Computing Geodesic Distances in Tree Space

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Abstract

We present two algorithms for computing the geodesic distance between phylogenetic trees in tree space, as introduced by Billera, Holmes, and Vogtmann (2001). We show that the possible combinatorial types of shortest paths between two trees can be compactly represented by a partially ordered set. We calculate the shortest distance along each candidate path by converting the problem into one of finding the shortest path through a certain region of Euclidean space. In particular, we show there is a linear time algorithm for finding the shortest path between a point in the all positive orthant and a point in the all negative orthant of $\mathbb{R}^k$ contained in the subspace of $\mathbb{R}^k$ consisting of all orthants with the first $i$ coordinates non-positive and the remaining coordinates non-negative for $0 \leq i \leq k$. The resulting algorithms for computing the geodesic distance appear to be the best available to date.

1 Introduction

Phylogenetic trees, or phylogenies, are used throughout biology to understand the evolutionary history of organisms ranging from primates to the HIV virus. Outside of biology, they are used in studying the evolution of languages and culture, for example. Often, reconstruction methods give multiple plausible phylogenetic trees on the same set of taxa, which we wish to compare using a quantitative distance measure. We would also like to have a statistical framework to better evaluate the generated trees. The tree space of Billera, Holmes, and Vogtmann [3] and its corresponding geodesic distance measure address both of these issues. In this paper, we give two practical algorithms for computing this distance.

There are many different algorithms to construct phylogenetic trees from biological data ([10] and its references), but their accuracy can be affected by such factors as the underlying tree shape [13] or the rate of mutation in the DNA sequences used [14]. To compare these methods through simulation, or to find the likelihood that a certain tree is generated from the data, researchers need to be able to compute a biologically meaningful distance between trees [14]. Several different distances between phylogenetic trees have been proposed (e.g. [7], [11], [12], [21], [22]). For example, the Nearest Neighbor Interchange (NNI) distance ([21] and [29]), which counts the number of rotations between trees, is considered one of the best distance measures, but is NP-hard to compute [8], making it impractical.

In response to the need for a distance measure between phylogenetic trees that naturally incorporates both the tree topology and the lengths of the edges, Billera et al. [3] introduced the geodesic distance. This distance measure is derived from the tree space, $T_n$, which contains all phylogenetic trees with $n$ leaves. The tree space is formed from a set of Euclidean regions, called orthants, one for each topologically different tree. Two regions are connected if their corresponding trees are considered to be neighbours. Each phylogenetic tree with $n$ leaves is represented as a

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point within this space. There is a unique shortest path, called the geodesic, between each pair of trees. The length of this path is our distance metric.

The most closely related work is by Staple [26] and Kupczok et al. [15], who developed algorithms to compute the geodesic distance based on the notes of Vogtmann [28]. Both of these algorithms are exponential in the number of different edges in the two trees. Although Kupczok et al. developed their algorithm \textsc{GeoMeTree} independently, it can be considered a direct improvement to the algorithm of Staple. We show in Section 5 that our algorithm performs significantly better than \textsc{GeoMeTree}, although it is still exponential. A polynomial time, $\sqrt{2}$-approximation of the geodesic distance was given by Amenta et al. [1].

Our primary contribution is two algorithms for computing the geodesic distance between two phylogenetic trees. We show these algorithms are significantly faster than the only explicit algorithm published to date. Furthermore, two main ideas were developed to construct these algorithms. First, the candidate shortest paths between trees can be represented as an easily constructible partially ordered set, giving information about the combinatorics of the tree space. Second, we can find the length of each candidate shortest path by translating the problem into one of finding the shortest path through a region of a lower dimensional Euclidean space. The solution to this new problem is a linear algorithm for a special case of the shortest Euclidean path problem in $\mathbb{R}^n$ with obstacles. Since the general problem is NP-hard for dimensions greater than 2, this result is also of interest to computational geometers. These two ideas can be combined using dynamic programming or divide and conquer methods to significantly reduce the search space, and thus make this distance computation practical for some biological data sets of interest.

The remainder of this paper is organized as follows. In Section 2, we describe the tree space and the geodesic distance between phylogenetic trees. The problem of finding the geodesic distance has both a combinatorial component, which is investigated in Section 3, and a geometric component, which is covered in Section 4. More specifically, we introduce a combinatorial framework in Section 3, which represents the candidate shortest paths between trees by an easily constructible partially ordered set (Theorem 3.7). In Section 4, we translate the problem of calculating the length of a candidate shortest path into a problem in Euclidean space (Theorem 4.4), and then show that this Euclidean problem can be solved in linear time. Section 5 combines the ideas of Sections 3 and 4 using dynamic programming or divide and conquer techniques to present two complete algorithms.

## 2 Tree Space and Geodesic Distance

This section describes the space of phylogenetic trees, $T_n$, and the geodesic distance. For further details, see [3]. A phylogenetic tree, or just tree, is a rooted tree, whose leaves are in bijection with a set of labels $X$ representing different organisms. For this paper, let $X = \{1,\ldots,n\}$. We often treat the root as a leaf, called 0. We consider both bifurcating (or binary) trees, in which each interior vertex has degree 3, and multifurcating (or degenerate) trees, in which this is not the case.

A split $A|B$ is a partition of $X \cup \{0\}$ into two non-empty sets $A$ and $B$, where $X$ is the leaf-set of some tree $T$ and 0 is its root. A split is in $T$ if it corresponds to some edge in $T$, in that one block of the partition consists of all the leaves below that edge, while the other block consists of the remaining leaves and the root. We say this split is induced by that edge in $T$. For example, in Figure 1, the split induced by the edge $e_3$ partitions the leaves into the sets $\{2,3\}$ and $\{0,1,4,5\}$. We will refer to splits induced by an edge ending in a leaf as trivial splits, and to all other splits as simply splits. A split of type $n$ is a partition of the set $\{0,1,\ldots,n\}$ into two blocks, each containing at least two elements. Let $E_T$ be the set of (non-trivial) splits of tree $T$. If $A \in E_T$ is a set of splits in $T$, then let $T/A$ be the tree $T$ with each edge that induces an element of $A$ contracted.
Two splits $e = X|X'$ and $e' = Y|Y'$ are compatible if one of $X \cap Y$, $X \cap Y'$, $X' \cap Y$ and $X' \cap Y'$ is empty. Equivalently, two splits are compatible if their inducing edges can exist in the same phylogenetic tree. For example, in Figure 1, the split $e_3 = \{2, 3\}|\{0, 1, 4, 5\}$ is compatible with the split $e_2 = \{2, 3, 4\}|\{0, 1, 5\}$, because $\{2, 3\} \cap \{0, 1, 5\} = \emptyset$. However, $e_3$ is incompatible with $f = \{1, 2\}|\{0, 3, 4, 5\}$. Two sets of mutually compatible splits of type $n$, $A$ and $B$, are compatible if $A \cup B$ is a set of mutually compatible splits.

