \leq T$ or $\mathcal{E}MD(A,B) \leq T$.

For any point $p \in \mathbb{R}^d$ and $r \geq 0$, we use $Ball(p,r) = \{q \in \mathbb{R}^d \mid ||q - p|| \leq r\}$ to indicate the ball of radius $r$ around $p$. Usually, the doubling dimension is defined for an abstract metric $(X, g)$ where $g$ is the distance function of $X$ [Chan et al., 2016]. In this paper, since we mainly focus on the applications for high-dimensional data with low intrinsic dimension, we directly describe the doubling dimension of point set in Euclidean space.

**Definition 3** (Doubling Dimension). The doubling dimension of a point set $P \subseteq \mathbb{R}^d$ is the smallest number $\rho$, such that for any $p \in P$ and $r \geq 0$, $P \cap Ball(p,2r)$ is always covered by the union of at most $2^\rho$ balls with radius $r$. 
Doubling dimension describes the expansion rate of $P$. For example, imagine a set of points uniformly distributed in a $d'$-dimensional flat in $\mathbb{R}^d$, and then the doubling dimension is $O(d')$ but the Euclidean dimension $d$ can be much higher.

**Claim 1.** Let $A$ and $B$ be two point sets in $\mathbb{R}^d$ with each one having the doubling dimension $\rho > 0$. Then the set $A \cup B$ has the doubling dimension at most $\rho + 1$.

This claim can be easily proved. Given any ball $\text{Ball}(p, 2r)$, we have $(A \cup B) \cap \text{Ball}(p, 2r) = (A \cap \text{Ball}(p, 2r)) \cup (B \cap \text{Ball}(p, 2r))$. Definition 3 implies that $(A \cup B) \cap \text{Ball}(p, 2r)$ is covered by at most $2^{\rho} + 2^\rho = 2^{\rho+1}$ balls with radius $r$. Therefore, Claim 1 is true.

The rest of the paper is organized as follows. In Section 2, we introduce a simplified variant of the net tree method to hierarchically decompose a given set of points in the space. By using the algorithm proposed in Section 2, we introduce our method for solving the EMD query problem (approximately) in Section 3. Finally, we evaluate the performance of our algorithm on real-world datasets in Section 4.

## 2 Hierarchical Gonzalez’s algorithm

In this section, we propose a hierarchical algorithm to decompose point set from coarse to fine. Roughly speaking, given a set $P$ of $n$ points in $\mathbb{R}^d$, we partition it to be covered by a set of balls where the number of the balls is bounded; then we recursively perform the same strategy for the points inside each individual ball until the radius becomes small enough. It is easy to see that this approach will induce a tree, where each node of the tree corresponds to an individual ball and its children form a decomposition of the points inside the ball.

The structure actually can be realized by constructing the **net tree** that has been particularly studied in the context of doubling metrics. [Har-Peled and Mendel, 2006] showed that the net tree can be constructed in $2^{O(\rho)} n \log n$ expected time if the point set has the doubling dimension $\rho$; their idea is based on a fast implementation of the well-known $k$-center clustering algorithm [Gonzalez, 1985] and the method of hierarchically well-separated tree (HST). However, their method needs to maintain and update some auxiliary data structures that are not very efficient for handling large-scale datasets in practice. Moreover, the method takes an extra $O(2^{O(\rho)} n)$ space for maintaining the data structures (besides the original $O(nd)$ for storing the input data).

**Our approach.** In a standard net tree, the nodes at the same level are required to satisfy two key properties: “covering property” and “packing property”. Informally speaking, at each level of the net tree, the covering property requires that each point of $P$ should be covered by a ball centered at one node (each node has a “representative” in $P$) with a specified radius; the packing property requires that the representatives of the nodes are “well separated” (i.e., their inter distances should be large enough). We observe that the “packing property” is not necessary to our EMD query problem. Our proposed algorithm can be viewed as a simplified variant of the net tree method, which only keeps the covering property and takes only a $O(nd)$ space complexity.

