Abstract

Given data, finding a faithful low-dimensional hyperbolic embedding of the data is a key method by which we can extract hierarchical information or learn representative geometric features of the data. In this paper, we explore a new method for learning hyperbolic representations that takes a metric-first approach. Rather than determining the low-dimensional hyperbolic embedding directly, we learn a tree structure on the data as an intermediate step. This tree structure can then be used directly to extract hierarchical information, embedded into a hyperbolic manifold using Sarkar’s construction (Sarkar, 2012), or used as a tree approximation of the original metric. To this end, we present a novel fast algorithm \textsc{TREP} such that, given a \(\delta\)-hyperbolic metric (for any \(\delta \geq 0\)), the algorithm learns a tree structure that approximates the original metric. In the case when \(\delta = 0\), we show analytically that \textsc{TREP} exactly recovers the original tree structure. We show empirically that \textsc{TREP} is not only many orders of magnitude faster than previous known algorithms, but also produces metrics with lower average distortion and higher mean average precision than most previous algorithms for learning hyperbolic embeddings, extracting hierarchical information, and approximating metrics via tree metrics.

1. Introduction

Extracting hierarchical information from data is a key step in understanding and analyzing the structure of the data in a wide range of areas from the analysis of single cell genomic data (Klimovskaia et al., 2019), to linguistics (Dhingra et al., 2018), computer vision (Khrulkov et al., 2019) and social network analysis (Verbeek & Suri, 2016). In single cell genomics, for example, researchers want to understand the developmental trajectory of cellular differentiation. To do so, they seek techniques to visualize, to cluster, and to infer temporal properties of the developmental trajectory of individual cells.

One way to capture hierarchical structure is represent the data as a tree. Even simple trees, however, cannot be faithfully represented in Euclidean space (Linial et al., 1995), regardless of the dimension of the Euclidean space. As a result, a variety of remarkably effective hyperbolic representation learning methods such as Nickel & Kiela (2017; 2018); Sala et al. (2018) have been developed. These methods learn an embedding in hyperbolic space first and then extract the resulting hyperbolic metric. These methods are successful because of the inherent connections between hyperbolic spaces and trees.

In this paper, we present a metric first approach to extracting hierarchical information and learning hyperbolic representations. The connection between hyperbolic spaces and trees suggests that the correct approach to learning hyperbolic representations is the metric first approach, to first learn a tree and then to embed this tree into hyperbolic space. More generally, The metric first approach to metric representation learning (Gilbert & Sonthalia, 2020) tells us that we should learn an appropriate metric first and then extract its representation rather than the other way around.

The quality of a hyperbolic representation is judged by the quality of the metric obtained. That is, we say that we have a good quality representation if the hyperbolic metric extracted from the hyperbolic representation is, in some way, faithful to the original metric on the data points. We note that finding a tree metric that approximates a metric is an important problem in its own right. Frequently, we would like to solve metric problems such as transportation, communication, and clustering on data sets; however, solving these problems with general metrics can be computationally challenging and we would like to approximate these metrics by simpler, tree metrics. This approach of approximating metrics via simple metrics has been extensively studied before. Examples include dimensionality reduction (Johnson & Lindenstrauss, 1984) and approximating metric by as simple graph metrics (Bartal, 1998; Peleg & Ullman, 1989).

To this end, in this paper we demonstrate that methods that...
learn a tree structure first outperform methods that learn hyperbolic embeddings directly. Additionally, we develop novel extremely fast algorithm Template:TREEREP that takes as input a \( \delta \)-hyperbolic metric and learns a tree structure that approximates the metric. This a new method that makes use of geometric insights obtained from the metric to infer the structure of the tree. To demonstrate the effectiveness of our method, we compare Template:TREEREP against previous methods such as Saitou & Nei (1987); Abraham et al. (2007); Chepoi et al. (2008) that also recover tree structures given a metric. We show that Template:TREEREP is not only faster, but produces better results than Abraham et al. (2007); Chepoi et al. (2008) and comparable results to Saitou & Nei (1987).

For learning hyperbolic representations, we demonstrate that Template:TREEREP is over 10,000 times faster than the optimization based methods from Nickel & Kiela (2017; 2018); Sala et al. (2018) while producing better quality results in most cases. This extreme decrease in the run time, with no loss in quality, is exciting as it allows us to extract hierarchical information from much larger data sets in single-cell sequencing, linguistics, and social network analysis, data sets for which such analysis was previously unfeasible.

The rest of the paper is organized as follows. Section 2 contains the relevant background information and Section 3 presents the geometric insights and the Template:TREEREP algorithm. In Section 4, we compare Template:TREEREP against the methods from Saitou & Nei (1987); Prim (1957); Chepoi et al. (2008); Abraham et al. (2007) in approximating metrics via tree metrics and against methods from Nickel & Kiela (2017; 2018); Sala et al. (2018) for learning low dimensional hyperbolic embedding. We show that the methods that learn a good tree to approximate the metric, in general, find better hyperbolic representations than those that embed into the hyperbolic manifold directly. Section 5 presents an intuitive analysis of this approach.

2. Preliminaries

Definition 1. Given a weighted graph \( G = (V, E, w) \) the shortest path metric \( d_G \) on \( V \) is defined as follows: \( \forall u, v \in V, d_G(u, v) \) is the length of the shortest path from \( u \) to \( v \).

Definition 2. Given a metric space, \( (X, d) \), two points \( x, y \in X \), and a continuous function \( f : [0, 1] \rightarrow X \), such that \( f(0) = x, f(1) = y \), and there is a \( \lambda \) such that \( d(f(t_1), f(t_2)) = \lambda |t_1 - t_2| \), the geodesic \( g(x, y) \) connecting \( x \) and \( y \) is the set \( f([0, 1]) \).

2.1. \( \delta \)-Hyperbolic Metrics

Gromov introduced the notion of \( \delta \)-hyperbolic metrics as a generalization of the type of metric obtained from negatively curved manifolds (Gromov, 1987).

Definition 3. Given a space \( (X, d) \), the Gromov product of \( x, y \in X \) with respect to a base point \( w \in X \) is

\[
(x, y)_w := \frac{1}{2} (d(w, x) + d(w, y) - d(x, y)) .
\]

The Gromov product is a measure of how close \( w \) is to the geodesic \( g(x, y) \) connecting \( x \) and \( y \).

Definition 4. A metric \( d \) on a space \( X \). Let \( \delta \geq 0 \) be the smallest number such that for every \( x, y, z \in X \) we have that

\[
(x, y)_w \geq \min (|(x, z)_w, (y, z)_w| - \delta).
\]

Then \( d \) is a \( \delta \)-hyperbolic metric on \( X \).

One example of a \( \delta \)-hyperbolic metric space is the hyperbolic manifold \( \mathbb{H}^k \) with \( \delta = \tanh^{-1}(1/\sqrt{2}) \) (Carnahan, 2010).

Definition 5. The hyperboloid model \( \mathbb{H}^k \) of the hyperbolic manifold is \( \mathbb{H}^k = \{ x \in \mathbb{R}^{k+1} : x_0 > 0, x_0^2 - \sum_{i=1}^{k} x_i^2 = 1 \} \).

If we set \( Q \) to be the diagonal matrix with \( Q_{11} = 1 \) and the other diagonal entries \(-1\), then the manifold \( \mathbb{H}^n \) is the upper sheet of \( x^T Q x = 1 \). The distance on this manifold can be calculated as \( d(x, y) = \cosh(x^T Q y) \).

2.2. Tree Metrics

Definition 6. The shortest path metric \( d_T \) on a weighted discrete tree \( T \) is called a tree metric.

Definition 7. Given a discrete graph \( G = (V, E, w) \) the metric graph \( (X, d) \) is the space obtained by letting \( X = E \times [0, 1] \) such that for any \( (e, t_1), (e, t_2) \in X \) we have that

\[
d((e, t_1), (e, t_2)) = \frac{w(e)}{|t_1 - t_2|} .
\]

This space is called a tree space if \( G \) is a tree. Here \( E \times \{0, 1\} \) are the nodes of \( G \).

Definition 8. A metric space \( T \) is a tree space (or a \( \mathbb{R} \)-tree) if any pair of its points can be connected with a unique geodesic segment, and if the union of any two geodesic segments \( g(x, y), g(y, z) \subset T \) having the only endpoint \( y \) in common, is the geodesic segment \( g(x, z) \subset T \).

There are multiple definitions of a tree space; they are, however, all connected via their metrics. Bermudo et al. (2013) tells us that a metric space is 0-hyperbolic if and only if it is an \( \mathbb{R} \)-tree or a tree space. This results lets us immediately conclude that Definitions 7 and 8 are equivalent. Similarly, Definition 1 implies that Definition 6 and 7 are equivalent. Hence all three definitions of tree spaces are equivalent. We note that trees are 0-hyperbolic, \( \delta = \infty \) corresponds to an arbitrary metric. Thus, \( \delta \) is a heuristic measure for how close a metric is to a tree metric.
2.3. Trees as Hyperbolic Representation

Sala et al. (2018) give an algorithm that is a modification of the algorithm in Sarkar (2012) that can, in linear time, embed any weighted tree into $\mathbb{H}^k$ with arbitrarily low distortion. The analysis in Sala et al. (2018) quantifies the trade-offs amongst the dimension $d$, the desired distortion, the scaling factor and the number of bits required to represent the distances in $\mathbb{H}^k$. We use these results to consider trees as a hyperbolic representations. One possible drawback of using trees as hyperbolic representations is that when we embed the trees, we may need a large number of bits of precision. However, recent work such as Yu & De Sa (2019) provide a solution to this issue.

