Computing the Gromov-Hausdorff Distance for Metric Trees

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The Gromov-Hausdorff (GH) distance is a natural way to measure distance between two metric spaces. We prove that it is NP-hard to approximate the GH distance better than a factor of 3 for geodesic metrics on a pair of trees. We complement this result by providing a polynomial time $O(\min\{n, \sqrt{rn}\})$ -approximation algorithm for computing the GH distance between a pair of metric trees, where r is the ratio of the longest edge length in both trees to the shortest edge length. For metric trees with unit length edges, this yields an $O(\sqrt{n})$ -approximation algorithm.¹

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1 INTRODUCTION

The Gromov-Hausdorff distance (or GH distance for brevity) [11] is one of the most natural distance measures between metric spaces, and has been used, for example, for matching deformable shapes [4, 16], and for analyzing hierarchical clustering trees [6]. Informally, the GH distance measures the *additive* distortion suffered when mapping one metric space to another using a cor-

¹This is an expanded version of the authors' previous conference paper [1].

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Fig. 1. Solid and hollow points sampled from distinct metric spaces; each metric space contains two distinct clusters with similar intra- and inter-cluster distances, but the points are sampled differently for each. Using correspondences between the two sets will lead to a small distortion. However, using bijections will map points from the same cluster to different clusters in the other metric space, leading to a much larger distortion.

respondence between their points. Even when working with spaces of equal size, correspondences such as those computed for GH distance are often preferable to, say, bijections, because the distance is less sensitive to slight stretching or the exact choice of points sampled from a larger space (see Figure 1). Multiple approaches have been proposed to estimate the GH distance [4, 15, 16].

Despite much effort, the problem of computing, either exactly or approximately, GH distance has remained elusive. The problem is not known to be NP-hard, and computing the GH distance, even approximately, for *graphic metrics*² is at least as hard as the graph isomorphism problem. Indeed, the metrics for two graphs have GH distance 0 if and only if the two graphs are isomorphic. Motivated by this trivial hardness result, it is natural to ask whether GH distance becomes easier in more restrictive settings such as geodesic metrics over trees, where efficient algorithms are known for checking isomorphism [2].

Related work. Most work on associating points between two metric spaces involves *embedding* a given high-dimensional metric space into an infinite host space of lower-dimensional metric spaces. However, there is some work on finding a bijection between points in two given finite metric spaces that minimizes typically multiplicative distortion of distances between points and their images, with some limited results on additive distortion.

Kenyon et al. [14] give an optimal algorithm for minimizing the multiplicative distortion of a bijection between two equal-sized finite metric spaces, and a parameterized polynomial-time algorithm that finds the optimal bijection between an arbitrary unweighted graph metric and a bounded-degree tree metric.

Papadimitriou and Safra [18] show that it is NP-hard to approximate the multiplicative distortion of any bijection between two finite three-dimensional point sets to within any additive constant or to a factor better than 3.

Hall and Papadimitriou [12] discuss the *additive distortion problem*—given two equal-sized point sets $S, T \subset \mathbb{R}^d$, find the smallest Δ such that there exists a bijection $f : S \rightarrow T$ such that $d(x, y) - \Delta \leq d(f(x), f(y)) \leq d(x, y) + \Delta$. They show that it is NP-hard to approximate by a factor better than 3 in $\mathbb{R}^3$, and also give a 2-approximation for $\mathbb{R}^1$ and a 5-approximation for the more general problem of embedding an arbitrary metric space onto $\mathbb{R}^1$. However, their setting differs from ours in two major ways: firstly, they consider finite metric spaces of equal size, whereas in this article the metric spaces may be uncountably infinite; secondly, they consider bijections between metric spaces, whereas in our work we deal with correspondences between metric spaces which are more general than bijections. In particular, an optimal correspondence between arbitrary spaces of equal size may not be a bijection (see Figure 1), so these hardness results do not apply to GH distance. Thus, their approach cannot be easily extended to our setting.

²A graphic metric measures the shortest path distance between vertices of a graph with unit length edges.

The interleaving distance between merge trees [17] was proposed as a measure to compare functions over topological domains that is stable to small perturbations in a function. Distances for the more general Reeb graphs are given in [3, 7]. These concepts are related to the GH distance (Section 4), which we will leverage to design an approximation algorithm for the GH distance for metric trees.

Our results. In this article, we give the first non-trivial results on approximating the GH distance between metric trees. First, we prove (in Section 3) that the problem remains NP-hard even for metric trees via a reduction from 3-PARTITION. In fact, we show that there exists no efficient algorithm with approximation ratio less than 3 unless $P = NP$. As noted above, we are not aware of any result that shows the GH distance problem being NP-hard even for general graphic metrics.

To complement our hardness result, we give an $O(\sqrt{n})$ -approximation algorithm for the GH distance between metric trees with n nodes and *unit length* edges. Our algorithm works with arbitrary edge lengths as well; however, the approximation ratio becomes $O(\min\{n, \sqrt{rn}\})$ where r is the ratio of the longest edge length in both trees to the shortest edge length. Even achieving the $O(n)$ -approximation ratio presented here for arbitrary r is a non-trivial task, and we hope this first non-trivial approximation result will stimulate further research on this and similar problems.

Our algorithm uses a reduction, described in Section 4, to the similar problem of computing the *interleaving distance* [17] between two *merge trees*. Given a function $f : \mathbb{X} \rightarrow \mathbb{R}$ over a topological space $\mathbb{X}$, the merge tree T_f describes the connectivity between components of the sublevel sets of f (see Section 2 for a more formal definition). Morozov et al. [17] proposed the interleaving distance as a way to compare merge trees and their associated functions.³ For us, interleaving distance provides a convenient way to measure distance after *rooting* the input trees so that correspondences are more nicely structured. We describe, in Section 5, an $O(\min\{n, \sqrt{rn}\})$ -approximation algorithm for interleaving distance between merge trees, and our reduction provides a similar approximation for computing the GH distance between two metric trees.

Note on independent work. After writing preliminary versions of the current report, we became aware of recent work by Schmiedl [19] in which he proves a lower bound of 3 for the approximation ratio of any polynomial-time approximation for GH distance in metric trees. As in our proof, his ultimately comes down to a reduction from 3-PARTITION. He also gives an approximation algorithm for arbitrary metrics, but the running time is not guaranteed to be polynomial in the size of the input.

2 PRELIMINARIES

Metric Spaces and the Gromov-Hausdorff Distance. A *metric space* $X = (X, \rho)$ consists of a (potentially infinite) set X and a function $\rho : X \times X \rightarrow \mathbb{R}_{\geq 0}$ such that the following hold: $\rho(x, y) = 0$ iff $x = y$; $\rho(x, y) = \rho(y, x)$; and $\rho(x, z) \leq \rho(x, y) + \rho(y, z)$.

Given sets A and B , a *correspondence* between A and B is a set $C \subseteq A \times B$ such that (i) for all $a \in A$, there exists $b \in B$ such that $(a, b) \in C$; and (ii) for all $b \in B$, there exists $a \in A$ such that $(a, b) \in C$. We use $\Pi(A, B)$ to denote the set of all correspondences between A and B .

Let $X_1 = (X_1, \rho_1)$ and $X_2 = (X_2, \rho_2)$ be two metric spaces. The *distortion* of a correspondence $C \in \Pi(X_1, X_2)$ is defined as

$$\text{Dist}(C) = \sup_{(x, y), (x', y') \in C} |\rho_1(x, x') - \rho_2(y, y')|.$$

³In fact, our hardness result can be easily extended to the GH distance between graphic metrics for trees and the interleaving distance between merge trees.

Fig. 2. Merge tree M_f (shown in red) for a function $f : \mathbb{X} \rightarrow \mathbb{R}$, where $\mathbb{X} = \mathbb{R}$. $\text{epi } f$ is shown in gray, and $\tilde{f}^{-1}(a)$ is the gray region below the blue horizontal lines in $\text{epi } f$.

The *GH distance* [15], d_{GH} , between $\mathcal{X}_1$ and $\mathcal{X}_2$ is defined as

$$d_{GH}(\mathcal{X}_1, \mathcal{X}_2) = \frac{1}{2} \inf_{C \in \Pi(\mathcal{X}_1, \mathcal{X}_2)} \text{Dist}(C).$$

Intuitively, d_{GH} measures how close can we get to an *isometric* (distance-preserving) embedding between two metric spaces. We note that there are different equivalent definitions of the GH distance (see, e.g. Theorem 7.3.25 of [5] and Remark 1 of [15]).

A *tree* $T = (V, E)$ consists of a set of *nodes* V and *edges* E connecting pairs of nodes such that some geometric realization of T is simply connected. Note our definition allows for nodes of degree 2. The *leaves* of T are the nodes of degree 1, and its *branching nodes* are the nodes of degree 3 or higher.

Given a tree $T = (V, E)$ and a length function $l : E \rightarrow \mathbb{R}_{\geq 0}$, we associate a metric space $\mathcal{T} = (T, d)$ with T as follows. T is a geometric realization of T . For $x, y \in T$, define $d(x, y)$ to be the length of the unique shortest path $\pi(x, y) \in T$. It is clear that d is a metric. The metric space thus obtained is a *metric tree*. We often do not distinguish between T and $\mathcal{T}$ and write $\mathcal{T} = (T, d)$.