Our algorithm also relies on the Gonzalez’s $k$-center clustering algorithm [Gonzalez, 1985], and we briefly introduce it for the sake of completeness. Initially, it selects an arbitrary point, say $c_1$, from the input $P$ and lets $S = \{c_1\}$; then it iteratively selects a new point that has the largest distance to $S$ among the points of $P$ and adds it to $S$, until $|S| = k$ (the distance between a point $q$ and $S$ is defined as $\text{dist}(q, S) = \min \{||q - p|| : p \in S\}$). Suppose $S = \{c_1, \ldots, c_k\}$, and then $P$ is covered by the $k$ balls $\text{Ball}(c_1, r), \ldots, \text{Ball}(c_k, r)$ with $r \leq \min \{|c_i - c_j| : 1 \leq i \neq j \leq k\}$. It is easy to know that the running time of the Gonzalez’s algorithm is $O(|S| nd)$.

Our main idea is hierarchically decomposing the given point set and running Gonzalez’s algorithm locally, and therefore we name the algorithm as **Hierarchical Gonzalez’s Algorithm** (see Algorithm 1). Denote by $\Delta$ the radius of the minimum enclosing ball of $P$. Initially, the whole point set $P$ is covered by a ball with radius $\Delta$. By applying Definition 3 twice, we know that $P$ is covered by $2^{2\rho}$ balls $\mathbb{B} = \{B_1, \ldots, B_{2^{2\rho}}\}$ with radius $\Delta/2$ (note that we can only claim these balls exist, but cannot find these balls explicitly).

If running the Gonzalez’s algorithm $2^{2\rho}$ rounds on $P$, and generate $2^{2\rho}$ clusters and their corresponding cluster centers of $P$; add $2^{2\rho}$ children nodes to $v$, where each child is associated with an individual cluster of $P$, and the corresponding cluster center. Each child is labeled as a $(i+1)$-level node.

### Algorithm 1 Hierarchical Gonzalez’s Algorithm

**Input:** A set $P$ of $n$ points in $\mathbb{R}^d$, a parameter $h > 0$, and the doubling dimension $\rho$.

1. Initialize an empty tree $\mathcal{H}$, and each node $v$ of $\mathcal{H}$ is associated with a point $p_v$ and a subset $P_v$ of $P$.
2. Arbitrarily select a point $p_0 \in P$. Let the root node of $\mathcal{H}$ be $v_0$. Also, $p_{v_0} = p_0$ and $P_{v_0} = P$. The root $v_0$ is labeled as the 0-th level node.
3. Starting from $v_0$, recursively grow each node $v$ of $\mathcal{H}$ as follows:
   a. Suppose the level of $v$ is $i \geq 0$. If $i = h$ or $P_v$ contains only one point, $v$ will be a leaf and stop growing it.
   b. Else, run the Gonzalez’s algorithm $2^{2\rho}$ rounds on $P_v$, and generate $2^{2\rho}$ clusters and their corresponding cluster centers of $P_v$; add $2^{2\rho}$ child nodes to $v$, where each child is associated with an individual cluster of $P_v$ and the corresponding cluster center. Each child is labeled as a $(i+1)$-level node.

**Doubling dimension** describes the expansion rate of $P$. For example, imagine a set of points uniformly distributed in a $d'$-dimensional flat in $\mathbb{R}^d$, and then the doubling dimension is $O(d')$ but the Euclidean dimension $d$ can be much higher. The idea is based on a fast implementation of the well-known $k$-center clustering algorithm [Gonzalez, 1985], and we briefly introduce it for the sake of completeness. Initially, it selects an arbitrary point, say $c_1$, from the input $P$ and lets $S = \{c_1\}$; then it iteratively selects a new point that has the largest distance to $S$ among the points of $P$ and adds it to $S$, until $|S| = k$ (the distance between a point $q$ and $S$ is defined as $\text{dist}(q, S) = \min \{|q-p| : p \in S\}$). Suppose $S = \{c_1, \ldots, c_k\}$, and then $P$ is covered by the $k$ balls $\text{Ball}(c_1, r), \ldots, \text{Ball}(c_k, r)$ with $r \leq \min \{|c_i - c_j| : 1 \leq i \neq j \leq k\}$. It is easy to know that the running time of the Gonzalez’s algorithm is $O(|S| nd)$.