Each edge, and hence split, $e \in E_T$, is also associated with a non-negative length $|e|_T$. For example, this length could represent the number of DNA mutations that occurred between speciation events. Two splits are considered the same if they have identical partitions, regardless of their lengths. For any $A \subseteq E_T$, let $\|A\| = \sqrt{\sum_{e \in A} |e|^2_T}$.

2.1 Tree Space

We now describe the space of phylogenetic trees, $\mathcal{T}_n$, as constructed by Billera et al. [3]. It is homeomorphic, but not isometric, to the tropical Grassmannian [24] and the Bergman fan of the graphic matroid of the complete graph [2]. This space contains all bifurcating and multifurcating phylogenetic trees with $n$ leaves. In this space, each tree topology with $n$ leaves is associated with a Euclidean region, called an orthant. The points in the orthant represent trees with the same topology, but different edge lengths. These orthants are attached, or glued together, to form the tree space.

We do not use the lengths of the edges ending in leaves in the definition of tree space, but can easily include them by considering geodesics through $\mathcal{T}_n \times \mathbb{R}^n_{+}$, as noted in Billera et al. [3].

Any set of $n - 2$ compatible splits corresponds to a unique rooted phylogenetic tree topology ([23 Theorem 3.1.4]). For any such split set $E_T$ corresponding to tree $T$, associate each split with a vector such that the $n - 2$ vectors are mutually orthogonal. The cone formed by these vectors is the orthant associated with the topology of $T$. Recall that the $k$-dimensional (nonnegative) orthant is the non-negative part of $\mathbb{R}^k$, denoted $\mathbb{R}^k_{+}$. A point $(x_1, ..., x_{n-2})$ in $\mathbb{R}^{n-2}$ represents the tree containing the edge associated with the $i$-axis that has length $x_i$, for all $1 \leq i \leq n-2$, as illustrated in Figure 2(a). If $x_i = 0$, then the tree is on a face of the orthant. In this case, we will say the tree does not contain the edge associated with the $i$-axis. The trees on the faces of each orthant have at least one edge of length 0. Furthermore, two orthants can share the same boundary face, and thus are attached. For example, in Figure 2(a), the trees $T_1$ and $T'_1$ are represented as two distinct points in the same orthant, because they have the same topology, but different edge lengths. The tree $T_0$ has only one edge, $e_1$, and thus is a point on the $e_1$ axis.

Notice that although Figure 2(a) is drawn in the plane, it actually sits in $\mathbb{R}^3$, with each of the axes or splits corresponding to a different dimension. In general, $\mathcal{T}_n$ sits in $\mathbb{R}^N$, where $N$ is the
number of possible splits. However, as no point in \( T_n \) has a negative coordinate in \( \mathbb{R}^N \), we will often let the positive and negative part of an axis correspond to different splits.

For any set \( A \) of compatible splits with lengths, let \( T(A) \) represent the tree containing exactly the edges that induce the splits in \( A \) and all trivial splits. The lengths of the edges in \( T(A) \) correspond to their respective lengths in \( A \). Let \( O(A) \) be the orthant of lowest dimension containing \( T(A) \). For any \( t \geq 0 \), let \( t \cdot A \) be the set of splits \( A \) whose lengths have all been multiplied by \( t \). If \( A \) and \( B \) are two sets of mutually compatible splits of type \( n \), such that \( A \cup B \) is also a set of mutually compatible splits, then we define the binary operator \( + \) on the orthants of \( T_n \) by \( O(A) + O(B) = O(A \cup B) \). For any union of disjoint orthants, \( \bigcup_{i=0}^{k} O(A_i) \), where \( B \) is a set of mutually compatible splits of type \( n \) such that \( B \) and \( A_i \) are compatible sets for all \( 0 \leq i \leq k \), define \( \left( \bigcup_{i=0}^{k} O(A_i) \right) + O(B) = \bigcup_{i=0}^{k} (O(A_i) + O(B)) = \bigcup_{i=0}^{k} O(A_i \cup B) \). If \( A \cap B = \emptyset \), we also use the direct sum notation \( \oplus \).

2.2 Geodesic Distance

There is a natural metric on \( T_n \). The distance between two trees in the same orthant is the Euclidean distance between them. The distance between two trees in different orthants is the length of the shortest path between them, where the length of a path is the sum of the Euclidean lengths of the intersections of this path with each orthant. For any trees \( T_1 \) and \( T_2 \) in \( T_n \), the geodesic distance, \( d(T_1, T_2) \), between \( T_1 \) and \( T_2 \) is the length of the geodesic, or locally shortest path, between \( T_1 \) and \( T_2 \) in \( T_n \). Billera et al. defined this distance, and proved that \( T_n \) is a CAT(0) space \( \text{[3, Lemma 4.1]} \), or has non-positive curvature \( \text{[5]} \), and thus the geodesic between any two trees in \( T_n \) is unique.

For example, in Figure 2(a), the geodesic between the trees \( T_1 \) and \( T_2 \) is represented by the dashed line. Figure 2(b) depicts 5 of the 15 orthants in \( T_1 \). This figure also illustrates that the edge lengths, in addition to the tree topologies, determine through which intermediate orthants the geodesic will pass.

2.3 The Essential Problem

The problem of finding the geodesic between two arbitrary trees in \( T_n \) can be reduced in polynomial time to the problem of finding the geodesic between two trees with no splits in common. This is
the problem considered in Sections 3 and 4. Furthermore, the lengths of the pendant edges can easily be included in the distance calculation, if desired.

Vogtmann [28] proved the following theorem, which explains how to decompose the problem of finding the geodesic when the trees share a common split. An alternative proof is given in [19]. Let $T_1$ and $T_2$ be two trees with a common split $e = X|Y$, where $0 \in X$, as shown in Figure 3(a). For $i \in \{1, 2\}$, let $T^A_i$ be the tree $T_i$ with edge $e$ and any edge below it in $T_i$ contracted. That is, any edge $a = X'|Y'$ such that $X' \subset Y$ or $Y' \subset Y$ is contracted, as shown in Figure 3(b). For $i \in \{1, 2\}$, let $T^B_i$ be the tree $T_i$ formed by contracting edge $e$ and all edges not contracted in $T^A_i$. That is, any edge $b = X'|Y'$ such that $X' \subset X$ or $Y' \subset X$ is contracted, as in Figure 3(c).

Figure 3: Forming the trees $T^A_i$ and $T^B_i$ from $T_i$ for $i \in \{1, 2\}$.

Theorem 2.1. If $T_1$ and $T_2$ have a common split $e$, and $T^A_i$ and $T^B_i$ are as described in the above paragraph for $i \in \{1, 2\}$, then $d(T_1, T_2) = \sqrt{d(T^A_1, T^A_2)^2 + d(T^B_1, T^B_2)^2 + (|e|_{T_1} - |e|_{T_2})^2}$.