3. Tree Representation

Algorithm 1 Metric to tree structure algorithm.

1: function ZONE1_RECURSION($T$, $d_T$, $d$, $L$, $v$)
2:  $T = (V, E, d') = \emptyset$
3:  Pick any three data points uniformly at random $x, y, z \in X$
4:  $T = \text{RECURSIVE\_STEP}(T, x, y, z, d, d_T)$
5:  return $T$
6: end function

Algorithm 2 Recursive parts of TreeRep.

1: function ZONE1\_RECURSION($T$, $d_T$, $d$, $L$, $v$)
2:  if Length($L$) == 0 then
3:    return $T$
4:  end if
5:  if Length($L$) == 1 then
6:    Let $u$ be the one element in $L$ and add edge $(u, v)$ to $E$
7:    Set edge weight $d_T(u, v) = d(u, v)$
8:    return $T$
9:  end if
10:  Pick any two $u, z$ from $L$ and remove them from $L$
11:  return RECURSIVE\_STEP($T$, $L$, $u, z, d, d_T$)
12: end function

13: function ZONE2\_RECURSION($T$, $d_T$, $d$, $L$, $u, v$)
14:  if Length($L$) == 0 then
15:    return $T$
16:  end if
17:  Set $z$ to be the closest node to $v$
18:  Delete edge $(u, v)$
19:  return RECURSIVE\_STEP($T$, $L$, $u, z, d, d_T$)
20: end function

To better understand the geometric insights used to develop TreeRep, we first focus on the problem of reconstructing the tree structure from a tree metric. These ideas will serve as the basis for the more general algorithm presented in Section 3.3. The complete pseudo-code for TreeRep is presented in Appendix 13. A high level version presented in Algorithm 1 and 2 is presented here.

3.1. The need for Steiner Nodes

A Steiner node is any node that you add to a graph that did not exist originally. In this section, we present a simple example that shows us that Steiner nodes are necessary for reconstructing the correct tree. Additionally, we will also demonstrate that forming a graph and then computing the MST will not recover the tree structure. Consider 3 points $x, y, z$ such that all pairwise distances are equal to 2. Then the graph is a triangle, and the MST is a path. Then the distance between the endpoints of the MST path is not correct. The correct tree is obtained by adding a new node $r$ and connecting $x, y, z$ to $r$, and making all the edge weights equal to 1. This example can be seen in Figure 1. Thus, we need Steiner nodes when reconstructing the tree structure.

3.2. TreeRep for 0-hyperbolic metrics

Theorem 1. Given $(X, d)$, a $\delta$-hyperbolic metric space, and $n$ points $x_1, \ldots, x_n \in X$, TreeRep returns a tree $(T, d_T)$. In the case that $\delta = 0$, $d_T = d$, and $T$ has the fewest possible nodes. TreeRep has a worst case run time $O(n^2)$. Furthermore the algorithm is embarrassingly parallelizable.

Remark 1. In practice we saw that the run time for TreeRep is much faster than $O(n^2)$. TreeRep is a divide and conquer algorithm. Hence, if the pieces that we divide the problem into are roughly the same size, then the expected running time is $O(n \log(n))$. However, such a running time is the expected running time. Usually, this expectation is over the randomness in the algorithm. Unfortunately, for TreeRep, this expectation is over the randomness in the algorithm and the randomness in the input data, so we need a distribution on the space of metrics. For example, if the input metric came from a path, then we have an $O(n \log(n))$ expected running time. However, if the input tree was a star graph (one center node and all other nodes attached to this center node), then in the first stage of the algorithm, we would add the center node, $r$. At every subsequent recursive stage, all remaining nodes would be sorted into zone 1 for $r$. Hence, TreeRep would take $O(n^2)$ time.

The proof of this theorem is by induction. For this discus-
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Figure 1. Figures showing the example that demonstrates the need for Steiner nodes.

Figure 2. Figures showing the tree $\hat{T}$ from Lemma 2 for Zone$_2(z)$ (a), Zone$_1(z)$ (b), Zone$_1(r)$ (c), and the Universal tree (d).

sion, we provide the conceptual pieces of the proof which we then assemble in detail in Appendix 7. The first main idea is that for any three points, we can construct the universal tree on three points in Lemma 1. Then we show (in Lemma 2) that adding a fourth point to a universal tree can be done consistently and, more importantly, the additional point falls into one of seven different zones. Finally, we show in Lemma 3 that for each node we add in a zone, the distances to all the other (non-universal) nodes in other zones are consistent, so we simply have to maintain consistency amongst the points within each zone. That is, it's sufficient to maintain local distance consistency.

**Lemma 1.** Given a metric $d$ on three points $x, y, z$, there exists a weighted tree $(T, d_T)$ on four nodes $x, y, z, r$, such that $r$ is adjacent to $x, y, z$, the edge weights are given by $d_T(x, r) = (y, z)_x$, $d_T(y, r) = (x, z)_y$, and $d_T(z, r) = (x, y)_z$, and the metric $d_T$ on the tree agrees with $d$.

**Definition 9.** The tree constructed in Lemma 1 is the universal tree on the three points $x, y, z$. The additional node $r$ is known as a Steiner node.

An example of the universal tree can be seen in Figure 2(d).

Let us now reinterpret Equation 2.1. We know that for any tree metric, and any four points $w, x, y, z$, we have that $(x, y)_w \geq \min((x, z)_w, (y, z)_w)$.

This inequality implies that the smaller two of the three numbers $(x, y)_w, (x, z)_w,$ and $(y, z)_w$ are equal. In this case, knowing which of the quantities are equal tells us the structure of the tree. This brings us to the analysis of the second main idea, local consistency. Lemmas 2, and 3, tell us that by using the information provided by the Gromov products, we can sort our data points into zones associated with the nodes of the universal tree, so that we only need to check local metric consistency to ensure global consistency.

**Lemma 2.** Let $(X, d)$ be a tree space. Let $w, x, y, z$ be four points in $X$ and let $(T, d_T)$ be the universal tree on $x, y, z$ with node $r$ as the Steiner node. Then we can extend $(T, d_T)$ to $(\hat{T}, d_{\hat{T}})$ to include $w$ such that $d_{\hat{T}} = d$.

The proof of Lemma 2 (in Appendix 7) shows that there are a number of ways to extend $T$ to include the new point $w$. Examples of the different ways can be seen in Figure 2. To clarify our discussion of the extension of $T$ and to extend our analysis to the general TREEREP algorithm, we introduce new terminology (such conditions are in the proof of Lemma 2).
Definition 10. Given a data set $V$ (consisting of data points, along with the distances amongst the points), a universal tree $T$ on $x,y,z \in V$ (with $r$ as the Steiner node), let us defining the following two zone types.

1. Zone$_1(r) = \{w \in V : (x,y)_w = (y,z)_w = (z,x)_w\}$
2. For a given permutation $\pi$ on $\{x,y,z\}$, Zone$_1(\pi x) = \{w \in V : (\pi x, \pi y)_w = (\pi x, \pi z)_w = d(w, \pi x)\}$
3. For a given permutation $\pi$ on $\{x,y,z\}$, Zone$_2(\pi x) = \{w \in V : (\pi x, \pi y)_w = (\pi x, \pi z)_w < d(w, \pi x)\}$

Using this terminology and our structural lemmas, we can describe a recursive algorithm that reconstructs the tree structure from a $0$-hyperbolic metric. Given a data set $V$ we pick three random points $x,y,z$ and construct the universal tree $T$. Then for all other $w \in V$, sort the $w$’s into their respective zones. Then for each of the seven zones we can recursively build new universal trees. For zones of type 1, pick any two points, $w_{i1}, w_{i2}$ and form the universal tree for $\pi x$ or $\pi y, \pi z$. If there is only one node in this zone, connect it to $\pi x$ or $\pi y$. For zones of type 2, pick any one point, $w_{i1}$ and form the universal tree for $\pi x, w_{i1}, r$. Examples of this can be seen in Figure 3. The following lemma proves that we only need to check consistency of the metric within each zone to ensure global consistency.

Lemma 3. Given $(X,d)$ a metric tree, and a universal tree $T$ on $x,y,z$ and a fourth point $w$, when sorting $w$ into its zone $(\text{Zone}_i(\pi x))$, TREEREP introduces an additive distortion of at most $\delta$ between $w$ and $\pi x, \pi y, \pi z$.