Our main idea is hierarchically decomposing the given point set and running Gonzalez’s algorithm locally, and therefore we name the algorithm as **Hierarchical Gonzalez’s Algorithm** (see Algorithm 1). Denote by $\Delta$ the radius of the minimum enclosing ball of $P$. Initially, the whole point set $P$ is covered by a ball with radius $\Delta$. By applying Definition 3 twice, we know that $P$ is covered by $2^{2\rho}$ balls $\mathbb{B} = \{B_1, \ldots, B_{2^{2\rho}}\}$ with radius $\Delta/2$ (note that we can only claim these balls exist, but cannot find these balls explicitly).

If running the Gonzalez’s algorithm $2^{2\rho}$ rounds, we obtain $2^{2\rho}$ points, say $\{s_{1,1}, s_{2,1}, \ldots, s_{2^{2\rho},1}\}$, and consider two cases: the points separately fall into different balls of $\mathbb{B}$ or not. For the first case, through the triangle inequality we know that $P$ is covered by $\bigcup_{j=1}^{2^{2\rho}} \text{Ball}(s_{j,1}, \Delta/2)$. For the other case (i.e., there exist two points, say $s_{j,1}$ and $s_{j,2}$, falling into one ball, and thus the distance $|s_{j,1} - s_{j,2}| \leq \Delta/2$), due to the nature of Gonzalez’s algorithm, we know that for each point $p \in P$, 

$$
\min_{1 \leq j \leq 2^{2\rho}} |p - s_{j,1}| \leq \min_{1 \leq j < j' \leq 2^{2\rho}} |s_{j,1} - s_{j,2}| \leq \Delta/2.
$$

Thus, for the second case, $P$ is also covered by $\bigcup_{j=1}^{2^{2\rho}} \text{Ball}(s_{j,1}, \Delta/2)$. Namely, we decompose $P$ into $2^{2\rho}$ parts and each part is covered by a ball with radius $\Delta/2$. In the following steps, we just recursively run the Gonzalez’s algorithm on each part locally. If we perform $\log_{2^{2\rho}}$ rounds with
a specified value $r > 0$, each point of $P$ will be covered by a ball with radius $r$ (w.l.o.g., we assume that $\log \frac{\Delta}{r}$ is an integer). Moreover, we can imagine that the algorithm generates a hierarchical tree $\mathcal{H}$ with height $h = \log \frac{\Delta}{r} + 1$, where the root (0-th level) corresponds to the set $P$ and each node at the $i$-th level, $1 \leq i \leq \log \frac{\Delta}{r}$, corresponds to a subset of $P$ that is covered by a ball with radius $\Delta / 2^i$. Obviously, each leaf node is covered by a ball with radius $r$, and the total number of leaves is $\min\{n, (2^\rho \log \frac{\Delta}{r})\} = \min\{n, (\frac{\Delta}{r})^{2\rho}\}$ (we stop growing the node if its corresponding subset has only one point).

**Running time.** For the $i$-th level of $\mathcal{H}$, denote by $n_1, n_2, \cdots, n_{2^ni}$ the number of points covered by the $2^ni$ nodes, respectively (obviously, $\sum_{j=1}^{2^ni} n_j = n$). For each node, we run the Gonzalez’s algorithm $2^\rho$ rounds locally. Therefore, the total running time cost at the $i$-th level is

$$\sum_{j=1}^{2^ni} O(2^\rho n_j d) = O(2^\rho nd). \quad (3)$$

Consequently, the total running time of Algorithm 1 is $O(2^\rho (\log \frac{\Delta}{r}) nd)$ if $h = \log \frac{\Delta}{r} + 1$.

**Space complexity.** In Section 3, we will show that we actually do not need to store the whole $\mathcal{H}$. Instead, we conduct the computations of EMD from top to bottom along $\mathcal{H}$. The space used for the $i$-th level can be released when the nodes at the $(i+1)$-th level all have been generated. That is, we just need to store at most two levels when constructing the tree $\mathcal{H}$ in Algorithm 1. Also, the space used for storing each level is always $O(nd)$. Therefore, the space complexity of Algorithm 1 is $O(nd)$.

Overall, we have the following theorem.

**Theorem 1.** If setting $h = \log \frac{\Delta}{r} + 1$, the hierarchical Gonzalez’s algorithm (Algorithm 1) generates a set of $\min\{n, (\frac{\Delta}{r})^{2\rho}\}$ balls covering $P$ with radius $r$, in $O(2^\rho (\log \frac{\Delta}{r}) nd)$ time. The space complexity is $O(nd)$.