As noted above, the length of the edges ending in leaves can be included in the distance calculations by considering the product space $T_n \times \mathbb{R}_+^n$, and the shortest distance, $d_l(T_1, T_2)$, between the trees in this space. In this case, if the length of the edge to leaf $i$ in tree $T$ is $|l_i|_T$ for all $1 \leq i \leq n$, then $d_l(T_1, T_2) = \sqrt{d(T_1, T_2)^2 + \sum_{i=1}^n (|l_i|_{T_1} - |l_i|_{T_2})^2}$.

Therefore, the essential problem is as follows, and we devote the rest of this paper to it.

**Problem.** Find the geodesic distance between $T_1$ and $T_2$, two trees in $T_n$ with no common splits.

### 3 Combinatorics of Path Spaces

The properties of the geodesic imply that it is restricted to certain orthants in the tree space. In this section, we model this section of tree space as a partially ordered set (poset), called the *path poset*, in which each element corresponds to one of the orthants in the tree space. This poset enables us to enumerate all orthant sequences that could contain the geodesic, as each such orthant sequence, called a *path space*, corresponds to a maximal chain in the path poset by Theorem 3.7.

For this section, assume that $T_1$ and $T_2$ are two trees in $T_n$ with no common splits. That is, $E_{T_1} \cap E_{T_2} = \emptyset$.

#### 3.1 The Incompatibility and Path Partially Ordered Sets

We now define the incompatibility poset, which depicts the incompatibilities between splits in $T_1$ and $T_2$. It will be used to construct the path poset. To define these posets, we introduce the following two split set definitions.
Let $A$ and $B$ be two sets of mutually compatible splits of type $n$, such that $A \cap B = \emptyset$. Define the compatibility set of $A$ in $B$, $C_B(A)$, to be the set of splits in $B$ which are compatible with all splits in $A$. Define the crossing set of $A$ in $B$, $X_B(A)$, to be the set containing exactly those splits in $B$ which are incompatible with at least one split in $A$. We will use the set of mutually compatible splits and the tree containing exactly those splits interchangeably here, thus writing $C_T(A)$ instead of $C_{E_T}(A)$ and $X_T(A)$ instead of $X_{E_T}(A)$.

If $D$ is a set of mutually compatible splits of type $n$ such that $D \subseteq A$, then:

1. $C_B(A) \subseteq C_B(D)$ (opposite monotonicity of the compatibility set),
2. $X_B(D) \subseteq X_B(A)$ (monotonicity of the crossing set),
3. $C_B(A)$ and $X_B(A)$ partition $B$ (partitioning).

A preposet or quasi-ordered set is a set $P$ and binary relation $\leq$ that is reflexive and transitive. See [25 Exercise 1] for more details. Define the incompatibility preposet, $\bar{P}(T_1, T_2)$, to be the preposet containing the elements of $E_{T_2}$ ordered by inclusion of their crossing sets. So, for any $f, f' \in E_{T_2}$, $f \leq f'$ in $\bar{P}(T_1, T_2)$ if and only if $X_{T_1}(f) \subseteq X_{T_1}(f')$. Define the equivalence relation $f \sim f'$ if and only if $f \leq f'$ and $f' \leq f$. Thus, all the splits in an equivalence class have the same crossing set, which we define to be the crossing set of that equivalence class.

**Definition 3.1.** The incompatibility poset, $P(T_1, T_2)$, consists of the equivalence classes defined by $\sim$ in the preposet $\bar{P}(T_1, T_2)$ ordered by inclusion of their crossing sets.

Generally, we will be informal, and treat the incompatibility poset as the elements of $E_{T_2}$ ordered by inclusion of their crossing sets. When we say two elements of $P(T_1, T_2)$ are equivalent, we mean that formally they are in the same equivalence class in the preposet $\bar{P}(T_1, T_2)$. Figure 4(c) gives an example of an incompatibility poset.

![Figure 4](image-url)

Figure 4: Example of an incompatibility poset and a path poset.

For any $A \in E_{T_2}$, define $\bar{A} \in E_{T_2}$ by

$$A \mapsto \bar{A} = \{ f \in E_{T_2} : X_{T_1}(f) \subseteq X_{T_1}(A) \}.$$  

Note that by definition, $X_{T_1}(A) = X_{T_1}(\bar{A})$. The map $X \mapsto \bar{X}$ is a closure operator on a set $I$ if for every subset $X \subseteq I$, it is extensive ($X \subseteq \overline{X}$), idempotent ($\overline{\overline{X}} = \overline{X}$), and isotone (if $X \subseteq Y$, then $\overline{X} \subseteq \overline{Y}$) [3]. From the definitions and the monotonicity of crossing sets, $A \mapsto \bar{A}$ is a closure operator on $E_{T_2}$.
Definition 3.2. The path poset of $T_1$ to $T_2$, $K(T_1, T_2)$, is the closed sets of $E_{T_2}$ ordered by inclusion.

The path poset represents the possible orthant sequences containing the geodesic between $T_1$ and $T_2$, and we next make clear this correspondence. The path poset is bounded below by $\emptyset$, and above by $E_{T_2}$. It is a sublattice of the lattice of order ideals of $P(T_1, T_2)$, but need not be graded [19]. Figure 4(d) gives an example of a path poset. For simplicity, we often just write $f_1 f_3$ instead of $\{ f_1, f_3 \}$, for example.

3.2 Path Spaces
The geodesic is contained in some sequence of orthants connecting the orthants containing $T_1$ and $T_2$. Billera et al. [3] defined a set of orthant sequences, such that at least one of them contains the geodesic. We call such orthant sequences path spaces. We characterize all maximal path spaces in Theorem 3.4, and show that they are in one-to-one correspondence with the maximal chains in $K(T_1, T_2)$ in Theorem 3.7.

Definition 3.3. For trees $T_1$ and $T_2$ with no common splits, let $E_0 \supset E_1 \supset \ldots \supset E_{k-1} \supset E_k$, and $F_0 \subset F_1 \subset \ldots \subset F_{k-1} \subset F_k$ be sets of splits such that $E_i$ and $F_i$ are compatible for all $0 \leq i \leq k$, $E_0 = E_{T_1}$, $F_k = E_{T_2}$, and $E_k = F_0 = \emptyset$. Then $\bigcup_{i=0}^{k} O(E_i \cup F_i)$ is a path space between $T_1$ and $T_2$.

Note that the inclusions are strict in this definition. A path space is a subspace of $T_n$ consisting of the closed orthants corresponding to the trees with interior edges $E_i \cup F_i$ for all $0 \leq i \leq k$. To simplify notation, let $O_i = O(E_i \cup F_i)$ and $O'_i = O(E'_i \cup F'_i)$. The intersection of $O_i$ and $O_{i+1}$ is the orthant $O(E_{i+1} \cup F_i)$. If the $i$th step transforms the tree with splits $E_{i-1} \cup F_{i-1}$ into the tree with splits $E_i \cup F_i$, then at this step we remove the splits $E_{i-1} \setminus E_i$ and add the splits $F_i \setminus F_{i-1}$.