Merge Trees and the Interleaving Distance. Let $f : \mathbb{X} \rightarrow \mathbb{R}$ be a continuous function from a connected topological space $\mathbb{X}$ to the set of real numbers. The *sublevel set* at a value $a \in \mathbb{R}$ is defined as $f_{\leq a} = \{x \in \mathbb{X} \mid f(x) \leq a\}$. A *merge tree* M_f captures the evolution of the topology of the sublevel sets as the function value is increased continuously from $-\infty$ to $+\infty$. Formally, it is obtained as follows. Let $\text{epi } f = \{(x, y) \in \mathbb{X} \times \mathbb{R} \mid y \geq f(x)\}$. Let $\tilde{f} : \text{epi } f \rightarrow \mathbb{R}$ be such that $\tilde{f}((x, y)) = y$. We may say $\tilde{f}((x, y))$ is the *height* of point $(x, y) \in \mathbb{X} \times \mathbb{R}$. For two points (x, y) and (x', y') in $\mathbb{X} \times \mathbb{R}$ with $y = y'$, let $(x, y) \sim (x', y')$ denote them lying in the same component of $\tilde{f}^{-1}(y) (= \tilde{f}^{-1}(y'))$. Then $\sim$ is an equivalence relation, and the merge tree M_f is defined as the quotient space $(\mathbb{X} \times \mathbb{R}) / \sim$.

The sublevel sets f_a of f merge as function value a increases, so we get a rooted tree where branching nodes represent the moments where two components merge and leaves represent the birth of a new component at a local minimum. Figure 2 shows an example of a merge tree for a one-dimensional function. Note that the merge tree extends to a height of ∞ . Our assumption that $\mathbb{X}$ is connected implies we have only one component in $f_{\leq N}$ for some sufficiently large $N > 0$, and M_f is, in fact, a single tree.

We define the *root* of merge tree M_f to be the node with the highest function value. The *ancestors* of a point $x \in M_f$ are the points lying on the unique path from x to the root of M_f as well as all points with greater height than the root. We define the *length* of any edge in a merge tree (other

Fig. 3. Part of trees M_f and M_g showing α and β .

than the edge to infinity) to be the height difference between its two endpoints. Ancestors of points in M_g are defined similarly.

Since each point $x \in M_f$ represents a component of a sublevel set at a certain height, we can associate this height value with x , denoted by $\hat{f}(x)$. Given a merge tree M_f and $\varepsilon \geq 0$, an ε -shift map $\sigma_f^\varepsilon : M_f \rightarrow M_f$ is the map that maps a point $x \in M_f$ to its ancestor at height $\hat{f}(x) + \varepsilon$, that is, $\hat{f}(\sigma_f^\varepsilon(x)) = \hat{f}(x) + \varepsilon$. Given $\varepsilon \geq 0$ and merge trees M_f and M_g , two continuous maps $\alpha : M_f \rightarrow M_g$ and $\beta : M_g \rightarrow M_f$ are said to be ε -compatible if they satisfy the following conditions :

$$\begin{aligned} \hat{g}(\alpha(x)) &= \hat{f}(x) + \varepsilon, \forall x \in M_f; & \hat{f}(\beta(y)) &= \hat{g}(y) + \varepsilon, \forall y \in M_g; \\ \beta \circ \alpha &= \sigma_f^{2\varepsilon}; & \alpha \circ \beta &= \sigma_g^{2\varepsilon}. \end{aligned} \quad (1)$$

See Figure 3 for an example. The *interleaving distance* [17] is then defined as

$$d_I(M_f, M_g) = \inf\{\varepsilon \geq 0 \mid \text{there exist } \varepsilon\text{-compatible maps } \alpha \text{ and } \beta\}.$$

Remark. We can relax the requirements on α and β from their normal definitions as follows.

(i) Instead of requiring *exact* value changes, we require

$$\hat{f}(x) \leq \hat{g}(\alpha(x)) \leq \hat{f}(x) + \varepsilon, \forall x \in M_f; \quad \hat{g}(y) \leq \hat{f}(\beta(y)) \leq \hat{g}(y) + \varepsilon, \forall y \in M_g.$$

(ii) If x_1 is an ancestor of x_2 in M_f , then $\alpha(x_1)$ is an ancestor of $\alpha(x_2)$ in M_g . A similar rule applies for β .

(iii) $\beta(\alpha(x))$ must be mapped to an ancestor of x and $\alpha(\beta(y))$ must be mapped to an ancestor of y .

Any pair of maps satisfying the original requirements also satisfies the relaxed requirements for the same value of ε . Conversely, for any pair of maps satisfying the relaxed requirements, we can *stretch up* the images for each map by instead mapping to the ancestors of the appropriate height of the original images, without changing the value of ε . Thus, both definitions of interleaving distance are equivalent. For convenience, when two ε -compatible maps are given to us we assume that they satisfy Equation (1), but we construct ε -compatible maps that satisfy the relaxed conditions mentioned, knowing that they can be “stretched” as just described to satisfy Equation (1).

If we know $\alpha(x)$ for a point x at height h , then we can compute $\alpha(y)$ for any ancestor y of x at height $h' \geq h$ by simply putting $\alpha(y) = \sigma_f^{h'-h}(\alpha(x))$. A similar claim holds for β . Thus, specifying the maps for the leaves of the trees suffices, because any point in the tree is the ancestor of at least one of the leaves. Hence, these maps have a representation that requires linear space in the size of the trees.

Morozov et al. [17] prove several facts about interleaving distance that will prove useful in this work. In particular, interleaving distance is a metric [17, Lemma 1]. Further, it is a *stable* distance measure with respect to small function perturbations; specifically, given two functions $f : \mathbb{X} \rightarrow \mathbb{R}$ and $g : \mathbb{X} \rightarrow \mathbb{R}$, we have $d_I(M_f, M_g) \leq \|f - g\|_\infty$ [17, Theorem 2].

3 HARDNESS OF APPROXIMATION

We now show the hardness of approximating the GH distance by a reduction from the following decision problem called *balanced partition* (or BAL-PART for brevity): given a multiset of positive integers $X = \{a_1, \dots, a_n\}$, and an integer m such that $1 \leq m \leq n$, is it possible to partition X into m multisets $\{X_1, \dots, X_m\}$ such that all the elements in each multiset sum to the same quantity $\mu = (\sum_{i=1}^n a_i)/m$? We prove below that BAL-PART is *strongly* NP-complete, that is, it remains NP-complete even if $a_i \leq n^c$ for some constant $c \geq 1$ for all $1 \leq i \leq n$.

LEMMA 3.1. BAL-PART is *strongly* NP-complete.

PROOF. We reduce 3-PARTITION, a strongly NP-complete problem [10] to BAL-PART. Given a multiset of positive integers $Y = \{a_1, \dots, a_n\}$ with $n = 3m$, 3-PARTITION asks to partition Y into m multisets $\{Y_1, \dots, Y_m\}$ of size 3 each so that the elements in each multiset sum to the same quantity. Given a 3-PARTITION instance, we construct an instance of BAL-PART as follows.

Basically, we add a sufficiently large number to each a_i so that if two multisets of the new numbers have the same sum, they have the same number of elements. In particular, let $\bar{a} = \sum_{i=1}^n a_i$. Then set $a'_i = a_i + \bar{a}$ and $X = \{a'_1, \dots, a'_n\}$. This reduction takes polynomial time, and the new numbers are polynomially larger than the original ones. We show that there exists an appropriate partition of Y iff there exists an appropriate partition of X .

Suppose there exists an appropriate partition $\{Y_1, \dots, Y_m\}$ of Y . Then setting $X_i = \{a'_j \mid a_j \in Y_i\}$ for $i = 1, \dots, m$ gives us the desired partition of X .

Conversely, suppose there exists an appropriate partition $\{X_1, \dots, X_m\}$ of X . Suppose $|X_i| = n_1 > |X_j| = n_2$ for some $i \neq j$. We thus have

$$\sum_{a'_k \in X_i} a_k + n_1 \bar{a} = \sum_{a'_k \in X_j} a_k + n_2 \bar{a} \Rightarrow (n_1 - n_2) \bar{a} = \sum_{a'_k \in X_j} a_k - \sum_{a'_k \in X_i} a_k \Rightarrow \sum_{a'_k \in X_j} a_k - \sum_{a'_k \in X_i} a_k \geq \bar{a}, \quad (2)$$

a contradiction since $\sum_{a'_k \in X_j} a_k < \bar{a}$. Thus, each partition X_i is of equal size. Since $n = 3m$, the size of each X_i is 3. $\square$

We now reduce an instance of BAL-PART, in which each $a_i \leq n^c$ for some constant $c \geq 1$, to GH-distance computation. Consider an instance $X = \{a_1, \dots, a_n\}$ and $1 \leq m \leq n$ of BAL-PART. If $m = 1$, then a balanced partition into one multiset trivially exists. If $m > 1$, we construct two trees T_1 and T_2 as follows. Let $\lambda > 8$ and $\rho < \lambda - 6$ be two positive constants. Let $T_{l,k}$ denote a star graph having k edges, each of length l . T_1 has a node r_1 incident to an edge (r_1, r'_1) of length ρ and to n edges $\{(r_1, p_1), \dots, (r_1, p_n)\}$ of length 1. Each node p_i is incident to another edge (p_i, p'_i) of length 1, and each p'_i is the center of a copy of T_{λ, a_i} . T_2 consists of a node r_2 incident to an edge (r_2, r'_2) of length ρ and to m edges $\{(r_2, q_1), \dots, (r_2, q_m)\}$ of length 2, where each q_i is the center of a distinct copy of $T_{\lambda+1, \bar{a}}$, and $\bar{a} = (\sum_{i=1}^n a_i)/m$. See Figure 4 for an illustration. We refer to the edges of each T_{λ, a_i} in T_1 and the edges of copies of $T_{\lambda+1, \bar{a}}$ in T_2 as *bottom* edges. Let $\mathcal{T}_1$ and $\mathcal{T}_2$ denote the metric trees associated with T_1 and T_2 , respectively. Since λ, ρ are constants and $a_i \leq n^c$ for all $1 \leq i \leq n$, this construction can be done in polynomial time.