**Remark 1 (If $\rho$ is not given).** In Algorithm 1, we require to input the doubling dimension $\rho$. Actually this is not necessary. Assume we know the value of $\Delta$ (i.e., the radius of the minimum enclosing ball of $P$). Then, for each node $v$ at the $i$-th level of $\mathcal{H}$, we just run the Gonzalez’s algorithm $l$ rounds until the obtained $l$ clusters have radius at most $\Delta / 2^{i+1}$; by the same manner of our previous analysis, we know that $l$ should be no larger than $2^\rho$. Therefore, we have the same time and space complexities as Theorem 1.

But it is expensive to compute the exact value of $\Delta$. One solution is to compute an approximate minimum enclosing ball of $P$ (e.g., the $O(\frac{1}{\epsilon} nd)$ time $(1 + \epsilon)$-approximation algorithm of Badoiu and Clarkson, 2003). Actually, we can solve this issue by a much simpler way. We can arbitrarily select a point $p$ and its farthest point $p'$ from $P$ (this step takes only linear time), and it is easy to see that $||p - p'|| \in [\Delta, 2\Delta]$; then we just replace $\Delta$ by the value $\tilde{\Delta} = ||p - p'||$ in the algorithm. Since $\tilde{\Delta} \leq 2\Delta$, the height of the tree $\mathcal{H}$ will be at most $\log \frac{\Delta}{r} + 1 \leq \log \frac{\Delta}{r} + 2$ (so we just increase the height by one).

### 3 EMD Query Algorithm

In this section, we consider solving the EMD query problem (approximately) by applying Algorithm 1. Recent hardness result reveals that it is quite unlikely to achieve an algorithm that solves the EMD query problem within a low time complexity. [Rohatgi, 2019] studied the hardness of computing EMD. Under the Hitting Set Conjecture, for every $\delta > 0$, he showed that there is no truly subquadratic time algorithm yielding a $(1 + 1/n^\delta)$-approximate EMD matching in $\omega(\log n)$ dimensions.

Therefore, we relax the requirement of Definition 2 slightly. Let $(A, B, T)$ be an instance of Definition 2. Suppose $\epsilon > 0$ is a given small parameter and $\Delta$ is the maximum radius of the minimum enclosing balls of $A$ and $B$. Our idea is to distinguish the instances “$\text{EMD}(A, B) > T + \epsilon\Delta$” and “$\text{EMD}(A, B) < T - \epsilon\Delta$”; the term “$\epsilon\Delta$” can be viewed as the induced approximation error. To realize this goal, we use the hierarchical structure $\mathcal{H}$ constructed in Algorithm 1 to estimate the value of $\text{EMD}(A, B)$ from coarse to fine, until these two instances can be distinguished. The height of $\mathcal{H}$ depends on the values of $\epsilon$ and $\text{EMD}(A, B) - T$. For ease of presentation, we name the following three cases:

- **Case 1:** $\text{EMD}(A, B) > T$;
- **Case 2:** $\text{EMD}(A, B) < T$;
- **Case 3:** $\text{EMD}(A, B) \in T \pm \epsilon\Delta$.

**Theorem 2.** If $\text{EMD}(A, B) > T + \epsilon\Delta$, Algorithm 2 will return “case 1”. If $\text{EMD}(A, B) < T - \epsilon\Delta$, the algorithm will return “case 2”. If $\text{EMD}(A, B) \in T \pm \epsilon\Delta$, the algorithm may return “case 1”, “case 2”, or “case 3”. The height of the tree $\mathcal{H}$ built in Algorithm 2 is at most $\min\{\log \frac{\Delta}{r} + 1, \log \frac{\Delta}{r} + 2\}$ where $\delta = |\text{EMD}(A, B) - T|$.

**Remark 2.** (i) The algorithm relies on Algorithm 1, and thus it also can be easily modified for solving the case that the doubling dimension is not given (see our analysis in Remark 1).

(ii) The running time of Algorithm 2 is data-dependent. The height of the tree $\mathcal{H}$ depends on how close $\text{EMD}(A, B)$ and $T$ are. Specifically, the closer the values, the higher the structure (and the higher the running time). As the subroutine, we can apply any existing EMD algorithm to compute $\text{EMD}(A_i, B_i)$ in Step 2(d) (we will discuss it with more details in our experiment section).