A path space is maximal if it is not contained in any other path space. Since [3 Proposition 4.1] proves that the geodesic is contained in a path space, it must be contained in some maximal path space. We now characterize the maximal path spaces using split compatibility.

Theorem 3.4. The maximal path spaces are exactly those path spaces $\bigcup_{i=0}^{k} O_i$ such that:

1. $E_i = C_{T_1}(F_i)$, for all $0 \leq i \leq k$.
2. $F_i = C_{T_2}(E_i)$, for all $0 \leq i \leq k$.
3. for all $1 \leq i \leq k$, the splits in $F_i \setminus F_{i-1}$ are minimal and equivalent elements in the incompatibility poset $P(T(E_{i-1}), T(E_{T_2} \setminus F_{i-1}))$

Notice that Conditions 2 and 3 imply that if $f \in F_i \setminus F_{i-1}$, then any other split $f'$ equivalent with $f$ is also in $F_i \setminus F_{i-1}$, and these are precisely the splits in $F_i \setminus F_{i-1}$. In contrast, an arbitrary path space has $E_i \subseteq C_{T_1}(F_i)$ and $F_i \subseteq C_{T_2}(E_i)$, but not necessarily equality.

Before giving a proof of Theorem 3.4, we define a relaxed path space. The only difference between a relaxed path space and a path space is that the inclusions need not be strict. We then show that any relaxed path space can be expressed as a path space.

Definition 3.5. For trees $T_1$ and $T_2$ with no common splits, let $E_{T_1} = E_0 \supset E_1 \supset \ldots \supset E_{k-1} \supset E_k = \emptyset$, and $\emptyset = F_0 \subset F_1 \subset \ldots \subset F_{k-1} \subset F_k = E_{T_2}$ be sets of splits such that $E_i$ and $F_i$ are compatible for all $0 \leq i \leq k$. Then $\bigcup_{i=0}^{k} O_i$ is a relaxed path space between $T_1$ and $T_2$.

Lemma 3.6. Let $S = \bigcup_{i=0}^{k} O_i$ be a relaxed path space. Then $S$ is also a path space.

Proof. If $S = \bigcup_{i=0}^{k} O_i$ is a relaxed path space, then one of the following cases holds:
• Case 1: For some $0 \leq j < k$, $E_j = E_{j+1}$ and $F_j \subseteq F_{j+1}$.
  Then $O_j \subseteq O_{j+1}$, and so $S = \left( \cup_{i=0}^{j-1} O_i \right) \cup \left( \cup_{i=j+1}^k O_i \right)$.

• Case 2: For some $0 \leq j < k$, $E_j \supseteq E_{j+1}$ and $F_j = F_{j+1}$.
  Then $O_j \supseteq O_{j+1}$, and so $S = \left( \cup_{i=0}^{j-1} O_i \right) \cup \left( \cup_{i=j+1}^k O_i \right)$.

Reindex the $E_i$’s and $F_i$’s in this new expression for $S$ so that their indices are consecutive from 0 to $k-1$. Redefine $k$ to be $k-1$. While Case 1 or Case 2 holds, repeat this process. Since $0 \leq k < \infty$ and we reduce $k$ by one at each step, we cannot repeat this process indefinitely. Therefore, for some $k$, neither Case 1 nor Case 2 holds for $S$, and thus for all $0 \leq j < k$, $E_j \supseteq E_{j+1}$ and $F_j \subset F_{j+1}$.

This implies that $S$ is a path space.

Proof of Theorem 3.4. Let $\mathcal{M}$ be the set of path spaces described in the theorem. We first show, by contradiction, that all path spaces in $\mathcal{M}$ are maximal. Suppose not. Then there exists some $M = \cup_{i=0}^{k} O_i \in \mathcal{M}$ that is strictly contained in the path space $S' = \cup_{i=0}^{k} O'_i$.

Suppose $O_j \subseteq O'_i$ for some $0 \leq j \leq k$ and some $0 \leq i' \leq k'$. Since $T_1$ and $T_2$ have no splits in common, $E_j \cap F'_i = F_j \cap E'_i = \emptyset$. This implies that $E_j \subseteq E'_i$ and $F_j \subseteq F'_i$. Also, $F'_i \subseteq C_{T_1}(E'_i) \subseteq C_{T_2}(E'_i) = F_j$, where the last equality follows from Condition 2 on the path spaces in $\mathcal{M}$. Hence, $F'_i = F_j$. This implies $E'_i \subseteq C_{T_1}(F'_i) = C_{T_2}(F_j) = E_j$, where the last equality follows from Condition 1. Therefore, $E'_i = E_j$, and hence $O_j = O'_i$.

Therefore, no orthant in $S'$ can strictly contain an orthant from $M$, so $S'$ is exactly the orthants forming $M$ as well as at least one other orthant. Let $j$ be the smallest index such that the orthant $O_{j-1}$ is in $M$ and $S'$, but $O'_j, O'_{j+1}, \ldots, O'_{j+t-1}$ are not in $M$ and $O_j = O'_{j+t}$. Since $O'_j$ is an orthant distinct from those in $M$, $E_{j-1} = E'_{j-1} \cup E'_j \subseteq E'_j + E_{j-1} = E_j$ and $F_{j-1} = F'_{j-1} \subseteq F'_{j} + F_{j-1} = F_j$. The crossing set in $E_{j-1}$ of the splits added as we transition from $O_{j-1}$ to $O'_j$ is contained in the set of splits dropped at this transition. That is, $X_{E_{j-1}}(E'_j \setminus F_{j-1}) \subseteq E_{j-1} \setminus E_j \subseteq E_{j-1} \setminus E_j$. But Conditions 1 and 3 imply that the crossing set of any element $f \in F_j \setminus F_{j-1}$ is exactly the splits dropped at the $j$-th step, or $X_{E_{j-1}}(f) = E_{j-1} \setminus E_j$. In particular, for every $f \in F'_j \setminus F_j \subset F'_j \setminus F_{j-1}$, we have $X_{E_{j-1}}(f) = E_{j-1} \setminus E_j$. This implies that $X_{E_{j-1}}(E'_j \setminus F_{j-1}) = E_{j-1} \setminus E_j$, which contradicts the strict inclusion that we just showed. So no path space in $\mathcal{M}$ is contained in another path space.

Let $S = \cup_{i=0}^{k} O_i$, be some path space that is not in $\mathcal{M}$. We will now prove that $S$ is contained in another path space, $S'$, and hence is not maximal. Since $S \notin \mathcal{M}$, at least one of the three conditions does not hold.

Case 1: There exists a $0 \leq j \leq k$ such that $E' = C_{T_1}(F_j) \setminus E_j$ is not empty. That is, Condition 1 does not hold.