LEMMA 3.2. If (X, m) is a yes instance of BAL-PART, then $d_{GH}(\mathcal{T}_1, \mathcal{T}_2) \leq 1$. Otherwise, $d_{GH}(\mathcal{T}_1, \mathcal{T}_2) \geq 3$.

PROOF. Suppose X can be partitioned into m subsets $X_1, \dots, X_m$ of equal weight $\bar{a} = (\sum_{i=1}^n a_i)/m$. We construct a correspondence C between $\mathcal{T}_1$ and $\mathcal{T}_2$ with distortion at most 2, implying that $d_{GH}(\mathcal{T}_1, \mathcal{T}_2) \leq 1$. A linearly interpolated bijection between the points of edges (r_1, r'_1) and (r_2, r'_2) , with r_1 mapping to r_2 and r'_1 mapping to r'_2 , is added to C . If $a_i \in X_j$, the linearly interpolated bijection between edges (r_1, p_i) and (r_2, q_j) is added to C , with p_i mapping to q_j . Also, using linear

Fig. 4. The trees $T_{l,k}$, T_1 , and T_2 .

interpolation, we map the *path* from p_i to each leaf of T_{λ, a_i} to distinct *edges* going from q_j to leaves of its copy of $T_{\lambda+1, \bar{a}}$; this is possible since $T_{\lambda+1, \bar{a}}$ has $\bar{a}$ leaves, and $\sum_{a \in X_j} a = \bar{a}$. Note that each edge (p_i, p'_i) may be mapped to a contiguous part of multiple edges in T_2 . Overall, the distortion induced by C is at most 2; this stems from the fact that C is piecewise linear, and the difference between the length of any node-to-node path in one tree and its image under C in the other tree is at most 2.

Suppose $d_{GH}(T_1, T_2) < 3$, and let C be a correspondence between T_1 and T_2 with distortion < 6 . Consider two leaves $l_1, l_2 \neq r'_2$ in T_2 . Then $d(l_1, l_2) \geq 2\lambda + 2$. Let l'_1, l'_2 be their corresponding images in T_1 under C . We argue that l'_1, l'_2 lie on distinct bottom edges of T_1 . Indeed, since $\text{Dist}(C) < 6$, the distance between l'_1 and l'_2 is $d(l'_1, l'_2) > d(l_1, l_2) - 6 \geq 2\lambda - 4$. If l'_1, l'_2 lie on the same edge of T_1 , then $d(l'_1, l'_2) \leq \lambda < 2\lambda - 4$, so they have to lie on distinct edges of T_1 . If either of l'_1, l'_2 lies on an edge $r_1 p_i$, for some $i \leq n$, then by construction, $d(l'_1, l'_2) \leq \lambda + 4 < 2\lambda - 4$ (recall that $\lambda > 8$). Finally, if either of l'_1, l'_2 lies on (r_1, r'_1) , then by the choice of ρ , $d(l'_1, l'_2) \leq \rho + \lambda + 2 < 2\lambda - 4$. Thus, both l'_1 and l'_2 lie on distinct bottom edges of T_1 . In particular, the corresponding image l'_1 in T_1 of any *one* leaf l_1 in T_2 must lie on a bottom edge of T_1 , because there exists some other leaf l_2 in T_2 by the assumption that $m > 1$. Hence, C induces a bijection χ between the leaves of T_1 and T_2 , where $\chi(l) = l'$ for $l \in T_2$ and $l' \in T_1$ is the leaf whose incident edge contains the image(s) of l under C . Note that if $l_i, l_j \in T_2$ are incident to q_i, q_j with $q_i \neq q_j$, then $\chi(l_i)$ and $\chi(l_j)$ are incident to $p_{i'}, p_{j'}$ with $p_{i'} \neq p_{j'}$; otherwise $d(l_i, l_j) = 2\lambda + 6$ and $d(\chi(l_i), \chi(l_j)) \leq 2\lambda$, thereby incurring a distortion of at least 6. Hence, the bijection χ can be used to partition X into m subsets $X_1, \dots, X_m$ of equal weight as follows: if $\chi(l) = l'$ for l incident to q_i and l' incident to p_j , then $a_j \in X_i$. Thus, (X, m) is a yes instance of BAL-PART. $\square$

We may also apply the reduction to metric trees with unit edge lengths by subdividing longer edges with an appropriate number of vertices. We thus have the following theorem.

THEOREM 3.3. *Unless $P = NP$, there is no polynomial-time algorithm to approximate the GH distance between two metric trees to a factor better than 3, even in the case of metric trees with unit edge lengths.*

4 GH AND INTERLEAVING DISTANCES

In this section, we show that the GH distance between two tree metric spaces T_1 and T_2 , and the interleaving distance between two appropriately defined trees induced by the T_i 's are within constant factors of each other.

Given a metric tree $\mathcal{T} = (T, d)$, let $V(T)$ denote the nodes of the tree. Given a point $s \in T$ (not necessarily a node), let $f_s : T \rightarrow \mathbb{R}$ be defined as $f_s(x) = -d(s, x)$. Equipped with this function, we

obtain a merge tree T^s from $\mathcal{T}$. Intuitively, T^s has the structure of rooting T at s , and then adding an extra edge incident to s with function value extending from 0 to $+\infty$. If s is an internal node of T or an interior point of an edge of T , s remains the root of T^s . But if s is a leaf of T , then s gets merged with the infinite edge and the node of T adjacent to s becomes the root of T^s .

Let $\mathcal{T}_1 = (T_1, d_1)$ and $\mathcal{T}_2 = (T_2, d_2)$ be two metric trees. Define

$$\Delta = \min_{u \in V(T_1), v \in V(T_2)} d_I(T_1^u, T_2^v). \quad (3)$$

We prove that Δ is within a constant factor of $d_{GH}(\mathcal{T}_1, \mathcal{T}_2)$. We first prove a lower bound on Δ .

LEMMA 4.1. $\frac{1}{2}d_{GH}(\mathcal{T}_1, \mathcal{T}_2) \leq \Delta$.

PROOF. Suppose $\Delta = d_I(T_1^s, T_2^t)$ for some $s \in V(T_1)$ and $t \in V(T_2)$. Set $f := f_s$ and $g := f_t$. Let $\alpha : T_1^s \rightarrow T_2^t, \beta : T_2^t \rightarrow T_1^s$ be Δ -compatible maps. We define the functions $\alpha^* : T_1^s \rightarrow T_2^t$ and $\beta^* : T_2^t \rightarrow T_1^s$ as follows:

$$\alpha^*(x) = \begin{cases} \alpha(x) & \text{if } g(\alpha(x)) \leq 0. \\ t & \text{otherwise.} \end{cases} \quad \beta^*(y) = \begin{cases} \beta(y) & \text{if } f(\beta(y)) \leq 0. \\ s & \text{otherwise.} \end{cases}$$

That is, if $\alpha(x)$ ($\beta(y)$, respectively) is an ancestor of t (s , respectively), then x (y , respectively) is mapped to the root t (s , respectively). We note that

$$\begin{aligned} f(x) &\leq g(\alpha^*(x)) \leq f(x) + \Delta, \\ g(y) &\leq f(\beta^*(y)) \leq g(y) + \Delta. \end{aligned} \quad (4)$$

Indeed, if $\alpha^*(x) = \alpha(x)$, then $g(\alpha^*(x)) = f(x) + \Delta$. Otherwise, $g(\alpha^*(x)) > 0$ and $g(\alpha^*(x)) = 0$. Since $f(x) \leq 0$, we obtain $g(\alpha^*(x)) < g(\alpha(x)) = f(x) + \Delta$. The same argument implies the second set of inequalities.

Consider the correspondence $C \in T_1 \times T_2$ induced by α^* and β^* defined as

$$C := \{(x, \alpha^*(x)) \mid x \in T_1\} \cup \{(\beta^*(y), y) \mid y \in T_2\}.$$

We prove that $\text{Dist}(C) \leq 4\Delta$.