4. Experiments

In this section, we demonstrate the effectiveness of TREEREP as a method for approximating metrics via tree metrics and the superiority of learning hyperbolic representations by first learning a tree structure first, and then embedding this tree. Additional details about the experiments and algorithms can be found in Appendix 12.2

3.3. TreeRep for General $\delta$-Hyperbolic Metrics

Having seen the main geometric ideas behind TREEREP, we want to extend the algorithm to return an approximating tree for any given metric. For an arbitrary $\delta$-hyperbolic metric, Lemma 2 does not hold in its current form. We can, however, modify it and leverage the intuition behind the original proof. Given four points $w,x,y,z$ we calculate, $(x,y)_w, (x,z)_w, (y,z)_w$. We do not satisfy one of the conditions of Lemma 2, if all three $(x,y)_w, (x,z)_w, (y,z)_w$ have distinct values. Nevertheless, we can still compute the maximum of these three quantities. Furthermore, since we have a $\delta$-hyperbolic metric, the smaller two products will be within $\delta$ of each other. Let us suppose that $(x,y)_w$ is the biggest. Then we place $w$ in Zone$_1(x)$ if and only if $d(z,w) = (y,z)_w$ or $d(z,w) = (x,z)_w$. Otherwise we place $w$ in Zone$_2(x)$. Note that when we have tree metric, we have that both $d(z,w) = (y,z)_w$ and $d(z,w) = (x,z)_w$.

In either case, as shown by Proposition 1, we are introducing a distortion of at most $\delta$ between $w$ and $y, z$. This suggests that when we do zone 2 recursive steps, we should pick the node that closest to $r$ as the third node for the universal tree. We see experimentally that this significantly improved the quality of the tree returned.

Proposition 1. Given a $\delta$-hyperbolic metric $d$, the universal tree $T$ on $x,y,z$ and a fourth point $w$, when sorting $w$ into its zone $(\text{Zone}_i(\pi x))$, TREEREP introduces an additive distortion of at most $\delta$ between $w$ and $\pi y, \pi z$.
for UPGMA, the additional assumption is that the metric is an ultrametric (i.e. a stronger triangle inequality holds). Hence we do not compare against such methods.

For the second task of learning hyperbolic embeddings, we compare TREEREP against Poincare Maps (PM) (Nickel & Kiela, 2017), Lorentz Maps (LM) (Nickel & Kiela, 2018), and PT (Sala et al., 2018). Here we can think of trees as hyperbolic embeddings, as using Sala et al. (2018), we can embed trees into $\mathbb{H}^k$ with arbitrarily low distortion. When comparing against such methods, we show that TREEREP is not only four to five orders of magnitude faster, but for low dimensions, and in many high dimensional cases, produces better quality embeddings.

We first perform a benchmark test for tree reconstruction from tree metrics in Section 4.1. Then, for both tasks, we test the algorithms on three different types of data sets. First, in Section 4.2, we create synthetic data sets by sampling random points from $\mathbb{H}^k$. Second, in Section 4.3, we will take real world biological data sets that are believed to have hierarchical structure. Third, in Section 4.4, we consider are metrics that come from real world unweighted graphs. In each case, we will show that TREEREP is an extremely fast algorithm that produces as good or better quality metrics. We will evaluate the methods on the basis of computational time, and the average distortion, as well as mean average precision (MAP) of the learned metrics.

In many cases, the metric learned by the various algorithms will be a scalar multiple of the actual metric, so we will solve for the scale $\alpha := \arg \min_c \| D - c \hat{D} \|_F$, before calculating the average distortion.

**Definition 11.** Let $d$ be a metric on the nodes of a graph $G = (V, E)$. For $v \in V$, let $N(v) = \{u_1, \ldots, u_{\deg(v)}\}$ be the neighborhood of $v$. Then let $B_{v, u_i} = \{u \in V \setminus \{u\} : d(u, v) \leq d(v, u_i)\}$. Then the mean average precision (MAP) is defined to be

$$\frac{1}{n} \sum_{v \in V} \frac{1}{\deg(v)} \sum_{i=1}^{\deg(v)} \frac{|N(v) \cap B_{v, u_i}|}{|B_{v, u_i}|}$$

Closer MAP is to 1, the closer $d$ is to approximating $d_G$.

**Definition 12.** Given two metrics $d_1, d_2$ on a finite set $X = x_1, \ldots, x_n$ the average distortion is:

$$\frac{1}{\binom{n}{2}} \sum_{i=1}^{n} \sum_{j \neq i} \frac{|d_1(x_i, x_j) - d_2(x_i, x_j)|}{d_2(x_i, x_j)}$$

As we can see from Figure 4, TREEREP is a much more viable algorithm at large scales. Additionally, the trees returned by NJ have double the number of nodes as the original trees. Contrarily, the trees returned by TREEREP and NJ are the only algorithms that are theoretically guaranteed to return a tree that is consistent with the original metric. Therefore, consistent with theoretical analysis, TREEREP returns a tree with the fewest number of nodes that is consistent with the input metric. TREEREP is only known algorithm that can exactly reconstruct the input tree from its metric at scale.

**4.1. Tree Reconstruction Experiments**

Before experimenting with general $\delta$-hyperbolic metrics, we benchmark our method on 0-hyperbolic metrics. To do this, we generate random synthetic 0-hyperbolic metrics. More details can be found in Appendix 12. Since TREEREP and NJ are the only algorithms that are theoretically guaranteed to return a tree that is consistent with the original metric, we will run this experiment with these two algorithms only. We compare the two algorithms based on their running times and the number of nodes in the trees.

Smaller average distortion implies greater similarity between $d_1$ and $d_2$.

**4.2. Random points on Hyperbolic Manifold**

We generate two different types of data sets. First, we hold the dimension $k$ constant and scale the coordinates. Second, we hold the magnitude of the coordinates constant and increase the dimension $k$. Note these metrics do not come with an underlying graph, so for MST, we create two different weighted graphs; a complete graph and a nearest neighbor graph, to give as input to MST.

For both types of data, Figures 5 and 6 show that as the scale and the dimension increase, the quality of the trees produced by TREEREP and NJ get better. Contrastingly, the quality of the trees produced by MST and CONSTRUCTTREE do not improve. Thus, demonstrating that TREEREP is an extremely fast algorithm that produces good quality trees...
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Figure 5. Graph showing the average distortion of the tree metric learned by TreeRep, NJ, MST, and CT and of the hyperbolic metric learned by LM and PT for 100 randomly sampled points from $\mathbb{H}^4$ for $k = 2^i$ for $i = 1, 2, \ldots, 10$.

Figure 6. Graph showing the average distortion of the tree metric learned by TreeRep, NJ, MST, and CT and of the hyperbolic metric learned by LM and PT for 100 randomly sampled points from $\mathbb{H}^{10}$ for scale $s = 2^i$ for $i = 1, \ldots, 10$.

Figure 7. Tree structure and embeddings for the Immunological distances from (Sarich, 1969).

4.3. Biological Data: scRNA seq and phylogenetic data

We also test on two real world biological data sets. The first data set consists of immunological distances from Sarich (1969). Given these distances, the goal is to recover the hierarchical phylogenetic structure. As seen in Figure 7, the trees returned by TreeRep and NJ recover this structure well, with sea lion and seal close to each other, and monkey and cat far away from everything else. Divergently, the trees and embeddings produced by MST, ConstructTree, PM, and PT make less sense as phylogenetic trees.

The second data set is the Zeisel sc RNA-seq data set (Zeisel et al., 2015). This data set is expected to be a tree as demonstrated in Dumitrascu et al. (2019). Here we used the various algorithms to learn a tree structure on the data or to learn an embedding into $\mathbb{H}^2$. The time taken and the average distortion are reported in Table 1. In this case, we see that TreeRep has the lowest distortion. Additionally, TreeRep is 20 times faster than NJ and is 20,000 to 40,000 times faster than PT and PM.

4.4. Unweighted Graphs

Metrics that come from unweighted graphs are the third data type that we consider. We use eight well known graph
Table 2. Time taken by various algorithms. For PT and LM this is the average time taken to learn a 10 dimensional embedding for the synthetic data sets. For TreeRep (TR), MST, and CT it is the average time taken over all 20 data sets.

|      | TR  | NJ  | MST | CT  | PT  | LM  |
|------|-----|-----|-----|-----|-----|-----|
| Time | 0.004 | 0.02 | 0.0002 | 0.076 | 312 | 971 |

For learning tree metrics to approximate general metrics, we see that NJ has the best MAP, with TreeRep and MST tied for second place. In terms of distortion, NJ is the best, TreeRep is second, while MST is third. However, NJ is extremely slow and is not viable at scale. Hence, in this case, we have two algorithms with good performance at large scale; TreeRep and MST, with TreeRep preforming better at scale. Additionally, MST did not perform well in the experiments in Sections 4.2 and 4.3.

For the task of learning hyperbolic representations, we see that PM, LM, and PT are much slower than the methods that learn a tree first. In fact, these algorithms were too slow to compute the hyperbolic embeddings for the larger data sets. Additionally, this extra computational effort does not always result in improved quality. In all cases, except for the Celebgan data set, the MAP returned by TreeRep is superior to the MAP of the 2-dimensional embeddings produced by PM, LM, and PT. In fact, in most cases, these 2-dimensional embeddings, have worse MAP than all of the tree first methods. Even when they learn 200-dimensional embeddings, PM, LM and PT have worse MAP than TreeRep on most of the data sets. Furthermore, except for PT200, the average distortion of the metric returned by TreeRep is superior to PT2, PM, an LM.\(^5\) Thus, showing the effectiveness of TreeRep at learning good Hyperbolic representations quickly.