We now construct a path space in which the splits $E'$ are dropped at the $j$-th step instead of an earlier one. Define $S' = \cup_{i=0}^{k} O'_i$, where

$$O'_i = \begin{cases} O_i + O(E') & \text{if } 0 \leq i \leq j \\ O_i & \text{if } j < i \leq k \end{cases}$$

Since $O_i \subseteq O'_i$ for all $i \neq j$ and $O_j \subseteq O_j + O(E')$, we have $S \subseteq S'$. It remains to show that $S'$ is a path space. By definition, $E'$ is compatible with $F_j \supseteq F_{j-1} \supseteq \ldots \supseteq F_0$, so $E'_i$ and $F'_i = F_i$ are compatible for all $0 \leq i \leq j$. The orthants remain unchanged for $j < i \leq k$. Since $E_{T_1} = E'_0 \supseteq E'_1 \supseteq \ldots \supseteq E'_j \supseteq \ldots \supseteq E'_k = \emptyset$, $S'$ is a relaxed path space, and hence a path space by Lemma 3.6.

Therefore, $S$ is strictly contained in the path space $S'$.

Case 2: There exists $0 \leq j \leq k$ such that $F' = C_{T_2}(E_j) \setminus F_j$ is not empty. That is, Condition 2 does not hold.
We will now construct a path space in which the splits $F'$ are added to the tree at the $j$-th step, instead of a later step. Define $S' = \bigcup_{i=0}^{k} \mathcal{O}'_i$, where

$$\mathcal{O}'_i = \begin{cases} 
\mathcal{O}_i & \text{if } 0 \leq i < j \\
\mathcal{O}_i + \mathcal{O}(F') & \text{if } j \leq i \leq k
\end{cases}$$

Since $\mathcal{O}_i \subseteq \mathcal{O}'_i$ for all $i \neq j$ and $\mathcal{O}_j \subseteq \mathcal{O}_j + \mathcal{O}(F')$, we have $S \subset S'$. It remains to show that $S'$ is a path space. By definition, $F'$ is compatible with $E_j \supset E_{j+1} \supset \ldots \supset E_k$, so $F'_i$ and $E_i = E_i$ are compatible for all $i \geq j$. The orthants remained unchanged for $0 \leq i < j$. Since $F'_0 \subset F'_1 \subset \ldots \subset F'_j \subset E'_j$, $S'$ is a relaxed path space, and hence a path space by Lemma 3.6. Thus, $S$ is strictly contained in the path space $S'$.

Case 3: Neither Case 1 nor Case 2 holds, and, for some $1 \leq j \leq k$, there exists $f \in F_j \setminus F_{j-1}$ and a minimal element $g$ in $P(T(E_{j-1}), T(E_{j-2}) \setminus F_{j-1}))$ such that $g < f$ in $P(T(E_{j-1}), T(E_{j-2}) \setminus F_{j-1}))$. That is, Conditions 1 and 2 hold, but Condition 3 does not hold. We will now construct a path space in which we add the splits $g$ and $f$ in two distinct steps, instead of during the same step. Define $S' = \bigcup_{i=0}^{k+1} \mathcal{O}'_i$, where

$$\mathcal{O}'_i = \begin{cases} 
\mathcal{O}_i & \text{if } 0 \leq i < j \\
(\mathcal{O}'_i \setminus X_{E_{i-1}}(g)) \cup F_{j-1} \cup g & \text{if } i = j \\
\mathcal{O}_{i-1} & \text{if } j < i \leq k - 1
\end{cases}$$

We will first show that $\mathcal{O}'_j$ is neither contained in nor contains any orthant from $S$. We must have $X_{E_{j-1}}(g) \neq \emptyset$, or else $g \in C_{T_2}(E_{j-1}) \setminus F_{j-1}$, implying Case 2 holds, which is a contradiction. This implies that $E_{j-1} \supset E_{j-1} \setminus X_{E_{j-1}}(g)$, or $E'_j \supset E'_j$. Since $g < f$ in $P(T(E_{j-1}), T(E_{j-2}) \setminus F_{j-1}))$, we have that $X_{E_{j-1}}(g) \subset X_{E_{j-1}}(f)$. To add $f$ at step $j$, we must drop any splits in $E_{j-1}$ that are incompatible with $f$, which implies $X_{E_{j-1}}(f) \subseteq E_{j-1} \setminus E_j$. This, along with the previous statement, implies that $X_{E_{j-1}}(g) \subseteq E_{j-1} \setminus E_j$. In turn, this implies that $E_j \subset E_{j-1} \setminus X_{E_{j-1}}(g)$, or $E'_{j+1} \subseteq E'_j$.

Therefore, we have shown that $E'_{j-1} \supset E'_j \supset E'_{j+1}$, as desired.

Since $g \in E_{j-1} \setminus F_{j-1}$, we have that $F'_{j-1} = F_{j-1} \subset F_{j-1} \cup g = F_j$, and hence it remains to show that $F'_j \subset F'_{j+1}$. First, we will show that $g \in F_j$. Since $g < f$, $X_{E_{j-1}}(g) \subset X_{E_{j-1}}(f) \subseteq E_{j-1} \setminus E_j$. This implies that $g \in C_{T_2}(E_j) = F_j$ by Condition 2. Next we will show that $F'_j = F_{j-1} \cup g \subset F_j = F'_{j+1}$. For any $f' \in F_{j-1} \cup g$, $X_{T_1}(f') \subseteq X_{T_1}(F_{j-1}) \cup X_{T_1}(g) \subseteq X_{T_1}(F_j)$ by definition of closure and $g \in F_j$. Along with the partitioning property, this implies that $X_{T_1}(f') \cap C_{T_1}(F_j) = \emptyset$, or $X_{T_1}(f') \subseteq E_j = \emptyset$ by Condition 1. Then $f' \in C_{T_1}(E_j) = F_j$, as desired. Furthermore, $X_{E_{j-1}}(F_{j-1} \cup g) = X_{E_{j-1}}(F_{j-1}) \cup X_{E_{j-1}}(g) = \emptyset \cup X_{E_{j-1}}(g) \subset X_{E_{j-1}}(f)$, and thus $f' \notin F_{j-1} \cup g$ by definition of the closure operator. So $f \in F_j \setminus F_{j-1} \cup g$, and hence $F'_j \subset F'_{j+1}$.

It remains to show that the splits in $\mathcal{O}'_j$ are mutually compatible. By the definitions, $C_{T_1}(F_{j-1} \cup g) = C_{T_1}(F_{j-1}) \cap C_{T_1}(g) \supset E_{j-1} \setminus X_{T_1}(g) \supset E_{j-1} \setminus X_{E_{j-1}}(g)$, and hence the splits of $\mathcal{O}'_j$ are mutually compatible. The other orthants remain unchanged, and thus $S$ is a path space. Therefore, $S'$ is a path space that strictly contains $S$, so $S$ is not maximal.