Indeed, consider any two pairs $(x_1, y_1), (x_2, y_2) \in C$. Let u be the least common ancestor of x_1 and x_2 in T_1 (if T_1 is rooted at s), and w the least common ancestor of y_1 and y_2 in T_2 (if T_2 is rooted at t). Note that since T_1 and T_2 are trees, there is a unique path $x_1 \rightsquigarrow u \rightsquigarrow x_2$ between x_1 and x_2 , such that $x_1 \rightsquigarrow u$ and $u \rightsquigarrow x_2$ are each monotone in function f values. This also implies that $d_1(x_1, u) = d_1(s, x_1) - d_1(s, u) = f(u) - f(x_1)$; similarly, $d_1(x_2, u) = f(u) - f(x_2)$. Symmetric statements hold for $y_1 \rightsquigarrow w \rightsquigarrow y_2$. Hence

$$\begin{aligned} d_1(x_1, x_2) &= d_1(x_1, u) + d_1(u, x_2) = 2f(u) - f(x_1) - f(x_2), \\ d_2(y_1, y_2) &= d_2(y_1, w) + d_2(w, y_2) = 2g(w) - g(y_1) - g(y_2). \end{aligned}$$

We then have

$$\begin{aligned} |d_1(x_1, x_2) - d_2(y_1, y_2)| &= |2f(u) - f(x_1) - f(x_2) - 2g(w) + g(y_1) + g(y_2)| \\ &\leq 2|f(u) - g(w)| + |f(x_1) - g(y_1)| + |f(x_2) - g(y_2)| \\ &\leq 2|f(u) - g(w)| + 2\Delta \text{ (by Equation (4))}. \end{aligned}$$

We now wish to bound $|f(u) - g(w)|$. Consider the case where $y_1 = \alpha^*(x_1), y_2 = \alpha^*(x_2)$. As we traverse the path $x_1 \rightsquigarrow u \rightsquigarrow x_2$, the image of this path under α^* is a path $y_1 \rightsquigarrow \alpha^*(u) \rightsquigarrow y_2$, where $y_1 \rightsquigarrow \alpha^*(u)$ and $\alpha^*(u) \rightsquigarrow y_2$ are each monotone in function g values. Hence, $\alpha^*(u)$ is an ancestor of y_1 and y_2 . Since w is the least common ancestor of y_1 and y_2 , we have that $\alpha^*(u)$ must be an ancestor of w . The same claim can be similarly proved for the remaining cases. Further, it can

be similarly shown that $\beta^*(w)$ must be an ancestor of u . Thus, $f(u) - \Delta \leq g(w) \leq f(u) + \Delta \Rightarrow |f(u) - g(w)| \leq \Delta$. We thus have

$$|d_1(x_1, x_2) - d_2(y_1, y_2)| \leq 4\Delta.$$

It then follows that $\text{Dist}(C) \leq 4\Delta$. Since $d_{GH}(\mathcal{T}_1, \mathcal{T}_2) \leq \frac{1}{2}\text{Dist}(C)$, the lemma follows. $\square$

Next, we prove an upper bound on Δ .

LEMMA 4.2. $\Delta \leq 14d_{GH}(\mathcal{T}_1, \mathcal{T}_2)$.

PROOF. Set $\delta = d_{GH}(\mathcal{T}_1, \mathcal{T}_2)$ and let $C^* : T_1 \times T_2$ be an optimal correspondence that achieves $d_{GH}(\mathcal{T}_1, \mathcal{T}_2)$. Note that in general $d_{GH}(\mathcal{T}_1, \mathcal{T}_2)$ may only be achieved in the limit. In that case, our proof can be modified by considering a near-optimal correspondence of distortion $\delta = d_{GH}(\mathcal{T}_1, \mathcal{T}_2) + \varepsilon$ for some arbitrary $\varepsilon > 0$.

Let s be one of the endpoints of a longest simple path in T_1 (i.e., the length of this path realizes the diameter of $\mathcal{T}_1$); s is necessarily a leaf of T_1 . Let (s, t) be a pair in C^* . Consider the merge trees T_1^s and T_2^t defined by the functions f_s and f_t , respectively. A result by Dey et al. [8, Corollary 6] (see also [9]) implies that

$$d_I(T_1^s, T_2^t) \leq 6\delta.$$

We prove below in Claim 4.3 that there is a vertex (in fact, a leaf) $z \in V(T_2)$ such that $d_2(t, z) \leq 8\delta$.

It is easy to verify that

$$\|f_t - f_z\|_\infty \leq d_2(t, z) \leq 8\delta.$$

On the other hand, by the stability theorem of the interleaving distance,

$$d_I(T_2^t, T_2^z) \leq \|f_t - f_z\|_\infty \leq 8\delta.$$

By the triangle inequality,

$$\begin{aligned} d_I(T_1^s, T_2^z) &\leq d_I(T_1^s, T_2^t) + d_I(T_2^t, T_2^z) \\ &\leq 6\delta + 8\delta \\ &\leq 14\delta. \end{aligned}$$

This completes the proof of the lemma. $\square$

CLAIM 4.3. *Let s be an endpoint of a longest simple path in T_1 , and let (s, t) be a pair in C^* . Then there is a vertex $z \in V(T_2)$ such that $d_2(t, z) \leq 8\delta$.*

PROOF. Assume that there is no tree node within 8δ distance to t . In this case, t must be in the interior of an edge $e \in E(T_2)$. Let u_1 and u_2 be the two points in e from opposite sides of t such that $d_2(t, u_1) = d_2(t, u_2) = 8\delta + \nu$, where $\nu > 0$ is an arbitrarily small value. Both u_1 and u_2 exist, as there is no tree node of T_2 within 8δ distance to t , and

$$d_2(u_1, u_2) = d_2(t, u_1) + d_2(t, u_2) = 16\delta + 2\nu.$$

Let $\tilde{u}_1, \tilde{u}_2 \in T_1$ be any corresponding points for u_1 and u_2 under C^* , that is, $(\tilde{u}_1, u_1), (\tilde{u}_2, u_2) \in C^*$. Since $\text{Dist}(C^*) \leq 2\delta$, we have

$$d_1(\tilde{u}_1, \tilde{u}_2) \geq 14\delta + 2\nu. \quad (5)$$

On the other hand, since $d_2(t, u_1) = d_2(t, u_2) = 8\delta + \nu$, we have that

$$d_1(s, \tilde{u}_1), d_1(s, \tilde{u}_2) \in [6\delta + \nu, 10\delta + \nu]. \quad (6)$$

We now obtain an upper bound on $d_1(\tilde{u}_1, \tilde{u}_2)$.

If $\tilde{u}_1$ and $\tilde{u}_2$ have ancestor/descendant relation in T_1^s , then $d_1(\tilde{u}_1, \tilde{u}_2) = |d_1(s, \tilde{u}_1) - d_1(s, \tilde{u}_2)|$ and by Equation (6), we thus have that $d_1(\tilde{u}_1, \tilde{u}_2) \leq 4\delta$, which contradicts Equation (5). Otherwise, if $\tilde{u}_1$ and $\tilde{u}_2$ do not have ancestor/descendant relation, let w be the nearest common ancestor of $\tilde{u}_1$ and

Fig. 5. w is the nearest common ancestor of $\tilde{u}_1$ and $\tilde{u}_2$ in T_1^s .

$\tilde{u}_2$ in T_1^s (see Figure 5). Let $c_0 = d_1(s, w)$. For simplicity, set $a = d_1(s, \tilde{u}_1)$ and $b = d_1(s, \tilde{u}_2)$. It then follows that

$$d_1(\tilde{u}_1, \tilde{u}_2) = a + b - 2c_0. \text{ Note, } a \geq c_0, b \geq c_0. \quad (7)$$

Since s is an endpoint of the longest path in T_1 , it follows that $c_0 \geq \min\{a - c_0, b - c_0\}$. Indeed, if this were not the case, then without loss of generality, suppose the other point s' of the diameter pair is not in the subtree of T_1^s rooted at $\tilde{u}_1$. We then have

$$d_1(\tilde{u}_1, s') = (a - c_0) + (b - c_0) > c_0 + (b - c_0) = d_1(s, s'), \quad (8)$$

a contradiction. By Equation (6), $a, b \geq 6\delta + \nu$. Thus,

$$c_0 \geq \min\{a - c_0, b - c_0\} \geq 6\delta + \nu - c_0 \Rightarrow c_0 \geq \frac{1}{2}(6\delta + \nu). \quad (9)$$

Combining Equations (7) and (9), we have

$$d_1(\tilde{u}_1, \tilde{u}_2) \leq a + b - 6\delta - \nu \leq 20\delta + 2\nu - 6\delta - \nu = 14\delta + \nu, \quad (10)$$

contradicting Equation (5). Thus, there exists $z \in V(T_2)$ such that $d_2(t, z) \leq 8\delta$. $\square$

Remark. The proof of Claim 4.3 actually shows that t lies within distance 8δ of at least one leaf, as we never use the fact that u_1 and u_2 lie on the same edge of T_2 . The only fact we use is that u_1 and u_2 lie on opposite sides of t at distance $8\delta + \nu$ each.

From Lemmas 4.1 and 4.2, we get the following.

THEOREM 4.4. *Let $\Delta = \min_{u \in V(T_1), v \in V(T_2)} d_I(T_1^u, T_2^v)$. Then*

$$\frac{1}{2}d_{GH}(\mathcal{T}_1, \mathcal{T}_2) \leq \Delta \leq 14d_{GH}(\mathcal{T}_1, \mathcal{T}_2).$$

In order to approximate $d_{GH}(\mathcal{T}_1, \mathcal{T}_2)$, we merely need to approximate the interleaving distance for each of the $O(n^2)$ pairs of merge trees obtained by rooting $\mathcal{T}_1$ and $\mathcal{T}_2$ at each of their vertices.