5. Metric First Discussion and Justification

Table 3 shows that for most of the data sets, learning a tree structure first and then embedding it into hyperbolic space, yields embeddings with better MAP and average distortion compared to methods that learn the embedding directly. One possible explanation for this phenomenon is that the optimization problems that seek the embeddings directly are not being solved optimally. That is, the algorithms get stuck at some local minimum. Another possibility is that there is a disconnect between the objective being optimized and the statistics calculated to judge the quality of the embeddings.

We propose that there are geometric facts about hyperbolic space that suggest embedding by first learning a tree is the correct approach. The tree-likeness of hyperbolic space has been studied from many different approaches. We present details from Hamann (2018); Dyubina & Polterovich (2001) and looks at the geometry of \(\mathbb{H}^k\) at its two extremes; large scale and small scale. Since \(\mathbb{H}^k\) is a manifold, we know that at small scales hyperbolic space looks like Euclidean space. Additionally, in the Poincare disk, the hyperbolic Riemannian metric is given by \(\frac{4}{(1-x^2-y^2)^2}(dx^2 + dy^2)\) and is just a re-scaling of the Euclidean metric. Thus, at small scales, hyperbolic space is similar to Euclidean space.

Hence to take advantage of hyperbolic representations (i.e., why learn a hyperbolic representation instead of a Euclidean one), we want to embed data into \(\mathbb{H}^k\) at scale. To study the large scale geometry of \(\mathbb{H}^k\), we consider the asymptotic cone for hyperbolic space \(\text{Con}(\mathbb{H}^k)\). In particular, we can think of the asymptotic cone as the “view of our space from infinitely far away”. See the more detailed discussion in Appendix 8 for examples and complete definitions. The following connects \(\text{Con}(\mathbb{H}^k)\) to \(\mathbb{R}\)-tree spaces.

**Theorem 2.** (Young, 2008) \(\text{Con}(\mathbb{H}^k)\) is a complete \(\mathbb{R}\)-tree.

Thus, we see that the large scale structure of hyperbolic space is a tree, indicating a strong connection between learning trees and learning hyperbolic embeddings. Furthermore, it can be shown that \(\text{Con}(\mathbb{H}^k)\) is a \(2^{\mathbb{R}\text{-}k}\)-universal tree. That is, any tree with finitely many nodes can be embedded into \(\text{Con}(\mathbb{H}^k)\) exactly. However, these are still embeddings into \(\text{Con}(\mathbb{H}^k)\). We would like to study embeddings into \(\mathbb{H}^k\).

**Definition 13.** A metric space \((T, d_T)\) admits an isometric embedding at infinity into the space \((X, d_X)\) if there exists a sequence of positive scaling factors \(\lambda_i \to \infty\) such that for every point \(t \in T\), there exists an infinite sequence \(\{x_{i}^{t}\}, i = 1, 2, \ldots\) of points in \(X\) such that for all \(t_1, t_2 \in T\)

\[
\lim_{i \to \infty} d_X(x_{i}^{t_1}, x_{i}^{t_2}) / \lambda_i = d_T(t_1, t_2)
\]

**Theorem 3.** (Dyubina & Polterovich, 2001) \(\text{Con}(\mathbb{H}^k)\) can be isometrically embedded at infinity into \(\mathbb{H}^k\).

Thus, we can embed any tree into \(\mathbb{H}^k\) with arbitrarily low distortion. A type of converse is also true.

**Definition 14.** A (geodesic) ray \(R\) is a (isometric) homeomorphic image of \([0, \infty)\), such that for any ball \(B\) of finite diameter, \(R\) lies outside \(B\) eventually.

Hamann (2018) showed that we can construct a rooted \(\mathbb{R}\)-tree \(T\) inside \(\mathbb{H}^k\), such that every geodesic ray in \(\mathbb{H}^k\) eventually converges to a ray of \(T\). Thus, showing that any configuration of points at scale in \(\mathbb{H}^k\) can be approximated...
by a tree. Additionally, larger the scale points can be better approximated by trees. More details can be found in Appendix 9. Thus, showing that learning a tree and then embedding this tree into $\mathbb{H}^k$ is equivalent to learning hyperbolic representations at scale.

This provides an explanation for why as the scale and dimension increased, TREEREP found a tree that better approximated the hyperbolic metric in Section 4.2. This also provides a justification for why learning a tree first, results in better hyperbolic representations.

### 6. Conclusion and Future Work

In conclusion, we have shown the effectiveness of TREEREP as a method for learning hyperbolic representations. We have seen that TREEREP is not only several orders of magnitude faster, but that this gain in speed does not come at the expense of quality. Hence making it possible for us to use to the power of hyperbolic representations for large data sets. Furthermore, our work experimentally verifies that the correct way to learn hyperbolic representations in $\mathbb{H}^k$ is to learn a tree metric first, using algorithms such as TREEREP. Additionally, we would like to generalize our representation to learn a $\delta$-hyperbolic representation for a small values of $\delta$. Future work includes devising an algorithm to construct a sparse graph $G$ that is consistent with a $\delta$-hyperbolic metric.
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7. Proofs

7.1. Tree Representation Proofs

**Lemma 1.** Given a metric $d$ on three points $x, y, z$, there exists a (weighted) tree $(T, d_T)$ on four nodes $x, y, z, r$, such that $r$ is adjacent to $x, y, z$, the edge weights are given by $w(x, r) = (y, z)_x$, $w(y, r) = (x, z)_y$, and $w(z, r) = (x, y)_z$, and the metric $d_T$ on the tree agrees with $d$.

**Proof.** The basic structure of this tree can be seen in Figure 2(d). To prove that the metrics agree we such need to see the following calculation.

$$d_T(x, y) = w(x, r) + w(r, y) = (y, z)_x + (x, z)_y$$

$$= \frac{1}{2}(d(x, y) + d(x, z) - d(y, z)) + d(x, y) + d(y, z) - d(x, z))$$

$$= d(x, y)$$

Here $d_T$ is the metric on the tree $T$. \qed

One important fact that we need is that if $(X, d)$ is a metric graph, then for any three distinct points $x, y, z \in X$, the geodesics connecting them intersect at a unique point. As seen in Lemma 1, we refer to this point a Steiner point $r$. It is now important to note that even though $r$ may not be a point in the data set we are given, but $r \in X$ (Bridson & Häfliger, 2013). Thus, in the following lemmas, whenever we find a Steiner point, we will assume that the metric $d$ is defined on $r$.

**Lemma 4.** If $d$ is a tree metric and $x, y, w$ are three points then

1. $(x, y)_w = 0$ if and only if $w \in g(x, y)$
2. $(x, y)_w = d(x, w)$ if and only if $(w, y)_x = 0$.
3. $(x, y)_w = d(y, w)$ if and only if $(w, x)_y = 0$.

Here $g(x, y)$ is the unique path connecting $x$ and $y$.

**Proof.** For 1. we see that

$$0 = (x, y)_w = \frac{1}{2}(d(w, x) + d(w, y) - d(x, y))$$

$$\Rightarrow d(x, y) = d(w, x) + d(w, y)$$

Thus we have that $w \in g(x, y)$.

For 2. we see that

$$(x, y)_w = d(x, w) \Rightarrow d(w, x) + d(w, y) - d(x, y)$$

$$= 2d(w, x)$$

$$\Rightarrow d(w, x) + d(x, y) - d(w, y) = 0$$

$$\Rightarrow 2(w, y)_x = 0$$

The proof for 3 is similar to that of 2. \qed

**Lemma 2.** Let $(X, d)$ be a tree space. Let $w, x, y, z$ be four points in $X$ and let $(T, d_T)$ be the universal tree on $x, y, z$ with node $r$ as the Steiner node. Then we can extend $(T, d_T)$ to $(\hat{T}, d_{\hat{T}})$ to include $w$ such that $d_{\hat{T}} = d$.

**Proof.** We note that there are four different possible cases for the configuration of $x, y, z, w$ depending on the relationship amongst the Gromov products. Each case determines a different placement of $r$, as follows:

1. If $(x, y)_w = (x, z)_w = (y, z)_w = 0$, then replace $r$ with $w$ to obtain $\hat{T}$.
2. If $(x, y)_w = (x, z)_w = (y, z)_w = c > 0$, then connect $w$ to $r$ via an edge of weight $c$ to obtain $\hat{T}$.
3. If there exists a permutation $\pi : \{x, y, z\} \rightarrow \{x, y, z\}$ such that,

$$(\pi x, \pi y)_w = (\pi x, \pi z)_w = c < (\pi y, \pi z)_w$$

and $d(\pi x, w) = (\pi x, \pi y)_w$, then connect $w$ to $\pi x$ via an edge of weight $c$ to obtain $\hat{T}$.
4. If there exists a permutation $\pi : \{x, y, z\} \rightarrow \{x, y, z\}$ such that,

$$(\pi x, \pi y)_w = (\pi x, \pi z)_w = c < (\pi y, \pi z)_w$$

and $d(\pi x, w) > (\pi x, \pi y)_w$, then add a Steiner point $\hat{r}$ on the edge $x, r$ with $d(\pi x, \hat{r}) = d(\pi x, w) - c$ and connect $w$ to $\hat{r}$ via an edge of weight $c$ to obtain $\hat{T}$.