Recall that in a poset $P$, $x < y$ is a cover relation, or $y$ covers $x$, if there does not exist any $z \in P$ such that $x < z < y$. A chain is a totally ordered subset of a poset. A chain is maximal when no other elements from $P$ can be added to that subset. See [25, Chapter 3] for an exposition of partially ordered sets.

**Theorem 3.7.** Let $g : K(T_1, T_2) \to T_n$ be given by $g(A) = \mathcal{O}_A$, where $\mathcal{O}_A = \mathcal{O}(C_{T_1}(A) \cup A)$, for any $A \in K(T_1, T_2)$. For any maximal chain $A_0 < A_1 < \ldots < A_k$ in $K(T_1, T_2)$, define $h(A_0 < A_1 < \ldots < A_k) = \ldots = 0$. For any maximal chain $A_0 < A_1 < \ldots < A_k$ in $K(T_1, T_2)$.
... < A_k) = \bigcup_{i=0}^{k} g(A_i). Then \( \bigcup_{i=0}^{k} g(A_i) = \bigcup_{i=0}^{k} O_{A_i} \) is a maximal path space and \( h \) is a bijection between maximal path spaces from \( T_1 \) to \( T_2 \) and maximal chains in \( K(T_1, T_2) \).

**Proof.** The map \( g \) is one-to-one, because if \( A \neq A' \), then \( X_{T_1}(A) \neq X_{T_1}(A') \), and hence \( C_{T_1}(A) \neq C_{T_1}(A') \) by the partitioning property. We now show that \( h \) maps maximal chains in \( K(T_1, T_2) \) to maximal path spaces.

Let \( \emptyset = A_0 < A_1 < \ldots < A_k = E_{T_2} \) be a maximal chain in \( K(T_1, T_2) \). For every \( 0 \leq i \leq k \), let \( F_i = A_i \) and \( E_i = C_{T_1}(A_i) \). We now show that \( \bigcup_{i=0}^{k} O_{A_i} \) is a path space. Since \( K(T_1, T_2) \) is the closed sets of \( E_{T_2} \) ordered by inclusion, \( A_i \subseteq A_{i+1} \) for all \( 0 \leq i < k \). This implies that \( \emptyset = F_0 \subset F_1 \subset \ldots \subset F_k = E(T_2) \), since \( F_i = A_i \) for all \( i \). It also implies that \( X_{T_1}(A_i) \subseteq X_{T_1}(A_{i+1}) \).

If \( X_{T_1}(A_i) = X_{T_1}(A_{i+1}) \), then \( A_{i+1} \subseteq A_i \), by definition of the closure and since \( A_i \) is a closed set. This is a contradiction, and therefore, \( X_{T_1}(A_i) \subset X_{T_1}(A_{i+1}) \). This implies \( E_i = C_{T_1}(A_i) \subsetneq C_{T_1}(A_{i+1}) = E_{i+1} \), and hence \( E_0 \supseteq E_1 \supseteq \ldots \supseteq E_k \). Also, \( E_0 = C_{T_1}(A_0) = C_{T_1}(\emptyset) = E_{T_1} \), and \( E_k = C_{T_1}(A_k) = C_{T_1}(E_{T_2}) = \emptyset \) since otherwise, \( T_2 \) could contain more than \( n - 2 \) splits. Finally, for all \( 0 \leq i \leq k \), \( E_i \) is compatible with \( F_i \) by definition. Therefore, \( \bigcup_{i=0}^{k} O(E_i \cup F_i) \) is a path space.

We will now show that \( \bigcup_{i=0}^{k} O_{A_i} \) satisfies the 3 conditions of Theorem 3.4, and hence is maximal. Since \( E_i = C_{T_1}(F_i) \), Condition 1 is met. As in any path space, \( F_i \subseteq C_{T_1}(E_i) \). For any \( f \in C_{T_2}(E_i) \), \( X_{T_1}(f) \cap E_i = \emptyset \). Since \( X_{T_1}(A_i) \) and \( C_{T_1}(A_i) \) partition \( E_{T_1} \) and \( E_i = C_{T_1}(A_i) \), then \( X_{T_1}(f) \subseteq X_{T_1}(A_i) \). So by definition \( f \in A_i = A_i = F_i \). Therefore, \( F_i \supseteq C_{T_2}(E_i) \) also, and Condition 2 holds.

To show Condition 3, suppose that for some \( 1 \leq j \leq k \), there exists \( f \in F_j \setminus F_{j-1} \) and a minimal element \( g \) in \( P(T(E_{j-1}), T(E_{T_2} \setminus F_{j-1})) \) such that \( g < f \) in \( P(T(E_{j-1}), T(E_{T_2} \setminus F_{j-1})) \). Then \( X_{T_1}(g) \subset X_{T_1}(f) \), so \( f \notin F_{i-1} \cup g \). This implies \( A_{i-1} = F_{i-1} < F_{i-1} \cup g < F_{i-1} \cup g \setminus \emptyset \leq F_i = A_i \), and hence \( A_i < A_{i-1} \) is not a cover relation, which is a contradiction. Therefore, Condition 3 also holds, and \( \bigcup_{i=0}^{k} O_{A_i} \) is a maximal path space.

So as claimed, if \( A_0 < A_1 < \ldots < A_k \) is a maximal chain, then \( h(A_0 < \ldots < A_k) \) is a maximal path space. It remains to show that \( h \) is a bijection. For any maximal path space \( \bigcup_{i=0}^{k} O_{A_i} \), \( F_i \subset F_{i+1} \) is a cover relation for all \( 0 \leq i < k \) since for any \( f \in F_{i+1} \setminus F_i \), \( F_i \cup f = F_{i+1} \) by Condition 3 of Theorem 3.4. This implies that \( \emptyset = F_0 < F_1 < \ldots < F_k = E(T_2) \) is a maximal chain in \( K(T_1, T_2) \) such that \( h(F_0 < F_1 < \ldots < F_k) = \bigcup_{i=0}^{k} O_{A_i} \), and hence \( h \) is onto. We have that \( h \) is one-to-one, because \( g \) is one-to-one. Therefore, \( h \) is a bijection, which establishes the correspondence.

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Figure 5: A family of trees whose path poset is exponential in the number of leaves.