COROLLARY 4.5. *If there is a polynomial time, c -approximation algorithm for the interleaving distance between two merge trees, then there is a polynomial time, $28c$ -approximation algorithm for the GH distance between two metric trees that runs the algorithm for interleaving distance $O(n^2)$ times.*

5 COMPUTING THE INTERLEAVING DISTANCE

Let M_f and M_g be merge trees of two functions f and g , respectively. For simplicity, we use f and g to denote the height functions on M_f and M_g as well. Let n be the total number of nodes in M_f and M_g , and let $r \geq 1$ be the ratio between the lengths of the longest and the shortest edges in M_f and M_g . We describe a $O(\min\{n, \sqrt{rn}\})$ -approximation algorithm for computing $d_I(M_f, M_g)$.

Candidate values and binary search. We first show that a candidate set Λ of $O(n^2)$ values can be computed in $O(n^2)$ time such that $d_I(M_f, M_g) \in \Lambda$. Given Λ , we perform a binary search on Λ .

Fig. 6. Trees M_f and M_g . Here $\delta_v = \min\{\frac{1}{2}\epsilon_1, \epsilon_2\}$.

At each step, we use a c -approximate decision procedure, for $c = c_1 \min\{n, \sqrt{rn}\}$ for some constant c_1 , that given a value $\epsilon > 0$ does the following: if $d_I(M_f, M_g) \leq \epsilon$, it returns a pair of $c\epsilon$ -compatible maps between M_f and M_g ; if $d_I(M_f, M_g) > \epsilon$, it will either return a pair of $c\epsilon$ -compatible maps between M_f and M_g or report that no pair of ϵ -compatible maps exist.

We perform the binary search using the c -approximate decision procedure in the following way: if the procedure returns a pair of $c\epsilon$ -compatible maps for a value $\epsilon \in \Lambda$, we continue the search using only lesser values of ϵ . Otherwise, we continue the search using only higher values of ϵ . When there are no more candidate values to search, we return the maps for the minimum value of ϵ that yielded a pair of maps.

The above procedure returns a pair of $c\epsilon$ -compatible maps where $d_I(M_f, M_g) \leq c\epsilon \leq cd_I(M_f, M_g)$. Indeed, the procedure does not run out of candidate values $\epsilon < d_I(M_f, M_g)$ until it has tried some $\epsilon' \leq d_I(M_f, M_g)$ for which the approximate decision procedure returned a pair of $c\epsilon'$ -compatible maps. We now describe the candidate set Λ .

Let V_f (V_g , respectively) be the set of nodes in M_f (M_g , respectively). We define $\Lambda = \Lambda_{11} \cup \Lambda_{22} \cup \Lambda_{12}$, where

$$\begin{aligned}\Lambda_{11} &= \{\tfrac{1}{2}|f(u) - f(v)| \mid u, v \in V_f\}, \\ \Lambda_{22} &= \{\tfrac{1}{2}|g(u) - g(v)| \mid u, v \in V_g\}, \\ \Lambda_{12} &= \{|f(u) - g(v)| \mid u \in V_f, v \in V_g\}.\end{aligned}$$

LEMMA 5.1. $d_I(M_f, M_g) \in \Lambda$.

PROOF. Suppose to the contrary that $d_I(M_f, M_g) = \epsilon \notin \Lambda$. Let $\alpha : M_f \rightarrow M_g$ and $\beta : M_g \rightarrow M_f$ be ϵ -compatible maps that realize $d_I(M_f, M_g) = \epsilon$. We will obtain a contradiction by choosing $\epsilon_0 > 0$ and constructing $(\epsilon - \epsilon_0)$ -compatible maps $\hat{\alpha}, \hat{\beta}$.

For any point $x \in M_f$, we define $\alpha_{\downarrow}(x) = \alpha(x)$ if $\alpha(x)$ is a node of M_g , otherwise $\alpha_{\downarrow}(x)$ is the lower endpoint of the edge of M_g containing $\alpha(x)$. Similarly we define the function $\beta_{\downarrow} : M_g \rightarrow M_f$.

For every node $v \in V_f$, $\alpha(v)$ ($\beta(\alpha(v))$, respectively) lies in the interior of an edge of M_g (M_f , respectively), because $\epsilon \notin \Lambda \cup \Lambda_{12}$ (Λ_{11} , respectively). We define

$$\delta_v = \min \left\{ \tfrac{1}{2} (f(\beta(\alpha(v))) - f(\beta_{\downarrow}(\alpha(v))), g(\alpha(v)) - g(\alpha_{\downarrow}(v))) \right\}.$$

See Figure 6. Similarly, we define δ_w for all $w \in V_g$. We set

$$\epsilon_0 = \min \left\{ \epsilon, \min_{v \in V_f \cup V_g} \delta_v \right\}.$$

Since $\epsilon \notin \Lambda$, we have $\epsilon_0 > 0$. We now construct $(\epsilon - \epsilon_0)$ -compatible maps $\hat{\alpha} : M_f \rightarrow M_g$ and $\hat{\beta} : M_g \rightarrow M_f$ (note $\epsilon_0 \leq \epsilon$, so $\epsilon - \epsilon_0$ is non-negative). We describe the construction of $\hat{\alpha}$; $\hat{\beta}$ is

Fig. 7. Figure showing u, v, x, y , and y' .

constructed similarly. By construction, for any node $u \in V_f$, $g(\alpha(u)) - g(\alpha_{\downarrow}(u)) \geq \varepsilon_0$, so we set $\hat{\alpha}(u)$ to be the point w on the edge of M_g containing $\alpha(u)$ such that $g(w) = f(u) + \varepsilon - \varepsilon_0$. Once we have defined $\hat{\alpha}(u)$ and $\hat{\alpha}(v)$ for an edge $uv \in M_f$, with $f(u) < f(v)$, we set $\hat{\alpha}(x)$, for a point $x \in uv$ with $f(x) = f(u) + \gamma$, to be

$$\hat{\alpha}(x) = \sigma_g^{\gamma}(\hat{\alpha}(u)).$$

That is, we set $\hat{\alpha}(x)$ to be the ancestor of $\hat{\alpha}(u)$ at height $f(u) + \varepsilon - \varepsilon_0 + \gamma = f(x) + \varepsilon - \varepsilon_0$. Now, it is not too hard to see that if x_1 is an ancestor of x_2 in M_f , then $\hat{\alpha}(x_1)$ is an ancestor of $\hat{\alpha}(x_2)$ (similarly for $\hat{\beta}$). Further, $\hat{\beta}(\hat{\alpha}(x_1))$ is a descendant of $\beta(\alpha(x_1))$ for all $x_1 \in M_f$ (a similar result holds for $\hat{\alpha} \circ \hat{\beta}$ and $\alpha \circ \beta$).

We claim that $\hat{\alpha}, \hat{\beta}$ are $(\varepsilon - \varepsilon_0)$ -compatible. Indeed, by construction, $g(\hat{\alpha}(x)) = f(x) + \varepsilon - \varepsilon_0$ for all $x \in M_f$, and $f(\hat{\beta}(y)) = g(y) + \varepsilon - \varepsilon_0$ for all $y \in M_g$. We now prove that

$$\hat{\beta} \circ \hat{\alpha} = \sigma_f^{2(\varepsilon - \varepsilon_0)}.$$

Suppose to the contrary there is a point $x \in M_f$ such that $y = \hat{\beta}(\hat{\alpha}(x)) \neq \sigma_f^{2(\varepsilon - \varepsilon_0)}(x)$. Since $f(y) = f(x) + 2(\varepsilon - \varepsilon_0)$, y must not be an ancestor of x . On the other hand, α, β are ε -compatible, so $y' = \beta(\alpha(x))$ is the ancestor of x at height $f(x) + 2\varepsilon$. By construction of $\hat{\alpha}$ and $\hat{\beta}$, y is a descendant of y' , in which case there is a node $u \in V_f$ that lies between y and y' . (If y and y' lie on the same edge of M_f , then y is also an ancestor of x .) Let $u = \beta_{\downarrow}(\alpha(x))$. Let v be the lower endpoint of the edge e containing x . See Figure 7. Since $\varepsilon \notin \Lambda$, $f(u) \neq f(v) + 2\varepsilon$ (i.e., $u \neq \beta(\alpha(v))$). There are two cases to consider:

- (i) $f(u) > f(v) + 2\varepsilon$. Then let $u = \beta(\alpha(z))$ for the point z lying between x and v at height $f(z) = f(u) - 2\varepsilon$. Furthermore, $f(x) \geq f(z) > f(x) - 2\varepsilon_0$ (if $f(x) - f(z) \geq 2\varepsilon_0$, then $f(y') - f(u) = f(x) - f(z) \geq 2\varepsilon_0$, contradicting the fact that $f(y') - f(y) = 2\varepsilon_0$). Therefore, we can choose a point $w \neq v$ on e such that $f(z) > f(w) > f(x) - 2\varepsilon_0$. We have $\hat{\beta}(\hat{\alpha}(w))$ is a descendant of $y = \hat{\beta}(\hat{\alpha}(x))$ (since w is a descendant of x). Moreover, $\beta(\alpha(w))$ is an ancestor of $\hat{\beta}(\hat{\alpha}(w))$. However, since $f(\beta(\alpha(w))) < f(u)$, $\beta(\alpha(w))$ lies between y and u . Thus, $\beta(\alpha(w))$ is not an ancestor of x (hence, w), that is, $\beta(\alpha(w)) \neq \sigma_f^{2\varepsilon}(w)$, contradicting the fact that α, β are ε -compatible.
- (ii) $f(u) < f(v) + 2\varepsilon$. In this case

$$f(\beta(\alpha(v))) - f(\beta_{\downarrow}(\alpha(v))) \leq f(\beta(\alpha(v))) - f(u) < f(y') - f(y) = 2\varepsilon_0 \leq 2\delta_v,$$

which contradicts the definition of δ_v .