To prove that these extensions of $T$ are consistent, first let us prove that there are exactly four cases. To do that, first note that since we have a 0-hyperbolic metric, at least two of the three Gromov products must be equal. Using the triangle inequality, we can see that for any three points $a, b, c$ the following holds

$$0 \leq (a, b)_c \leq d(a, c).$$

That is, either we are in the first two cases and three of products are equal, or we have that two of the products are equal. In the case that two of the products are equal, the permutation $\pi$ tells us which of the two are equal and we further subdivide into the case whether $d(\pi x, w) = (\pi x, \pi y)_w$ or $d(\pi x, w) > (\pi x, \pi y)_w$ as we cannot have $d(\pi x, w) < (\pi x, \pi y)_w$.

Therefore, there are at most four possible configuration cases and it remains to show that the new tree $d_{\hat{T}}$ is consistent with $d$ on the four points. In each case, we present the high level intuition for why these modification result in a consistent tree. The low level details about the metric numbers can easily be checked.
Case 1: If \((x, y)_w = (x, z)_w = (y, z)_w = 0\), then we replaced \(r\) with \(w\) in \(\hat{T}\). In this case, using Lemma 4, we see that \(w\) must lie on all tree geodesics \(g(x, y), g(x, z), g(y, z)\). Since the metric comes from a tree, these three geodesics can only intersect at one point \(r\). Thus, we must replace \(r\) with \(w\).

To see that the metric is consistent, we need to verify that \(d(w, x) = d_{\hat{T}}(r, x)\). To see we have the following:

\[
d_{\hat{T}}(r, x) = (y, z)_x
= (y, z)_x + (x, y)_w + (x, z)_w - (y, z)_w
= d(w, x)
\]

Case 2: If

\[(x, y)_w = (x, z)_w = (y, z)_w = c > 0,
\]

then we can see that \((x, w)_r = (y, w)_r = (z, w)_r = 0\). In this case, \(r\) lies on geodesics \(g(x, y), g(x, z), g(x, w), g(y, w), g(y, z), g(z, w)\). Thus, we must have a star shaped graph with \(r\) in the center.

To see that the metric is consistent we just need to verify that \(d(w, x) = d_{\hat{T}}(w, x)\). To see we have the following calculation.

\[
d_{\hat{T}}(w, x) = d_{\hat{T}}(w, r) + d_{\hat{T}}(r, x)
= (x, y)_w + (y, z)_x
= (x, y)_w + (x, z)_w + (y, z)_w
= d(w, x)
\]

Case 3: In this case suppose condition 4 is true. Without loss of generality assume that \(\pi\) is the identity map. In each case, we have a tree that looks like a tree in Figure 2. In this case, we can do the calculations and see that \((w, y)_r = (w, z)_r = 0\). That is, the geodesics \(g(w, y), g(w, z), g(y, z), g(x, y), g(x, z)\) all intersect at the same point. Thus, again telling us our tree structure.

To check that the metric is consistent, we need to verify that \(d(w, y) = d_{\hat{T}}(w, y) = d_{\hat{T}}(w, r) + d_{\hat{T}}(r, y)\). Before we can do that, let us first verify that

\[
d_{\hat{T}}(w, r) = (y, z)_w
\]

To verify this we need to the following calculation

\[
d_{\hat{T}}(w, r) = d_{\hat{T}}(r, \hat{r}) + d_{\hat{T}}(\hat{r}, w)
= c + d_{\hat{T}}(x, r) - d_{\hat{T}}(x, \hat{r})
= c + (y, z)_x - (d(x, w) - c)
= 2c + (y, z)_x - d(x, w)
= (x, y)_w + (x, z)_w + (y, z)_x - d(w, x)
= (y, z)_w
\]

We then can see that

\[
d_{\hat{T}}(w, y) = d_{\hat{T}}(w, r) + d_{\hat{T}}(r, y)
= (y, z)_w + (x, z)_y
= (y, z)_w + (x, y)_w - (x, z)_w + (x, z)_y
= d(w, y)
\]

Note \(d_{\hat{T}}(w, r) = (y, z)_w\) and the consistency of the metric implies that \(d(w, x) = (y, z)_w\). Finally, we can see \((w, y)_r = 0\) as follows.

\[
2(w, y)_r = d(w, r) + d(r, y) - d(w, y)
= (z, y)_w + (x, z)_y - d(w, y)
= \frac{1}{2}(d(w, z) - d(w, y) + d(x, y) - d(x, z)
= (x, z)_w - (x, y)_w
= 0
\]

Note that this also implies that \((w, x)_r > 0\).

Case 4: In this case, suppose condition 3 is true. Without loss of generality assume that \(\pi\) is the identity map. Then in this case, we still have that \((w, y)_r = (w, z)_r = 0\), but in addition we have that \((w, y)_x = (w, z)_x = 0\). Thus, again telling us our tree structure.

In this case, to verify that the metric is consistent, we need to check that \(d(w, y) = d_{\hat{T}}(w, y) = d_{\hat{T}}(w, x) + d_{\hat{T}}(x, y)\). To see this we have the following calculations.

\[
d_{\hat{T}}(w, x) + d_{\hat{T}}(x, y) = (x, y)_w + d(x, y)
= 2(x, y)_w - (x, z)_w + d(x, y)
= d(w, y) + (w, z)_x
\]

Thus, now it suffices to show that \((w, z)_x = 0\), which can be seen using the following calculations.

\[
(x, z)_w = d(w, x) \Rightarrow 0 = d(w, x) + d(x, z) - d(w, z)
= (w, z)_x = 0
\]

This also implies that \((w, z)_r = 0\).

The proof of Lemma 2 shows that there are a number of ways to extend \(T\) to include the new point \(w\). To clarify our discussion of the extension of \(T\), we introduce new terminology.

**Definition 15.** Given a data set \(V\) (consisting of data points, along with the distances amongst the points), a universal tree \(T\) on \(x, y, z \in V\) (with \(r\) as the Steiner node), let us
defining the following three zone types. The first type is associated only with the Steiner node $r$, while the other two types are defined for each of the original nodes $x, y, z$.

1. Zone$_1(r)$ is all $w \in V$ such that condition 2 is true in Lemma 2.
2. For a given permutation $\pi$, Zone$_1(\pi x)$ is all $w \in V$ such that condition 3 is true in Lemma 2 with $\pi$.
3. For a given permutation $\pi$, Zone$_2(\pi x)$ is all $w \in V$, such that condition 4 is true in Lemma 2 with $\pi$.

Note that there are seven zones total.

**Lemma 5.** Let $(X, d)$ be a metric tree. Let $x, y \in X$ and let $r \in g(x, y)$ if and only if $X \setminus \{r\}$ has at least two disconnected components and $x, y$ are in distinct components.

**Proof.** Suppose $r \in g(x, y)$. In metric trees, we know that there exist unique simple path between any two points. Therefore, if, after removing $r$, a path connecting $x, y$ remained (i.e., they are in the same component), then there are two simple paths connecting $x, y$ in $X$, which is not possible.

Suppose $x, y$ are in two separate components of $X \setminus \{r\}$, then because $X$ is path connected, the geodesic between $x$ and $y$ must pass through $r$. □

**Lemma 3.** Given $(X, d)$ a metric tree, and a universal tree $T$ on $x, y, z$, we have the following

1. If $w \in \text{Zone}_1(x)$, then for all $\hat{w} \notin \text{Zone}_1(x)$, we have that $x \in g(w, \hat{w})$.
2. If $w \in \text{Zone}_2(x)$, then for all $\hat{w} \notin \text{Zone}_1(x)$ for $i = 1, 2$, then we have that $r \in g(w, \hat{w})$.

**Proof.** First let us prove statement 1. To do this, let us analyze the possible zones to which $\hat{w}$ belongs.

**Case 1:** Suppose $\hat{w} \in \text{Zone}_1(y)$ (similar for $\hat{w} \in \text{Zone}_1(z)$). Then we have that $d(\hat{w}, y) = (x, y)\hat{w}$. This, implies that $(\hat{w}, x)_y = 0$. Thus, by Lemma 4, we have that $y \in g(\hat{w}, x)$. Similarly we have that $x \in g(w, y)$.

Now since $w \in \text{Zone}_2(x)$, we know that $g(x, w) \cap g(x, y) = \{x\}$. Similarly, know that $g(x, y) \cap g(y, \hat{w}) = \{y\}$. Then using Lemma 5, on removing $x$, we see that $w$ and $y$ are different connected components. Then since $x \notin g(\hat{w}, y)$, we see that $\hat{w}, y$ is in one connected component. Thus, $w, \hat{w}$ in different components. Thus, $x \in g(w, \hat{w})$ by Lemma 5.

**Case 2:** Suppose $\hat{w} \in \text{Zone}_2(y)$ (similar for $\hat{w} \in \text{Zone}_2(z)$). Now let $r$ be the Steiner node of the universal tree on $x, y, z$. In this case we know from Lemma 2 that $r \in g(\hat{w}, x)$ and that $g(w, x) \cap g(x, r) = \{x\}$.

Now since $w \in \text{Zone}_1(x)$, we know that $g(x, w) \cap g(x, r) = \{x\}$. Similarly, know that $g(x, r) \cap g(r, \hat{w}) = \{r\}$. Then using Lemma 5, on removing $x$, we see that $w$ and $r$ are different connected components. Then since $x \notin g(\hat{w}, r)$, we see that $\hat{w}, r$ is in one connected component. Thus, $w, \hat{w}$ are in different components. Thus, $x \in g(w, \hat{w})$ by Lemma 5.