The number of elements in a path poset \( K(T_1, T_2) \) can be exponential in the number of leaves in \( T_1 \) and \( T_2 \). For example, for any even positive integer \( n \), consider the trees \( T_1 \) and \( T_2 \) depicted in Figures 5(a) and 5(b). Their incompatibility poset is given in Figure 5(c). Let \( W \) be the set of minimal elements in \( P(T_1, T_2) \). Then \( |W| = \frac{n^2 - 2}{2} \). Each subset of \( W \) is a distinct closed set, and hence an element in \( K(T_1, T_2) \). This implies there are at least \( 2^{\frac{n^2 - 2}{2}} \) elements in \( K(T_1, T_2) \), and hence also an exponential number of maximal chains.
4 Geodesics in Path Spaces

Given a path space, this section shows how to find the locally shortest path, or path space geodesic, between \( T_1 \) and \( T_2 \) within that space in linear time. We do this by transforming the problem into a Euclidean shortest-path problem with obstacles ([17] and references) in Theorem 4.4. We next reformulate the problem as a touring problem [9]. A touring problem asks for the shortest path through Euclidean space that visits a sequence of regions in the prescribed order. Lemmas 4.8 and 4.9 give conditions on the path solving the touring problem. The linear algorithm for computing the path space geodesic is given in Section 4.2.1, with Theorem 4.10 proving its correctness.

4.1 Two Equivalent Euclidean Space Problems

Let \( T_1 \) and \( T_2 \) be two trees with no common splits, and let \( S = \bigcup_{i=0}^{k} \mathcal{O}(E_i \cup F_i) \) be a path space between them. Define the path space geodesic between \( T_1 \) and \( T_2 \) through \( S \) to be the shortest path between \( T_1 \) and \( T_2 \) contained in \( S \). Let \( d_S(T_1, T_2) \) be the length of this path.

We will now show that the path space geodesic between \( T_1 \) and \( T_2 \) through a path space containing \( k + 1 \) orthants is contained in a subspace of \( \mathcal{T}_n \) isometric to a subset of a lower or equal dimension Euclidean space, \( V(\mathbb{R}^k) \). For \( 0 \leq i \leq k \), define the orthant

\[
V_i = \{(x_1, ..., x_k) \in \mathbb{R}^k : x_j \leq 0 \text{ if } j \leq i \text{ and } x_j \geq 0 \text{ if } j > i\}.
\]

Let \( V(\mathbb{R}^k) = \bigcup_{i=0}^{k} V_i \).

We prove three properties of path space geodesics, and hence also geodesics, in Proposition 4.1 and Corollary 4.3. These properties will imply that if a set splits shrink to or start growing from 0 length at the same point on the path space geodesic, then we know the length of each edge at any other point on the path space geodesic. Analogous properties were proven by Vogtmann [28] for geodesics.

**Proposition 4.1.** The path space geodesic is a straight line in each orthant that it traverses.

**Proof.** If not, replace the path within each orthant with a straight line, which enters and exits the orthant at the same points as the original path, to get a shorter path.

**Proposition 4.2.** Moving along the path space geodesic, the length of each non-zero edge changes in the trees on it at a constant rate with respect to the geodesic arc length.

**Proof.** By Proposition 4.1, each edge must shrink or grow at a constant rate with respect to the other edges within each orthant, but these rates can differ between orthants. So it suffices to consider when the geodesic goes through the interiors of the two adjacent orthants \( \mathcal{O}_i = \mathcal{O}(E_i \cup F_i) \) and \( \mathcal{O}_{i+1} = \mathcal{O}(E_{i+1} \cup F_{i+1}) \), and bends in the intersection of these two orthants. Let \( \mathbf{a} \) be the point at which the geodesic enters \( \mathcal{O}_i \), and let \( \mathbf{b} \) be the point at which the geodesic leaves \( \mathcal{O}_{i+1} \).

The edges \( E_i \setminus E_{i+1} \) are dropped and the edges \( F_{i+1} \setminus F_i \) are added as the geodesic moves from \( \mathcal{O}_i \) to \( \mathcal{O}_{i+1} \). Thus the edges \( E_i \setminus E_{i+1} \) and \( F_{i+1} \setminus F_i \) all have length 0 in the intersection \( \mathcal{O}(E_{i+1} \cup F_i) \).

Let \( m = |E_{i+1} \cup F_i| \), the dimension of \( \mathcal{O}_i \cap \mathcal{O}_{i+1} \). Consider the subset \( S = H_a \cup H_b \) of \( \mathcal{O}_i \cup \mathcal{O}_{i+1} \), where \( H_a \) is the affine hull of \( \mathbf{a} \cup (\mathcal{O}_i \cap \mathcal{O}_{i+1}) \) intersected with \( \mathcal{O}_i \) and \( H_b \) is the affine hull of \( \mathbf{b} \cup (\mathcal{O}_i \cap \mathcal{O}_{i+1}) \) intersected with \( \mathcal{O}_{i+1} \). This subset can be isometrically mapped into two orthants in \( \mathbb{R}^{m+1} \) as follows. For each tree \( T \in H_a \), let the first \( m \) coordinates be given by the projection of \( T \) onto \( \mathcal{O}_i \cap \mathcal{O}_{i+1} \). Let the \((m + 1)\)-st coordinate be the length of the projection of \( \mathcal{O}_i \cap \mathcal{O}_{i+1} \). More specifically, let the edges in \( E_{i+1} \cup F_i \) be \( e_1, e_2, ..., e_m \). Then we map \( T \) to the point \((|e_1|_T, |e_2|_T, ..., |e_m|_T, s) \) in \( \mathbb{R}^{m+1} \), where \( s = \sqrt{\sum_{e \in E_{i+1} \cup F_i} |e|^2} \). Similarly, for each tree \( T \in H_b \),
Corollary 4.3. Let $T$ be a tree on the path space geodesic between $T_1$ and $T_2$ through the path space $\bigcup_{i=0}^{k} \mathcal{O}(E_i \cup F_i)$. Suppose $T \in \mathcal{O}_i$. Then if $1 \leq j \leq i$, we have $\frac{|f_1|_{T_1}}{|f_1|_{T_2}} = \frac{|f_2|_{T_2}}{|f_2|_{T_1}}$ for any $f_1, f_2 \in F_j \setminus F_{j-1}$, and if $i < j \leq k$, we have $\frac{|e_1|_{T_1}}{|e_1|_{T_2}} = \frac{|e_2|_{T_2}}{|e_2|_{T_1}}$ for any $e_1, e_2 \in E_{j-1} \setminus E_j$.

Proof. Proposition 4.2 implies that the length of each edge in $T_1$ shrinks at a constant rate until it reaches 0 as we travel along the path space geodesic, and the length of each edge in $T_2$ grows at a constant rate from 0 starting at some point along the path space geodesic. Since for any $1 \leq j \leq k$, the edges $E_{j-1} \setminus E_j$ reach length 0 at the same point along the path space geodesic, each edge in $E_{j-1} \setminus E_j$ must be changing at a constant rate with respect to the lengths of the other edges in $E_{j-1} \setminus E_j$. Similarly, since the edges $F_j \setminus F_{j-1}$ start growing from 0 at the same point along the path space geodesic, each edge in $F_j \setminus F_{j-1}$ is changing at a constant rate with respect to the lengths of the other edges in $F_j \setminus F_{j-1}$.