Hence, we conclude that y is an ancestor of x , that is, $\hat{\beta} \circ \hat{\alpha} = \sigma_f^{2(\varepsilon - \varepsilon_0)}$. Similarly, one can argue that $\hat{\alpha} \circ \hat{\beta} = \sigma_g^{2(\varepsilon - \varepsilon_0)}$, implying that $\hat{\alpha}, \hat{\beta}$ are $(\varepsilon - \varepsilon_0)$ -compatible maps as claimed.

Putting everything together, we conclude that $\varepsilon \in \Lambda$. $\square$

We now describe the decision procedure to answer the question “is $d_I(M_f, M_g) \leq \varepsilon$?” approximately. Given a parameter $\varepsilon > 0$, an edge is called ε -long, or *long* for brevity, if its length is strictly greater than 2ε . We first describe an exact decision procedure for the case when all edges in both trees are long, and then describe an approximate decision procedure for the case when the two trees have short edges.

Trees with long edges. We remove all degree-two nodes in the beginning. A *subtree* rooted at a point x in a merge tree M , denoted M^x , includes all the points in the merge tree that are descendants of x and an edge from x that extends upward to height ∞ . For a node $u \in V$, let $C(u)$ denote the children of u and let $p(u)$ denote its parent. Assume $d_I(M_f, M_g) \leq \varepsilon$, and let $\alpha : M_f \rightarrow M_g$ and $\beta : M_g \rightarrow M_f$ be a pair of ε -compatible maps. As in the proof of Lemma 5.1, we define the functions $\alpha_\downarrow$ and $\beta_\downarrow$ but restricted only to the vertices of M_f and M_g . That is, for a node $v \in V_f$, we define $\alpha_\downarrow(v)$ to be the lower endpoint of the edge containing $\alpha(v)$ —if $\alpha(v)$ is a node, then $\alpha_\downarrow(v)$ is $\alpha(v)$ itself. Similarly, we define $\beta_\downarrow(w)$, for a node $w \in V_g$.

The following two properties of $\alpha_\downarrow$ and $\beta_\downarrow$ will be crucial for the decision procedure.

LEMMA 5.2. *If all edges in M_f and M_g are ε -long, then the following hold: (i) For a node $v \in V_f$, $|f(v) - g(\alpha_\downarrow(v))| \leq \varepsilon$, and (ii) for a node $w \in V_g$, $|g(w) - f(\beta_\downarrow(w))| \leq \varepsilon$.*

PROOF. We will prove part (i); part (ii) is similar. By definition, $g(\alpha_\downarrow(v)) \leq f(v) + \varepsilon$. Suppose $g(\alpha_\downarrow(v)) < f(v) - \varepsilon$. Let v' be a point in M_g lying on the edge containing $\alpha(v)$ and $\alpha_\downarrow(v)$ with height $f(v) - \varepsilon - \varepsilon_0$, for some sufficiently small ε_0 . Then $\beta(v')$ lies in one of the subtrees rooted at the children of v , say M_1 . Consider a descendant u of v at height $g(v') - \varepsilon$ lying in a different subtree M_2 rooted at v 's child. Such a descendant exists, because all edges are ε -long. Since by definition and our choice of v' there does not exist any node in M_g between $\alpha(v)$ and v' , we have $\alpha(u) = v'$. But then $\beta(\alpha(u)) = \beta(v')$ lies in M_1 , and hence is not an ancestor of $u \in M_2$; in other words, $\beta(\alpha(u)) \neq \sigma_f^{2\varepsilon}(u)$. This contradicts the fact that α and β are ε -compatible. Thus, $g(\alpha_\downarrow(v)) \geq f(v) - \varepsilon$, and the claim follows. $\square$

LEMMA 5.3. *If all edges in M_f and M_g are ε -long, then $\alpha_\downarrow$ and $\beta_\downarrow$ are bijections with $\beta_\downarrow = \alpha_\downarrow^{-1}$ (and $\alpha_\downarrow = \beta_\downarrow^{-1}$).*

PROOF. We will first show that $\beta_\downarrow = \alpha_\downarrow^{-1}$. Suppose to the contrary there exists a vertex $v \in V_f$ such that $\beta_\downarrow(\alpha_\downarrow(v)) = w \neq v$. Let $\alpha_\downarrow(v) = u$, for $u \in V_g$. From Lemma 5.2 we have $|f(v) - f(w)| \leq 2\varepsilon$. Since all edges are longer than 2ε and $v \neq w$, v cannot be an ancestor/descendant of w in M_f . By definition of $\alpha_\downarrow$, $\alpha(v)$ is an ancestor of $\alpha_\downarrow(v) = u$. Thus, $\beta(\alpha(v))$ is an ancestor of $\beta(u)$. Further, $|f(v) - g(u)| \leq \varepsilon$ (Lemma 5.2) and $\beta(\alpha(v)) = \sigma_f^{2\varepsilon}(v)$ (since α, β are ε -compatible). Hence, $\beta(u)$ lies between v and $\beta(\alpha(v))$ on the edge e whose lower endpoint is v as e is ε -long. Thus, $\beta(u)$ is an ancestor of v . See Figure 8. Also by definition of $\beta_\downarrow$, $\beta(u)$ is an ancestor of $\beta_\downarrow(u) = w$. Thus, w is a descendant of v , a contradiction since v cannot be an ancestor of w .

We thus have $\beta_\downarrow = \alpha_\downarrow^{-1}$. Similarly, we can show that $\alpha_\downarrow = \beta_\downarrow^{-1}$. This also implies that $\alpha_\downarrow$ and $\beta_\downarrow$ are bijections. $\square$

We define an indicator function $\Phi : V_f \times V_g \rightarrow \{0, 1\}$ such that

$$\Phi(u, v) = \begin{cases} 1, & \text{if } d_I(M_f^u, M_g^v) \leq \varepsilon, \\ 0, & \text{otherwise.} \end{cases}$$

Fig. 8. Figure showing $\beta(u) = \beta(\alpha_{\downarrow}(v))$ is an ancestor of v .

The following lemma gives a recursive definition of $\Phi(u, v)$.

For two integers, k and ℓ with $k \leq \ell$, let $[k, \ell] = \{k, k+1, \dots, \ell\}$.

LEMMA 5.4. *Suppose all the edges in M_f and M_g are ε -long. Let $(u, v) \in V_f \times V_g$, and let u_i and v_j denote the i -th and j -th child, respectively, of u and v . We have $\Phi(u, v) = 1$ if and only if the following conditions hold: (i) $|f(u) - g(v)| \leq \varepsilon$, (ii) $|C(u)| = |C(v)|$, and (iii) there exists a permutation π of $[1 : |C(u)|]$ such that $\Phi(u_i, v_{\pi(i)}) = 1$ for all $i \in [1 : |C(u)|]$.*

PROOF. Suppose $\Phi(u, v) = 1$, and let α, β be the corresponding ε -compatible maps. Suppose property (i) does not hold, and let $f(u) > g(v) + \varepsilon$ without loss of generality. Thus, $\beta(v)$ maps to one of the multiple edges incident to u , and there exists at least one edge $e = (u, w)$ with $w \in C(u)$ such that none of e 's points (other than u) is in the image of β . However, $\beta(\alpha(w)) = \sigma_f^{2\varepsilon}(w)$ must lie in the interior of e (since e is ε -long), a contradiction. To prove that (ii) holds, note that by Lemma 5.3 and monotonicity of $\alpha_{\downarrow}$ and $\beta_{\downarrow}$, there exist bijections $\alpha_{\downarrow}, \beta_{\downarrow}$ between the vertices of M_f^u and M_g^v such that if $u_1 \in C(u_2)$ for a vertex $u_2 \in M_f^u$, then $\alpha_{\downarrow}(u_1) \in C(\alpha_{\downarrow}(u_2))$ (a symmetric statement holds for $\beta_{\downarrow}$ and vertices in M_g^v). Thus, $\alpha_{\downarrow}, \beta_{\downarrow}$ induce bijections between $C(u)$ and $C(v)$, and hence $|C(u)| = |C(v)|$. Finally, for (iii), let $\alpha_{\downarrow}(u') = v'$ for some $u' \in C(u), v' \in C(v)$. Then by definition of $\alpha_{\downarrow}$ and $\beta_{\downarrow}$, $\alpha(M_f^{u'}) \subseteq M_g^{v'}$ and $\beta(M_g^{v'}) \subseteq M_f^{u'}$. This means that the restriction of the pair of ε -compatible maps α and β to $M_f^{u'}$ and $M_g^{v'}$, respectively, remain ε -compatible for $M_f^{u'}$ and $M_g^{v'}$. Thus, $\Phi(u', v') = 1$, and the permutation π is defined by $\alpha_{\downarrow}, \beta_{\downarrow}$.