To prove Theorem 2, we need to prove the following Lemma 1 and 2 first.

Let $\Delta$ be the maximum radius of the minimum enclosing balls of $A$ and $B$. Note that the diameter of $P = A \cup B$ could be much larger than $\Delta$. But Lemma 1 tells us that after the first level, the approximate error only depends on $\Delta$.

**Lemma 1.** (i) The value $\tilde{\Delta}$ obtained in Step 1 of Algorithm 2 is between $\Delta$ and $2\Delta$. (ii) At the first level of $\mathcal{H}$, the set $P$ is decomposed into $2^\rho (\rho + 1)$ balls where each ball has the radius at most $2\Delta$.

\footnote{Given two sets of vectors $A, B \subseteq \{0, 1\}^{O(\log n)}$ where each set contains $n$ vectors, the Hitting Set (HS) problem is to ask whether there exists some $a \in A$ such that the inner product $a \cdot b \neq 0$ for every $b \in B$. The HS Conjecture states that there is no algorithm solving the HS problem in $O(n^{2 - \epsilon})$ time for any $\epsilon > 0$.}
Algorithm 2 Hierarchical EMD Query Algorithm

Input: Two point sets $A$ and $B$ in $\mathbb{R}^d$, and the doubling dimension $\rho$. $T > 0$ is a given threshold, and $\epsilon > 0$.
1. Compute the approximate radii of the minimum enclosing balls of $A$ and $B$ (via the method mentioned in Remark 1), and denote them as $\Delta_A$ and $\Delta_B$ respectively. Let $\Delta = \max\{\Delta_A, \Delta_B\}$.
2. Let $P = A \cup B$. Construct the tree $\mathcal{H}$ level by level (from top to bottom) via Algorithm 1 (replace $\rho$ by $\rho + 1$ according to Claim 1).
   (a) Let $i$ be the index of the current level at $\mathcal{H}$. If $i = \log \frac{\Delta}{\epsilon} + 3$, stop the loop and output “Case 3”.
   (b) Let $v_i^1, v_i^2, \ldots, v_i^N$ be the nodes at the $i$-th level ($N = 2^{2^\rho}$). Correspondingly, each node $v_i^j$ is associated with a point $p_{v_i^j}$ and a subset $P_{v_i^j}$ of $P$.
   In addition, let $n_i^j$ be the total weight of $A \cap P_{v_i^j}$ and $m_i^j$ be the total weight of $B \cap P_{v_i^j}$.
   (c) Initialize two empty sets of points $A_i$ and $B_i$. For each $v_i^j$, $1 \leq j \leq N$, if $n_i^j \geq m_i^j$, add $p_{v_i^j}$ to $A_i$ and assign a weight $n_i^j - m_i^j$ to it; else, add $p_{v_i^j}$ to $B_i$ and assign a weight $m_i^j - n_i^j$ to it.
   (d) Compute $\text{EMD}(A_i, B_i)$ by an existing EMD algorithm. If $\text{EMD}(A_i, B_i) > T + \frac{1}{2^i - 1}\Delta$, stop the loop and output “Case 1”; else if $\text{EMD}(A_i, B_i) < T - \frac{1}{2^i - 1}\Delta$, stop the loop and output “Case 2”.

Proof. Let $\Delta_A$ and $\Delta_B$ be the radii of the minimum enclosing balls of $A$ and $B$, respectively. So $\Delta = \max\{\Delta_A, \Delta_B\}$.
It is easy to prove the statement (i). Since $\Delta_A \in [\Delta_A, 2\Delta_A]$ and $\Delta_B \in [\Delta_B, 2\Delta_B]$, we directly have $\Delta = \max\{\Delta_A, \Delta_B\} \in [\Delta, 2\Delta]$.
We can view the set $P = A \cup B$ as an instance of 2-center clustering where each of $A$ and $B$ can be covered by a ball with radius $\Delta$. So if we run the Gonzalez’s algorithm $2^{2^{\rho+1}} > 2$ rounds, we obtain a set of $2^{2^{\rho+1}}$ balls with radius $\leq 2\Delta$ (since the Gonzalez’s algorithm yields a 2-approximation of $k$-center clustering). Thus the statement (ii) is true.