**Case 3:** $\hat{w} \in \text{Zone}_2(x)$. Let $r$ be the Steiner node for the universal tree on $x, y, z$. Now my Lemma 2, we know that $x \in g(w, \hat{w})$. Thus, again by removing $x$ and using Lemma 5, $r$ and $w$ are in different. We also have that by Lemma 2 $x \notin g(\hat{w}, r)$. Thus $\hat{w}, r$ are in the same connected component of $X \setminus \{x\}$. Thus, $w$ and $\hat{w}$ are in different connected components. Thus, by Lemma 5, $x \in g(w, \hat{w})$.

Thus in all cases, we can see that $x \in g(w, \hat{w})$.

Now let us prove statement 2. Without loss of generality assume that

$$\hat{w} \in \text{Zone}_1(y)$$

for $i = 1, 2$. Then from Lemma 2, we know that $r \notin g(w, x)$ and $r \notin g(\hat{w}, y)$, but $r \in g(x, \hat{w})$. Thus, using Lemma 5 on removing $r, x$ and $y$ and in different components and $w$ is in the same component as $x$ and $\hat{w}$ is in the same component as $y$. Thus, again using Lemma 5, we have that $r \in g(w, \hat{w})$. □

**Theorem 1.** Given $(X, d)$ a $\delta$-hyperbolic metric space, and $n$ points $x_1, \ldots, x_n \in X$, TREEREP returns a tree $(T, d_T)$. In the case that $\delta = 0$, $d_T = d$, and $T$ has the fewest possible nodes. TREEREP has worst case run time $O(n^2)$. Furthermore the algorithm is embarrassingly parallelizable.

**Proof.** The proof of this theorem follows directly from our structural lemmas. More precisely, we show that for $\delta = 0$, TREEREP returns a consistent metric via induction on $n$, the number of data points.

**Base Case:** The case when $n \leq 3$ is covered by Lemma 1. And, the case when $n = 4$ is covered by Lemma 2.

**Inductive Hypothesis:** Assume that for all $k \leq n$, our data set of $k$ points is consistent with a 0-hyperbolic metric $d$, then TREEREP returns a tree $(T, d_T)$ that is consistent with $d$ on the $k$ points.

**Inductive Step:** Assume that $w$ is the last vertex attached to $T$. By the inductive hypothesis, we know that without $w$, $(T, d_T)$ is consistent on with $d$ so we only need to show that it is consistent with the addition of $w$. 


Now let \( x, y, z \) be the universal tree used to sort \( w \) in the penultimate recursive step. Let \( r \) be the Steiner node. Then by Lemma 2, we know that \( d_T(w, x) = d(w, x) \), \( d_T(w, y) = d(w, y) \), and \( d_T(w, z) = d(w, z) \).

Now without loss of generality assume that \( w \) was sorted in a zone for \( x \). That is, \( w \in Zone_i(x) \) for \( i = 1, 2 \).

**Case 1:** If \( w \in Zone_1(x) \). Then from Lemma 1, we know that for all \( \tilde{w} \notin Zone_1(x) \), we have that \( x \in g(w, \tilde{w}) \).

Thus, having \( d_T(x, w) = d(x, w) \) and \( d_T(x, \tilde{w}) = d(x, \tilde{w}) \) is sufficient to show consistency.

Now, since \( w \) was placed last there is at most one other point \( \tilde{w} \) in \( Zone_1(x) \), and \( d_T(w, \tilde{w}) = d(w, \tilde{w}) \) due to Lemma 1.

**Case 2:** If \( w \in Zone_2(x) \). Then from Lemma 2, we know that for all \( \tilde{w} \notin Zone_i(x) \), for \( i = 1, 2 \) we have that \( r \in g(w, \tilde{w}) \). Thus, having \( d_T(r, w) = d(r, w) \) and \( d_T(r, \tilde{w}) = d(r, \tilde{w}) \) is sufficient to show consistency.

Suppose \( \tilde{w} \in Zone_1(x) \). Then from Lemma 1, we have that \( x \in g(w, \tilde{w}) \). Thus, having \( d_T(x, w) = d(x, w) \) and \( d_T(x, \tilde{w}) = d(x, \tilde{w}) \) is sufficient to show consistency.

Finally, since \( w \) was the last node placed there are no other nodes in \( Zone_2(x) \).

Thus, we have the the tree returned by TREEREP is consistent with the input metric \( d \).

Notice that whenever we add a Steiner node \( r \) we fix the position of at least one data point node. We then look at \( O(n) \) Gromov inner products. Thus, we have a worst case running time of \( O(n^2) \).

Additionally, the part where we place nodes into their respective zones can be done in parallel. Thus, if we have \( K \) threads then the running time is \( O\left(\frac{n^3}{K}\right) \) for the worst running times.

The final part of the theorem is that we return the tree with the smallest possible nodes. Whenever we look at any triangle formed by three points \( x, y, z \), we place a Steiner node \( r \). Now, if none of the distances from \( x, y, z \) to \( r \) is 0, then this Steiner node must exist in all tree consistent with \( d \). If one of these distances is 0, we contracted that edge and got rid of \( r \). Thus, along with the local consistency argument above this shows that all Steiner nodes that we have placed are necessary (the local consistency argument implies that no two of the Steiner nodes placed could in fact be made into one node due to the nodes beings in different regions). Thus, we have the fewest possible nodes.

### 7.2. Tree Approximation Proofs

**Proposition 1.** Given a \( \delta \)-hyperbolic metric \( d \), the universal tree \( T \) on \( x, y, z \) and a fourth point \( w \), when sorting \( w \) into its zone \( Zone_i(\pi x) \), TREEREP introduces an additive distortion of \( \delta \) between \( w \) and \( \pi y, \pi z \).

**Proof.** Without loss of generality assume that \( \pi \) is the identity. In this case, we know that \( d_T(w, r) = (y, z)_w \), and that \( d_T(y, r) = (x, z)_y \). Thus, we have the following:

\[
|d_T(w, y) - d(w, y)| = |d_T(w, r) + d_T(r, y) - d(w, y)|
\]

\[
= |(y, z)_w + (x, z)_y - d(w, y)|
\]

\[
= \frac{1}{2} |d(w, z) + d(y, x) - d(w, y) - d(x, y)|
\]

\[
= |(x, y)_w - (x, z)_w|
\]

\[
\leq \delta
\]

\[\square\]

### 8. Geometry: Asymptotic Cones

**Definition 16.** An ultrafilter \( F \) on \( X \) is a subset of \( \mathcal{P}(X) \) such that

1. If \( A \in F \) and \( A \subseteq B \) then \( BF \)
2. \( A, B \in F \) then \( A \cap B \in F \)
3. For any \( A \subseteq X \), exactly 1 of \( A, X \setminus A \) is in \( F \)
4. \( \emptyset \notin F \).

One way to view \( F \) is as defining a probability measure on \( X \). In particular, we will view the sets in \( F \) to be large and the sets not in \( F \) to be small. Hence, we can define a measure \( \nu \) such that for all \( A \in F \) we have that \( \nu(A) = 1 \) and for all \( A \notin F \) we have that \( \nu(A) = 0 \).

In this way, we can see that \( \nu \) is a finitely additive measure on \( X \). One common method to define ultrafilters is to take a point \( x \in X \) and let \( F \) be the set of all sets that contain \( x \). In this case, the measure \( \nu \) has a point mass at \( x \) and zero mass elsewhere. Such filters are known as principal ultrafilters.

Given a measure \( \nu \) on \( \mathbb{N} \), we can use it to define limits and convergence in \( X \). In particular, we have that a sequence \( x_i \) converges to \( x \), if for all \( \epsilon > 0 \) we have that

\[
\nu \left( \{ x_i : |x_i - x| < \epsilon \} \right) = 1
\]

We will denote limits of this form as \( \lim_{\nu} x_i = x \).

We will make use of ultrafilters to construct the asymptotic cone. We will do this via looking at a non-principal ultrafilter on \( \mathbb{N} \). We consider non-principal ultrafilters as we...
want to get a view from infinity, and we do not want to be in the case when one particular index in \( \mathbb{N} \) has the entire mass. Hence we restrict ourselves to non-principal ultrafilters. One nice characterization of non-principal ultrafilters is that they are exactly the ultrafilters that have no finite sets.

Now that we have mathematical framework in which we can take limits, let us define our asymptotic cone. Let \( \omega \) be a non-principal ultrafilter on \( \mathbb{N} \). Let \( \{b_i\}_{i \in \mathbb{N}} \) be a sequence of base points and let \( \{\lambda_i\}_{i \in \mathbb{N}} \) be a sequence of scaling factors that go to infinity. Let \( d \) be the metric on our space \( X \). Then let

\[
X_{\omega,b_i,\lambda_i} = \{y_i : y_i \in X \text{ and } d(b_i, y_i) \leq \text{const}_{\{y_i\}} \lambda_i\}
\]

While this space looks huge we will define an equivalence relation and mold out by this relation to obtain better structure on this space. Given two points \( y = \{y_i\}, z = \{z_i\} \in X_{\omega,b_i,\lambda_i} \), we say that \( y \sim z \) if

\[
\lim_{\omega} \frac{d(y_i, z_i)}{\lambda_i} = 0
\]

We can now define our asymptotic cone \( \text{Con}_\omega(X) = X(\omega, b_i, \lambda_i) / \sim \). We can also define a metric on this space as follows, given \( y = \{y_i\}, z = \{z_i\} \in \text{Con}_\omega(X) \)

\[
d_\omega(y, z) := \lim_{\omega} \frac{d(y_i, z_i)}{\lambda_i}
\]

Let us look at a few examples to get a handle on what \( \text{Con}_\omega(X) \) looks like.