We now prove the opposite direction. Suppose properties (i), (ii), and (iii) hold. Let (α_i, β_i) be the pair of ε -compatible maps between $M_f^{u_i}$ and $M_g^{v_{\pi(i)}}$. Then, a pair of ε -compatible maps (α, β) between M_f^u and M_g^v is obtained as follows: $\alpha(x) = \{\alpha_i(x) \mid x \in M_f^{u_i}\}$ (β is defined similarly). Note that points on the infinite edge from u (v , respectively) upward are *shared* among all $M_f^{u_i}$ ($M_g^{v_j}$, respectively), whereas all other points in M_f^u (M_g^v , respectively) are present in only one $M_f^{u_i}$ ($M_g^{v_j}$, respectively). However, since $|f(u) - g(v)| \leq \varepsilon$, *shared* points are mapped to *shared* points and we have $|\alpha(x)| = 1$ ($|\beta(y)| = 1$), respectively for all $x \in M_f^u$ ($y \in M_g^v$, respectively). Thus, α and β are functions and satisfy all the required properties. Hence, $\Phi(u, v) = 1$. $\square$

Decision procedure. We compute Φ for all pairs of nodes in $V_f \times V_g$ in a bottom-up manner and return $\Phi(r_f, r_g)$ where r_f (r_g , respectively) is the root of M_f (M_g , respectively). Let $(u, v) \in V_f \times V_g$.

Suppose we have computed $\Phi(u_i, v_j)$ for all $u_i \in C(u)$ and $v_j \in C(v)$. We compute $\Phi(u, v)$ as follows. If (i) or (ii) of Lemma 5.4 does not hold for u and v , then we return $\Phi(u, v) = 0$. Otherwise, we construct the bipartite graph $G_{uv} = \{C(u) \cup C(v), E = \{(u_i, v_j) \mid \Phi(u_i, v_j) = 1\}\}$ and determine in $O(k^{5/2})$ time whether G_{uv} has a perfect matching, using the algorithm by Hopcroft and Karp [13]. Here, $k = |C(u)| = |C(v)|$. If G_{uv} has a perfect matching $M = \{(u_1, v_{\pi(1)}), \dots, (u_k, v_{\pi(k)})\}$, we

Fig. 9. A naive map.

set $\Phi(u, v) = 1$, else we set $\Phi(u, v) = 0$. If $\Phi(u, v) = 1$, we use the ε -compatible maps for $M_f^{u_i}, M_g^{v_{\pi(i)}}$, for $1 \leq i \leq k$, to compute a pair of ε -compatible maps between M_f^u and M_g^v , as discussed in the proof of Lemma 5.4.

For a node $u \in V_f \cup V_g$, let k_u be the number of its children. The total time taken for running Hopcroft and Karp [13] is

$$\sum_{u \in V(T_1)} \sum_{v \in V(T_2)} O(k_u k_v \sqrt{k_v}) = \sum_{u \in V(T_1)} k_u \sum_{v \in V(T_2)} O(k_v \sqrt{k_v}) \leq O(n^{3/2}) \sum_{u \in V(T_1)} k_u \leq O(n^{5/2}).$$

Hence, we obtain the following.

LEMMA 5.5. *Given two merge trees M_f and M_g and a parameter $\varepsilon > 0$ such that all edges of M_f and M_g are ε -long, then whether $d_I(M_f, M_g) \leq \varepsilon$ can be determined in $O(n^{5/2})$ time. If the answer is yes, a pair of ε -compatible maps between M_f and M_g can be computed within the same time.*

Trees with short edges. Given two merge trees, a naive map is to map the lowest among all the leaves in both the trees to a point at height equal to the height of the higher of the two roots of M_f and M_g (see Figure 9). Thus, all the points in one tree will be mapped to the infinitely long edge on the other tree. This map produces a distortion equal to the height of the trees, which can be arbitrarily larger than the optimum. Nevertheless, this simple idea leads to an approximation algorithm.

Here is an outline of the algorithm. After carefully *trimming* off short subtrees from the input trees, the algorithm decomposes the resulting trimmed trees into two kinds of regions: those with nodes and those without nodes. If the interleaving distance between the input trees is small, then there exists an isomorphism between trees induced by the regions without nodes. Using this isomorphism, the points in the nodeless regions are mapped without incurring additional distortion. Using a counting argument and the naive map described above, it is shown that the distortion incurred while mapping the regions with nodes and the trimmed regions is bounded.

More precisely, given M_f, M_g and $\varepsilon > 0$, define the *extent* $e(x)$ of a point x (which is not necessarily a tree node) in M_f or M_g as the maximum height difference between x and any of its descendants. Suppose each edge is at most ε long. Let M'_f and M'_g be subsets of M_f and M_g consisting only of points with extent at least $2(\sqrt{2ns} + 1)\varepsilon$, adding nodes to the new leaves of M'_f and M'_g as necessary. Note that M'_f and M'_g themselves are trees; however, they might contain nodes of degree 2. See Figure 10 for an example.

Fig. 10. Trimming a tree: (left) original tree, red points have extent $< 2(\sqrt{2ns} + 1)\epsilon$; (right) trimmed tree, nodes added at the bottom (hollowed nodes).

LEMMA 5.6. *If $d_I(M_f, M_g) \leq \epsilon$, then $d_I(M'_f, M'_g) \leq \epsilon$.*

PROOF. Let $\alpha : M_f \rightarrow M_g$ and $\beta : M_g \rightarrow M_f$ be ϵ -compatible maps. Let α' and β' be restrictions of the functions' domains to M'_f and M'_g , respectively. We argue that the ranges of α' and β' lie in M'_g and M'_f , respectively. Suppose otherwise. Then without loss of generality, there is a point $x \in M'_f$ with $y = \alpha(x)$ not in M'_g . Because $x \in M'_f$, its extent in M_f is at least $2(\sqrt{2ns} + 1)\epsilon$. Therefore, there exists a descendant x' of x in M_f with $f(x') = f(x) - 2(\sqrt{2ns} + 1)\epsilon$. Because y is not in M'_g , the extent of y must be less than $2(\sqrt{2ns} + 1)\epsilon$ and there exists no descendant y' of y with $g(y') = g(y) - 2(\sqrt{2ns} + 1)\epsilon = f(x) - 2(\sqrt{2ns} + 1)\epsilon + \epsilon = f(x') + \epsilon$. Since $g(\alpha(x')) = f(x') + \epsilon$, $\alpha(x')$ is not a descendant of $\alpha(x)$, which contradicts the assumption that α, β are ϵ -compatible maps. $\square$

The above lemma can be easily generalized to say that removing points in both trees with extent less than or equal to any fixed value does not increase the distance between them.

We now define *matching points* in M'_f and M'_g . Let H be the set of function values for leaves and branching nodes in M'_f or M'_g , and let $H' \subseteq H$ be the subset of H consisting of function values h for which $(h, h + 2\epsilon]$ does not intersect H . A point x in M'_f is a matching point if $f(x) \in H'$. Similarly, a point y in M'_g is a matching point if $g(y) \in H'$. By this definition, no two matching points share a function value within 2ϵ of each other unless they share the exact same function value. Furthermore, if x is a matching point, then all points with the same function value as x on both M'_f and M'_g are matching points. There are $O(n^2)$ matching points.

Suppose $d_I(M'_f, M'_g) \leq \epsilon$, and let $\alpha' : M'_f \rightarrow M'_g$ and $\beta' : M'_g \rightarrow M'_f$ be a pair of ϵ -compatible maps. Call a matching point x in M'_f and a matching point y in M'_g with $f(x) = g(y)$ *matched* if $\alpha'(x)$ is an ancestor of y .

LEMMA 5.7. *Let x be any matching point in M'_f . The matched relation between matching points in M'_f at height $f(x)$ and matching points in M'_g at height $f(x)$ is a bijective function.*

PROOF. No two distinct matching points y_1 and y_2 on M'_g with $f(x) = g(y_1) = g(y_2)$ share the same ancestor with function value $f(x) + \epsilon$, because they have no branching node ancestors with low enough function value. Therefore, a matching point in M'_f can be matched to only one matching point in M'_g .

Let x_1 and x_2 be two distinct matching points from M'_f with $f(x) = f(x_1) = f(x_2)$. If $\alpha'(x_1)$ and $\alpha'(x_2)$ are ancestors of a common matching point y , then $\alpha'(x_1) = \alpha'(x_2)$ and thus x_1 and x_2 must have a common ancestor x' at height $f(x) + 2\epsilon$. However, x_1 and x_2 have no branching node

Fig. 11. The left tree shows matching points on tree M'_f and the right tree shows $\tilde{M}_f$.

ancestor with low enough function value for x' to exist. Hence, the matching relation must be injective from matching points in M'_f to M'_g .

Finally, consider any matching point y on M'_g with $g(y) = f(x)$. Point $x'_1 = \beta'(y)$ is the ancestor of a matching point x_1 on M'_f with $f(x_1) \geq g(y)$. (Note that by the same argument as the beginning of this proof, only one such matching point x_1 can exist.) Point $y' = \alpha'(x'_1)$ is an ancestor of y with $g(y') \leq g(y) + 2\varepsilon$. Point y is the only descendant of y' with function value $f(x)$. Point $\alpha'(x_1)$ must be an ancestor of y , meaning x_1 and y are matched. Thus, the matching relation is surjective. $\square$

We now define a rooted tree $\tilde{M}_f$ to be a rooted tree consisting of one node per matching point on M'_f . Let $p(v)$ be the matching point for node v . $\tilde{M}_f$ has node v as an ancestor of node u if $p(v)$ is an ancestor of $p(u)$ (see Figure 11). Define $\tilde{M}_g$ similarly. The size of $\tilde{M}_f$ and $\tilde{M}_g$ is $O(n^2)$. Intuitively, $\tilde{M}_f$ and $\tilde{M}_g$ represent the trees induced by matching points. By the definition of interleaving distance and Lemma 5.7, $\tilde{M}_f$ and $\tilde{M}_g$ are isomorphic if M'_f and M'_g satisfy that $d_I(M'_f, M'_g) \leq \varepsilon$.