Lemma 2. In Algorithm 2, for each $1 \leq i \leq \log \frac{\Delta}{\epsilon} + 3$, $\text{EMD}(A_i, B_i) \in \text{EMD}(A, B) \pm \frac{1}{2^i - 1}\Delta$.
Proof. First, we consider another two sets of points $\hat{A}_i$ and $\hat{B}_i$, where each of them contains the same set of points $\{p_{v_i^1}, p_{v_i^2}, \ldots, p_{v_i^N}\}$. To differentiate the points in $\hat{A}_i$ and $\hat{B}_i$, we denote each point $p_{v_i^j}$ as $a_i^j$ (resp., $b_i^j$) in $\hat{A}_i$ (resp., $\hat{B}_i$). For the set $\hat{A}_i$ (resp., $\hat{B}_i$), each point $a_i^j$ (resp., $b_i^j$) is associated with the weight $n_i^j$ (resp., $m_i^j$). We can imagine that each $a_i^j$ is a set of $n_i^j$ unit-weight overlapping points; namely, there is a bijection between “$a_i^j$” and $A \cap P_{v_i^j}$. The similar bijection also exists between “$b_i^j$” and $B \cap P_{v_i^j}$. Moreover, since the whole set $P_{v_i^j}$ is covered by a ball with radius $\Delta$, through the triangle inequality, we have

$$\text{EMD}(\hat{A}_i, \hat{B}_i) \leq \text{EMD}(A, B) \pm \frac{1}{2^i - 1}\Delta \tag{4}$$

Next, we only need to prove $\text{EMD}(A_i, B_i) = \text{EMD}(\hat{A}_i, \hat{B}_i)$. Due to the space limit, we omit the proof of the following claim and leave it to our full paper.

Claim 2. There exists a set of flows $\bar{F} = \{\bar{f}_{ji} \mid 1 \leq j, l \leq N\}$ yielding the optimal EMD from $A_i$ to $B_i$, such that for any $1 \leq j \leq N$, $\bar{f}_{jj} = \min\{n_i^j, m_i^j\}$.

Claim 2 shows that the flow from $a_i^j$ to $b_i^j$ is $\min\{n_i^j, m_i^j\}$. W.l.o.g., we assume $n_i^j \leq m_i^j$, then we can safely delete the point $a_i^j$ and replace $m_i^j$ with $m_i^j - n_i^j$ without changing the value of $\text{EMD}(A_i, B_i)$. If we perform this change for each pair $(a_i^j, b_i^j)$ for $1 \leq j \leq N$, the point sets $A_i$ and $B_i$ will become $A_i$ and $B_i$ eventually. Therefore, $\text{EMD}(A_i, B_i) = \text{EMD}(\hat{A}_i, \hat{B}_i)$, and consequently (4) implies $\text{EMD}(A_i, B_i) \in \text{EMD}(A, B) \pm \frac{1}{2^i - 1}\Delta$.

Proof. (of Theorem 2) At the $i$-th level in the tree $\mathcal{H}$, we have $\text{EMD}(A_i, B_i) \in \text{EMD}(A, B) \pm \frac{1}{2^i - 1}\Delta$ via Lemma 2. Also, since $\Delta/2 \leq \Delta \leq \Delta$, we know that

$$\text{EMD}(A, B) - \frac{1}{2^i - 1}\Delta \leq \text{EMD}(A_i, B_i) \leq \text{EMD}(A, B) + \frac{1}{2^i - 1}\Delta \tag{5}$$

If the first event “$\text{EMD}(A, B) > T + \epsilon\Delta$” happens, the left hand-side of (5) implies

$$\text{EMD}(A_i, B_i) > T + \epsilon\Delta - \frac{1}{2^i - 1}\Delta \geq T - \frac{1}{2^i - 1}\Delta. \tag{6}$$

So the algorithm will never output “case 2”. Moreover, when $i \geq \log \frac{\Delta}{\epsilon} + 3$ with $\delta = |\text{EMD}(A, B) - T|$, we have

$$\text{EMD}(A_i, B_i) > \text{EMD}(A, B) - \frac{1}{2^i - 1}\Delta \tag{7}$$

and $\delta > \frac{\Delta}{2^i - 3} > \frac{1}{2^i - 2}. \tag{8}$

(7) comes from the left hand-side of (5). Combining (8) and (9), we have $\text{EMD}(A_i, B_i) > T + \frac{1}{2^i - 1}\Delta$. That is, the algorithm will output “case 1” before $i$ reaches $\log \frac{\Delta}{\epsilon} + 3$.