1. Example 1: Let us first consider \( X = \mathbb{R}^n \). We know that \( \mathbb{R}^n \) is scale invariant. This results in \( \text{Con}_\omega(\mathbb{R}^n) \) being equivalent to \( \mathbb{R}^n \). In fact, if we assume that \( b_i \equiv 0 \), then the map \( x \mapsto \{\lambda_i x\} \) is an isometry from \( \mathbb{R}^n \) to \( \text{Con}_\omega(\mathbb{R}^n) \).

2. Example 2: Suppose \( X \) is a bounded metric space. In this case \( \text{Con}_\omega(X) \) is a single point.

**Definition 17.** A metric space \( (X, d_x) \) can be isometrically embedded into a metric space \( (Y, d_y) \) if there exists a map \( f : X \to Y \) such that for all \( x_1, x_2 \in X \) we have that

\[
d_x(x_1, x_2) = d_y(f(x_1), f(x_2))
\]

Such a map \( f \) is known as an isometry.

**Definition 18.** A metric space \( (X, d) \) is homogenous if for all \( x, y \in X \) there exists an isometry \( f : X \to X \) such that \( f(x) = y \).

**Definition 19.** Given a \( \mathbb{R} \)-tree \( T \), the valency of a point \( x \in T \) in an \( \mathbb{R} \)-tree is the number of connected components in \( T \setminus \{x\} \). Let the valence of a the tree, denoted \( \text{val}(T) \), be the maximum valence of any point in \( T \).

**Definition 20.** A \( \mathbb{R} \)-tree \( T \) is a \( \mu \)-universal if every \( \mathbb{R} \)-tree \( \tilde{T} \) with \( \text{val}(\tilde{T}) \leq \mu \) can be isometrically embedded into \( T \).

Here we can see that we can embed any finite tree into a \( 2^{\aleph_0} \)-universal tree \( T \). Hence, if could isometrically embed \( T \) into \( \text{Con}(\mathbb{H}^n) \) then we can embed any tree into \( \text{Con}(\mathbb{H}^n) \). This and more turns out to be true.

**Theorem 4.** (Dyubina & Polterovich, 2001) Any \( 2^{\aleph_0} \)-universal \( \mathbb{R} \)-tree can be isometrically embedded into the asymptotic cone for any complete simply connected manifold of negative curvature.

### 9. Geometry: Geodetic Tree

In general, it is rare to be able isometrically embed one space into another. Hence, we have the following weaker definition.

**Definition 21.** We say that we can quasi isometrically embed a metric space \( (X, d_x) \) into a metric space \( (Y, d_y) \) if there exists a map \( f : X \to Y \) and real numbers \( c, \lambda \in \mathbb{R} \) such that \( \lambda \geq 1, c > 0 \) and for all \( x_1, x_2 \in X \) we have that

\[
\frac{1}{\lambda} d_x(x_1, x_2) - c \leq d_y(f(x_1), f(x_2)) \leq \lambda d_x(x_1, x_2) + c
\]

Such isometries are called \((\lambda, c)\)-quasi-isometries.

It has been shown that any \( \delta \)-hyperbolic metric space \( (X, d) \) with bounded growth admits a quasi-isometric embedding into \( \mathbb{H}^k \) (Bonk & Schramm, 2000).

**Definition 22.** We say that a ray \( R \) is quasi geodetic if instead of being an isometric image of \([0, \infty)\), we have that \( R \) is an quasi-isometric image of \([0, \infty)\).

**Definition 23.** A ray is eventually (quasi) geodetic if it has a subray that is (quasi) geodetic.

**Theorem 5.** (Hamann, 2018) For all \( \lambda \geq 1, c \geq 0 \) there is a constant \( \kappa = \kappa(\delta, \lambda, c) \), such that for every two points \( x, y \in \mathbb{H}^k \), every \((\lambda, c)\)-quasi-geodesic between them lies in a \( \kappa \)-neighborhood around every geodesic between \( x \) and \( y \) and vice versa.

**Definition 24.** Two geodesic rays \( \pi_1, \pi_2 \) are equivalent if for any sequence \( (x_n) \) of points on \( \pi_1 \), we have \( \lim \inf_{n \to \infty} d(x_n, \pi_2) \leq M \) for all \( M < \infty \)

**Definition 25.** The boundary \( \partial \mathbb{H}^k \) of \( \mathbb{H}^k \) is the equivalence class of all geodesic rays.

**Theorem 6.** (Hamann, 2018) There is an \( \mathbb{R} \)-tree \( T \subset \mathbb{H}^k \) such that the canonical map \( \gamma \) from \( \partial T \) to \( \partial X \) exists and has the following properties.

1. It is surjective;
2. there is a constant \( M < \infty \) depending only on \( k \) such that \( \gamma^{-1}(\eta) \) has at most \( M \) elements for each \( \eta \in \partial \mathbb{H}^k \).
Theorem 7. (Hamann, 2018) Let \( T \) be the \( \mathbb{R} \)-tree in Theorem 6 with root \( r \). There exist constants \( \lambda \geq 1 \), \( c \geq 0 \) such that every ray in \( T \) starting at the root is a \((\lambda, c)\)-quasi-geodetic ray in \( \mathbb{H}^k \).

The above two theorems tell us that given any geodesic ray \( R \) in \( \mathbb{H}^k \) there exists a ray in \( T \) that is equivalent to \( R \) (via \( \sim \) in Definition 24). Furthermore this ray in \( T \) is \((\lambda, c)\)-quasi-geodetic ray in \( \mathbb{H}^k \). Thus, due to Theorem 5 any configuration of points at scale in \( \mathbb{H}^k \) can be approximated by a tree such that the larger the scale, better the approximation.

10. TREEREP Best

So far all numbers for the TREEREP algorithm that we have reported are averages. But due to the speed of the algorithm, we can actually run the experiment multiple times and pick the tree with the best metric.

11. Improving Distortion

We have seen that in the case of unweighted graphs TREEREP produces better MAP than PM, LM, and PT. However, PT tends to have better average distortion. Hence, we want to be able to improve the distortion. Once we have learned the tree structure we can set up an optimization problem to learn the edge weights on the tree to improve the distortion. Specifically, since the metric comes from the tree, for any pair of data points, there is exactly one path connecting the two data points. Thus, regardless of the edges weights, this path is the shortest path between the data points. Thus, we can set up an optimization problem of the following form:

\[
\arg \min_{W} \| AW - D \|_2.
\]

Here \( W \) is a vector containing the edge weights, \( D \) is a vector containing the original metric, and \( A \) is a matrix that encodes all of the paths. This optimization problem however, is unfeasible as \( n \) gets longer. So instead we sample some rows of \( A \) and solve a heuristic problem. As can be seen from Table 5, we are still faster than NJ but now have improved our distortion without sacrificing MAP.

12. Experiment and Practical Details

12.1. TreeRep

There a few practical details that must be discussed in relation to the TREEREP algorithm.

1. Pre-allocate the matrix for the weights of edges of the tree as a dense matrix. Doing this greatly speeds up computations. Note the proof of Lemma 2, show that we need at most \( n \) Steiner nodes. Thus, the tree has about \( 2n \) nodes. Since the input to the algorithm is a dense \( n \times n \) matrix, we already need \( O(n^2) \) memory. Thus, having a dense \( 2n \times 2n \) matrix is still linear memory usage in the size of the input.

2. When doing zone 2 recursions pick the node closest to \( r \) as the new \( z \) as suggested by Proposition 1.

3. The placement of nodes into their respective zones can be done in parallel. For all of the experiments in the paper, we used 8 threads to do the placement for the experiments in Sections 4.1, 4.3, and 4.4, and 1 thread in Section 4.2.

4. All of the numbers reported are averages over 20 iterations. We could have also picked the best over 20 iterations as our algorithm is fast enough for this to be viable.

5. When checking for equality, instead of checking for exact equality, we checked whether two numbers are within 0.1 of each other.

6. It is possible for some of the edge weights to be set to a negative number. In this case, after the algorithm terminated we set those edge weights to 0.

12.2. Neighbor Join

The following implementation of NJ was used: http://crsl4.github.io/PhyloNetworks.jl/latest/. We set the options so as to not have any negative edge weights.

12.3. MST

Prim’s algorithm for calculating MST was used. We used the implementation at https://github.com/JuliaGraphs/LightGraphs.jl

12.4. LevelTree and ConstructTree

To the best of the authors knowledge there does not exist a publicly available implementations of these algorithms. Both of these algorithms were implemented by the authors.

Note that LevelTree claims to be a \( O(n) \) algorithm, but this only true, once we have calculated the sphere \( S_n \) needed for the algorithm. However, it takes \( O(n^2) \) time to calculate the spheres \( S_n \) (equivalent to solving single source all destination shortest path problem).