Decision procedure. We are now ready to describe the decision procedure. We first construct the subtrees M'_f and M'_g of M_f and M_g , respectively, consisting of points with extent at least $2(\sqrt{2ns} + 1)\varepsilon$. Next, we compute matching points on M'_f and M'_g and construct the trees $\tilde{M}_f$ and $\tilde{M}_g$ on these matching points, as defined above.

Using the algorithm of [2, chap. 3, p. 85], we determine in time linear in the size of the trees whether $\tilde{M}_f$ and $\tilde{M}_g$ are isomorphic. If the answer is no, we return no. By Lemma 5.7, $d_I(M_f, M_g) > \varepsilon$ in this case. Otherwise, we construct the following functions $\alpha : M_f \rightarrow M_g$ and $\beta : M_g \rightarrow M_f$ and return them. Recall, it suffices to perform assignments where the function value increases by at most $c\varepsilon$. For each pair of matching points x and y matched by the isomorphism, the algorithm sets $\alpha(x) = y$ and $\beta(y) = x$. Now, let (ξ_1, ξ_2) be any maximal range of function values without any branching nodes or leaves in M'_f or M'_g with $\xi_2 - \xi_1 > 2\varepsilon$. Let x' be any point in M'_f with $f(x') \in (\xi_1, \xi_2)$. Point x' has a unique matching point descendant x at height ξ_1 , by the definition of matching points. The algorithm sets $\alpha(x')$ to the point y' in M'_g where y' is the ancestor of $\alpha(x)$ with $g(y') = f(x')$, and it sets $\beta(y') = x'$. For every remaining point x'' in M'_f , the algorithm sets $\alpha(x'')$ to $\alpha(x)$ where x is the lowest matching point ancestor of x'' . $\beta(y'')$ is defined similarly for remaining points y'' in M'_g that were not paired with some x' . We call such points x'' and y'' lazily assigned. See Figure 12. Finally, each point z in $M_f - M'_f$ has $\alpha(z)$ set to $\alpha(x)$ where x is the lowest ancestor of z in M'_f . Similar assignments are done for points in $M_g - M'_g$.

Fig. 12. Figure showing points x, y, x', y', x'', y'' .

LEMMA 5.8. (i) For each lazily assigned point $x'' \in M'_f$,

$$g(\alpha(x'')) \leq f(x'') + 2(\sqrt{2ns} + 1)\varepsilon.$$

(ii) For each lazily assigned point $y'' \in M'_g$,

$$f(\beta(y'')) \leq g(y'') + 2(\sqrt{2ns} + 1)\varepsilon.$$

PROOF. We only prove (i); (ii) is symmetric. The higher of the two roots of M'_f and M'_g is a matching point, and so are all the points at that height. Thus, all lazily assigned points have a matching point ancestor. We show that the nearest such ancestor cannot be too much higher up.

Let x be a matching point. We show that there exists a region (ξ_1, ξ_2) as defined above with

$$f(x) - 2(\sqrt{2ns} + 1)\varepsilon \leq \xi_2 \leq f(x).$$

Consider sweeping over the function values downward starting at $f(x)$ and let ξ_2 be the largest function value possible for a region as defined above. If the sweep line ever goes a distance greater than 2ε without encountering a branching node or leaf in M'_f or M'_g , then an ξ_2 is found. Therefore, there will be at least one branching node or leaf x' in M'_f or M'_g per descent of 2ε until ξ_2 is found.

Suppose $\xi_2 < f(x) - 2(\sqrt{2ns} + 1)\varepsilon$. Let $l = \sqrt{2ns} + 1$, and $f' = f(x) - 2l\varepsilon$.

Let $\{P_1, P_2, \dots\}$ be a set of paths from each branching node of M'_f or M'_g encountered during the sweep to leaves of M_f and M_g such that for each pair of paths, both paths are disjoint except possibly at the higher endpoint of one of the two paths. Such a set of paths can be found by greedily selecting an arbitrary path for each branching node as it is encountered. In addition, let $\{Q_1, Q_2, \dots\}$ be a set of pairwise-disjoint paths from leaves of M'_f and M'_g to leaves of M_f and M_g . Because each point in M'_f and M'_g has extent at least $2l\varepsilon$, the lower endpoint of each of these paths lies below height f' . Since edge lengths are at most $s\varepsilon$, there are at least $(f(x') - f')/s\varepsilon$ nodes in M_f or M_g on the path P_i or Q_j from each branching node or leaf x' at height $f(x') \in [f', f(x))$, not counting x' itself. In total, these paths contain at least

$$\sum_{i=1}^l \frac{(l-i)2\varepsilon}{s\varepsilon} = \frac{l(l-1)}{s}$$

nodes, not counting their higher endpoints. Each node counted above appears on at most one path P_i and at most one path Q_j , for at most two paths total, so

$$\frac{l(l-1)}{s} \leq 2n \Rightarrow l(l-1) \leq 2ns,$$

a contradiction since $l = \sqrt{2ns} + 1$. Therefore, either $\xi_2 \geq f(x) - 2(\sqrt{2ns} + 1)\varepsilon$, or the trees M'_f and M'_g do not extend below height $f(x) - 2(\sqrt{2ns} + 1)\varepsilon$. In either case, the lemma follows. $\square$

LEMMA 5.9. *Let M_f and M_g be two merge trees and let $\varepsilon > 0$ be a parameter. There is an $O(n^2)$ time algorithm that returns a pair of $4(\sqrt{2ns} + 1)\varepsilon$ -compatible maps between M_f and M_g , if $d_I(M_f, M_g) \leq \varepsilon$ and the maximum length of a tree edge is $s\varepsilon$. If $d_I(M_f, M_g) > \varepsilon$, then the algorithm may return no or return a pair of $4(\sqrt{2ns} + 1)\varepsilon$ -compatible maps.*

PROOF. Constructing the trees $\tilde{M}_f$ and $\tilde{M}_g$, the corresponding isomorphism between them (if it exists), and the maps α and β between M_f and M_g (if they exist) takes time $O(n^2)$.

Except for the lazily assigned points, all the points in M'_f and M'_g are mapped by α and β , respectively, to points at the same function value. By Lemma 5.8, each point in M'_f and M'_g has its function value changed by at most $2(\sqrt{2ns} + 1)\varepsilon$. Points in $M_f - M'_f$ ($M_g - M'_g$, respectively) have their nearest ancestors in M'_f (M'_g , respectively) at function value at most $2(\sqrt{2ns} + 1)\varepsilon$ away. Since α and β map them to the images of their nearest ancestors, their function values change by at most $2 \cdot 2(\sqrt{2ns} + 1)\varepsilon$. $\square$

Remark. (i) Since the minimum edge length is $\leq 2\varepsilon$, the maximum edge length is $s\varepsilon$, and the ratio between the lengths of the longest and shortest edges is r ; we have $r \geq s/2$.

(ii) If $s = \Omega(n)$, we modify the above algorithm slightly—we skip the trimming step, but keep the rest the same. It can be shown, as in Lemma 5.8, that the height of a point and its image differ by at most $2n\varepsilon$. In particular, the proof no longer requires as complicated a counting argument, because any path contains at most n nodes.

Putting it together. By Lemmas 5.5 and 5.9, the decision procedure takes $O(n^{5/2})$ time. If it returns no, then $d_I(M_f, M_g) > \varepsilon$. If it returns yes, then it also returns $O(\min\{n, \sqrt{rn}\}\varepsilon)$ -compatible maps between them. Hence, we conclude the following.

THEOREM 5.10. *Given two merge trees M_f and M_g with a total of n vertices, there exists an $O(n^{5/2} \log n)$ -time algorithm with an approximation factor of $O(\min\{n, \sqrt{rn}\})$ for computing the interleaving distance between them, where r is the ratio between the lengths of the longest and the shortest edge in both trees.*

Combining Theorem 5.10 with Corollary 4.5, we have the following.

COROLLARY 5.11. *Given two metric trees $\mathcal{T}_1$ and $\mathcal{T}_2$ with a total of n vertices, there exists an $O(n^{9/2} \log n)$ -time algorithm with an approximation factor of $O(\min\{n, \sqrt{rn}\})$ for computing the GH distance between them, where r is the ratio between the lengths of the longest and the shortest edge in both trees.*

6 CONCLUSION

We have presented the first hardness results for computing the GH distance between metric trees. We have also given a polynomial-time approximation algorithm for the problem. But the current gap between the lower and upper bounds on the approximation factor is polynomially large. While we would like to reduce this gap, doing so seems very difficult. On the algorithmic side of things in particular, trying for anything less than an $O(\sqrt{n})$ -approximation appears to prevent our use of algorithms for graph isomorphism, the strongest algorithmic tool used in the above algorithm. We hope that our current investigation will stimulate more research on the theoretical and algorithmic aspects of embedding or matching under additive metric distortion.

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