Similarly, for the second event “$\text{EMD}(A, B) < T - \epsilon\Delta$”, the algorithm will output “case 2” before $i$ reaches $\log \frac{\Delta}{\epsilon} + 3$.
For the third event “$\mathcal{EMD}(A, B) \in T_{\pm \epsilon \Delta}$”, the algorithm could output “case 1” or “case 2” before $i$ reaches $\log \frac{1}{\epsilon} + 3$. It is also possible that the algorithm keeps running until $i = \log \frac{1}{\epsilon} + 3$, and then it will output “case 3”.

4 Experiments

All the experimental results were obtained on a server equipped with 2.4GHz Intel CPU and 8GB main memory; the algorithms are implemented in Matlab R2019a. We apply two widely used EMD algorithms, the NETWORK SIMPLEX algorithm [Ahuja et al., 1993] and the SINKHORN algorithm [Cuturi, 2013], to compute $\mathcal{EMD}(A_i, B_i)$ in Step 2(d) of our HIERARCHICAL EMD QUERY ALGORITHM. Moreover, we use these two algorithms as the baselines for EMD query. Given an instance $(A, B, T)$, let $time_{our}$ be the running time of our algorithm, and $time_{Net}$ (resp., $time_{Sink}$) be the running time of computing $\mathcal{EMD}(A, B)$ by using NETWORK SIMPLEX (resp., SINKHORN). We use the ratios $time_{our}/time_{Net}$ and $time_{our}/time_{Sink}$ to measure the performance of our algorithm (namely the lower the ratio, the better the performance).

Datasets. We use two popular benchmark datasets. The MNIST dataset [LeCun et al., 1998] contains $n = 60,000$ handwritten digit images from 0 to 9, where each image is represented by a 784-dimensional vector. We arbitrarily select 10 pairs of digits to form 10 instances for EMD query, where each digit corresponds to a set of 6000 images. The CIFAR-10 dataset [Krizhevsky et al., 2009] consists of $n = 60,000$ color images of 10 classes (e.g., airplane, bird), with each class having 6000 images and each image being represented by a 3072-dimensional vector. We randomly select 10 pairs of images to generate 10 instances for the EMD query problem.

Results and analysis. For each instance $(A, B)$, we first use NETWORK SIMPLEX (resp., SINKHORN) to compute their EMD (denote by $T_0$); then we vary the threshold $T$ from $2^{-10}T_0$ to $2^{10}T_0$, and set the values of $\epsilon$ to be $\{0.01, 0.03, 0.05\}$. Since it is difficult to obtain the exact doubling dimension $\rho$ for real-world datasets (and the data may contain noise and thus not strictly follow the definition of doubling dimension), we directly set a value $l \in \{2^2, 2^4, 2^6\}$ to be the number of children of each node in the tree $\mathcal{H}$. We plot the average running time ratio histograms on $time_{our}/time_{Net}$ and $time_{our}/time_{Sink}$ in Figure 1. From Figure 1, we can see that the ratios are all lower than 0.5, which indicates that our algorithm can save at least half of the running time comparing with the baselines NETWORK SIMPLEX and SINKHORN. Also, for most of the instances, when $\epsilon$ increases, the running time of our algorithm will slightly decrease (because the height of the tree $\mathcal{H}$ is reduced).

We also show the precision of our method on the MNIST and CIFAR-10 datasets respectively in Table 1 and 2, where the precision measures the frequency that our method returns the right result with respect to the three cases defined in Section 3. Our method can achieve the average precision $\geq 0.86$ for all the instances. When $l$ increases, the precision will increase as well. Moreover, our experimental results remain very stable. For each instance, we run 10 trials and the standard deviation of the precision is less than $1.5 \times 10^{-2}$.

5 Future Work

Following this work, several interesting problems deserve to be studied in future. For example, how to generalize our method for other measures instead of EMD (e.g., Kullback–Leibler divergence)? Moreover, is there any method to solve the EMD query problem without the assumption of low doubling dimension?
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