12.5. PM and LM

The following options were used. The number of epochs was to set to be higher than default. Everything else was left at default. One note about PM and LM is that their objective function is set up to optimize for MAP and not average distortion.
Tree! I am no Tree! I am a Low Dimensional Hyperbolic Embedding

| Table 4. TreeRep Best Numbers |
|-------------------------------|
| No Opt | Heuristic Opt | Full Opt |
| Graph | MAP | Distortion | MAP | Distortion | MAP | Distortion |
| Celegans | 0.508 | 0.173 | 0.539 | 0.138 | 0.547 | 0.119 |
| Diseasome | 0.912 | 0.134 | 0.911 | 0.106 | 0.890 | 0.092 |
| CS PhD | 0.987 | 0.134 | 0.984 | 0.119 | 0.968 | 0.121 |
| Yeast | 0.841 | 0.171 | 0.833 | 0.150 | 0.808 | 0.135 |
| Grid-worm | 0.727 | 0.154 | 0.728 | 0.125 | - | - |
| GRQC | 0.699 | 0.175 | 0.694 | 0.152 | - | - |

Table 5. MAP and average distortion for the TreeRep and MST after doing the heuristic optimization. The time taken for both optimizations is the same.

| Graph | Time | Distortion | MAP | Distortion | MAP |
|-------|------|------------|-----|------------|-----|
| Celegans | 0.69 | 0.157 | 0.504 | 0.195 | 0.357 |
| Diseasome | 1.56 | 0.121 | 0.891 | 0.111 | 0.774 |
| CS PhD | 1.2 | 0.152 | 0.971 | 0.170 | 0.989 |
| Yeast | 4.2 | 0.163 | 0.813 | 0.171 | 0.862 |
| Grid Worm | 32 | 0.164 | 0.707 | 0.151 | 0.768 |
| GRQC | 68 | 0.157 | 0.676 | 0.159 | 0.669 |

1. -lr 0.3
2. -epochs 1000
3. -burnin 20
4. -nlegs 50
5. -fresh
6. -sparse
7. -train_threads 2
8. -ndproc 4
9. -batchsize 10

For PM we used -manifold poincare, for LM we used -manifold lorentz. The code is taken from https://github.com/facebookresearch/poincare-embeddings

12.6. PT

The following options were used. We used the -learn-scale option as based on the discussion in the appendix of Sala et al. (2018) learning the scale results in better quality metrics. Additionally, we add a burnin phase to the optimization. Finally, based on the discussion in (Sala et al., 2018), the objective function for PT has a lot of shallow local minimas. Thus, we added momentum and used Adagrad for the optimization to try and avoid these local minimums.

1. -learn-scale
2. --burn-in 100
3. --momentum 0.9
4. --use-adagrad
5. -l 5.0
6. --epochs 1000
7. --batch-size 256
8. --subsample 64

The code is taken from https://github.com/HazyResearch/hyperbolics

12.7. Hardware

All experiments were run on Google cloud instances. For PM, LM and PT we created a fresh instance for each algorithm. Each instance for an algorithm only had the bare minimum installed to run those algorithms. We used n1-highmem-8 instances. The specification of each of the instances are as follows:

1. 8 cores each with 6.5 GB of ram.
2. Ubuntu-1604-xenial-v20190913 operating system.
3. 100 standard persistent disk.

For TreeRep, NJ, CT, LT and MST, we ran all code via a Jupyter notebook interface running Julia 1.1.0. All experiments (except for the experiments with Enron and Wordnet), we done on instances with the same specification as above.

For Enron and Wordnet, we need more memory to store the distance matrices. Thus, used instances with the following specifications.

1. 24 cores each with 6.5 GB of ram.
2. Ubuntu-1604-xenial-v20190913 operating system.
3. 100 standard persistent disk.

12.8. Synthetic 0-hyperbolic metrics

To produce random synthetic 0-hyperbolic metrics, we do the following. First, we take a complete binary tree of depth \( i \). We then compute its double tree. Then for each node in this tree we sample a number \( C \) from 2 to 10 and replace the node with a clique of size \( C \). We then pick a random
node in the tree and compute the breadth first search tree from that node. We then assign edge uniformly randomly, sampled from $[0,1]$.

### 12.9. Synthetic Data Sets

Here we sampled coordinates from the standard normal $N(0,1)$. The final coordinate $x_0$ is set so that the point lies on the hyperboloid manifold. In the presence of a scale we just multiplied each coordinate by that scale before calculating $x_0$. We ran TREEREP with 1 thread.

### 12.10. Phylogenetic and Single Cell Data

The immunological distances can be seen in Figure 9. The matrix is symmeterized by averaging across the diagonal. In this case, we ran TREEREP 10 times and picked the tree with the lowest average distortion.

The figures for the trees are produced using an adaptation of Sarkar’s construction for Euclidean space. The code from PT also produces a picture. This picture can be seen in Figure 8. As we can see, this figure is similar to the one in the main text.

For the Zeisel data we did the same pre-processing as done in Dumitrascu et al. (2019). For PM and MST, we use 10 nearest neighbor graph.

### 12.11. Unweighted Graphs

Some of the graphs are disconnected. The largest connected component of each graph was used.

For $\delta$ calculation, we normalized the distances so that the maximum distance was 1 and then calculated $\delta$. For C elegans, Diseasesome, and Phds, this calculation is exact.

For Yeast, Grid-worm and GRQC, we fixed the base point to be $w=1$ and then calculated $\delta$. It is known from theory that for any fixed base point the $\delta$ is at least half of the $\delta$ for the whole metric (Bridson & Häfliger, 2013). Thus, we get the inequality.

All experiments with a “-” were terminated after 4 hours.

### 12.12. Calculating $\alpha$

Can be calculated directly using

$$\alpha = \frac{Tr(D^* D)}{\|D\|_F^2}$$

### 13. Tree Representation Pseudo-code

**Algorithm 3** Recursive parts of TreeRep.

1. function ZONE1.RECURSION($T$, $d_T$, $d$, $L$, $v$)
2. if Length($L$) == 0 then
3. return $T$
4. end if
5. if Length($L$) == 1 then
6. Set $u = \text{pop}(L)$ and add edge $(u,v)$ to $E$
7. Set edge weight $d_T(u,v) = d(u,v)$
8. return $T$
9. end if
10. Set $z = \text{the closest node to } v$.
11. Delete edge $(u,v)$
12. return RECURSIVE_STEP($T,L,v,u,z,d_T$)
13. end function

14. function ZONE2.RECURSION($T$, $d_T$, $d$, $L$, $u$, $v$)
15. if Length($L$) == 0 then
16. return $T$
17. end if
18. Set $z = \text{the closest node to } v$.
19. Delete edge $(u,v)$
20. return RECURSIVE_STEP($T,L,v,u,z,d_T$)
21. end function

---

Figure 8. Figure for Sarich data produced by PT code

Figure 9. Immunological distances from (Sarich, 1969)
Algorithm 4 Metric to tree structure algorithm.

1: function TREE_STRUCTURE(X, d)
2:   T = (V, E, d') = ∅
3:   Pick any three data points uniformly at random
   x, y, z ∈ X.
4:   T = RECURSIVE_STEP(T, X, x, y, z, d, d_T)
5:   return T
6: end function

7: function RECURSIVE_STEP(T, X, x, y, z, d, d_T)
8:   Let Z1(r → [], x → [], y → [], z → []), Z2(x → [], y → [], z → []).
9:   Place an additional node r in V and add edges
   xr, yr, zr to E
10:  Set the weights d_T(x, r) = (y, z), d_T(y, r) = (x, z), and d_T(z, r) = (x, y).
11:  for all remaining data points w ∈ X do
12:     a = (x, y)_w, b = (y, z)_w, c = (z, x)_w, m = 0,
13:        m2 = 0
14:        if a == b == c then
15:           push(w, Z1[r])
16:           Set d_T(w, r) = (x, y)_w
17:        else if a == maximum(a, b, c) then
18:           π = (x → z, y → y, z → x)
19:           m = b, m2 = c
20:           Set d_T(w, r) = a
21:        else if b == maximum(a, b, c) then
22:           π = (x → x, y → y, z → z)
23:           m = a, m2 = c
24:           Set d_T(w, r) = b
25:        else if c == maximum(a, b, c) then
26:           π = (x → y, y → x, z → z)
27:           m = a, m2 = b
28:           Set d_T(w, r) = c
29:        end if
30:        if d(w, πx) == m or d(w, πx) == m2 then
31:           push(w, Z1[πx])
32:        else
33:           push(w, Z2[πx])
34:        end if
35:     end for
36:     // recurse on each of the zones
37:     T = ZONE1_RECURSION(T, d_T, d, Z1[r], r)
38:     T = ZONE1_RECURSION(T, d_T, d, Z1[x], x)
39:     T = ZONE1_RECURSION(T, d_T, d, Z1[y], y)
40:     T = ZONE1_RECURSION(T, d_T, d, Z2[x], x, r)
41:     T = ZONE2_RECURSION(T, d_T, d, Z2[y], y, r)
42:     T = ZONE2_RECURSION(T, d_T, d, Z2[z], z, r)
43:     return T
44: end function