Therefore, there is one degree of freedom for each set of edges dropped, or alternatively for each set of edges added, at the transition between orthants. Thus, the path space geodesic lies in a space of dimension equal to the number of transitions between orthants. We will now show that each path space geodesic lives in a space isometric to $V(\mathbb{R}^k)$. For example, in Figure 6(a), the path space $Q$ consists of the orthants $\mathcal{O}((e_1, e_2, e_3))$, $\mathcal{O}((f_1, e_2, e_3))$, and $\mathcal{O}((f_1, f_2, f_3))$. We apply Theorem 4.4 to see that the geodesic through $Q$ is contained in the shaded region of $\mathbb{R}^2$ shown in Figure 6(b).

Figure 6: An isometric map between a path space and $V(\mathbb{R}^2)$.

Theorem 4.4. Let $Q = \bigcup_{i=0}^{k} \mathcal{O}(E_i \cup F_i)$ be a path space between $T_1$ and $T_2$, two trees in $T_n$ with no common splits. Then the path space geodesic between $T_1$ and $T_2$ through $Q$ is contained in a space isometric to $V(\mathbb{R}^k)$.
Proof. For all $1 \leq j \leq k$, let $A_j = E_{j-1} \setminus E_j$ and let $B_j = E_1 \setminus F_{j-1}$. Then $\{A_j\}_{j=1}^k$ and $\{B_j\}_{j=1}^k$ are partitions of $E_{T_1}$ and $E_{T_2}$ respectively. By Corollary 4.3, any tree $T' \in Q$ on the path space geodesic satisfies the following property for each $1 \leq j \leq k$:

1. if $T' \in \mathcal{O}_i$ and $j \leq i$, then there exists a $c_j = c_j(T') \geq 0$, depending on $T'$, such that $\frac{|f_j|_{T_2}}{|f_j|_{T_1}} = c_j$ for all $f \in B_j$,

2. if $T' \in \mathcal{O}_i$ and $j > i$, then there exists a $d_j = d_j(T') \geq 0$, depending on $T'$, such that $\frac{|e|_{T_2}}{|e|_{T_1}} = d_j$ for all $e \in A_j$.

Let $Q' \subset T_n$ be the set of trees satisfying this property. For $0 \leq i \leq n$, define $h_i : Q' \cap \mathcal{O}_i \to V_i$ by

$h_i(T') = h_i(T(c_1 \cdot B_1 \cup \ldots \cup c_i \cdot B_i \cup d_{i+1} \cdot A_{i+1} \cup \ldots \cup d_k \cdot A_k))$

$= (-c_1||B_1||, \ldots, -c_i||B_i||, d_{i+1}||A_{i+1}||, \ldots, d_k||A_k||)$.

We claim that $h_i$ is a bijection from $Q' \cap \mathcal{O}_i$ to the orthant $V_i$ in $V(\mathbb{R}^k)$. The orthant $\mathcal{O}_i$ contains trees with $N = |B_1| + |B_2| + \ldots + |B_i| + |A_{i+1}| + \ldots + |A_k|$ edges, and hence is an $N$-dimensional orthant. All trees in $\mathcal{O}_i$ contain exactly the edges $\{B_1, \ldots, B_i, A_{i+1}, \ldots, A_k\}$, so without loss of generality we can assign each edge to a coordinate axes so that the edges in $B_1$ are assigned to coordinates $1$ to $|B_1|$, the edges in $B_2$ are assigned to coordinates $|B_1| + 1$ to $|B_1| + |B_2|$, the edges in $A_{i+1}$ are assigned to the coordinates $|B_1| + |B_2| + \ldots + |B_i| + 1$ to $|B_1| + |B_2| + \ldots + |B_i| + |A_{i+1}|$, etc. Let $e_j$ be the edge assigned to the $j$-th coordinate. By abuse of notation, for all $1 \leq j \leq i$, let $B_j$ be the $N$-dimensional vector with a 0 in every coordinate except those corresponding to the edges in $B_j$, which contain the lengths of those edges in $T_2$. Similarly, for all $i < j \leq k$, let $A_j$ be the $N$-dimensional vector with a 0 in every coordinate except those corresponding to the edges in $A_j$, which contain the lengths of those edges in $T_1$. For example, $B_1$ is the $N$-dimensional vector $(|f_1|_{T_2}, |f_2|_{T_2}, \ldots, |f_1|_{B_1}|_{T_2}, 0, \ldots, 0)$.

Then $Q' \cap \mathcal{O}_i$ is generated by the vectors $\left\{ \frac{B_1}{||B_1||}, \frac{B_2}{||B_2||}, \ldots, \frac{B_i}{||B_i||}, \frac{A_{i+1}}{||A_{i+1}||}, \ldots, \frac{A_k}{||A_k||} \right\}$. Since these generating vectors are pairwise orthogonal, they are independent, and hence $Q' \cap \mathcal{O}_i$ is a $k$-dimensional orthant contained in $\mathcal{O}_i$. Furthermore, for all $1 \leq j \leq i$, $\frac{B_j}{||B_j||}$ corresponds to the tree $T \left( \frac{1}{||B_j||} \cdot B_j \right)$, and for all $i < j \leq k$, $\frac{A_j}{||A_j||}$ corresponds to the tree $T \left( \frac{1}{||A_j||} \cdot A_j \right)$. For all $1 \leq j \leq k$, let $u_j$ be the $k$-dimensional unit vector with a 1 in the $j$-th coordinate. Then for $1 \leq j \leq i$,

$h_i \left( \frac{B_j}{||B_j||} \right) = h_i \left( T \left( \frac{1}{||B_j||} \cdot B_j \right) \right) = -\frac{1}{||B_j||} \cdot ||B_j||u_j = -u_j.$

Similarly, for all $i < j \leq k$,

$h_i \left( \frac{A_j}{||A_j||} \right) = h_i \left( T \left( \frac{1}{||A_j||} \cdot A_j \right) \right) = \frac{1}{||A_j||} \cdot ||A_j||u_j = u_j.$

The basis of $V_i$ is $\{-u_1, \ldots, -u_i, u_{i+1}, \ldots, u_k\}$, so $h_i$ maps each basis element of $Q' \cap \mathcal{Q}_i$ to a unique basis element of $V_i$. Thus, $h_i$ is a linear transformation, whose corresponding matrix is the identity matrix, and hence a bijection between $Q' \cap \mathcal{Q}_i$ and $V_i$ for all $i$. Furthermore, since the determinant of the matrix of $h_i$ is 1, $h_i$ is also an isometry. So $Q'$ is piecewise linearly isometric to $V(\mathbb{R}^k)$.

For all $0 \leq i \leq n$, the inverse of $h_i$ is $g_i : V_i \to Q'$ defined by $g_i(-x_1, -x_2, \ldots, x_k) = T'$, where $x_j \geq 0$ for all $1 \leq j \leq k$ and $T'$ is the tree with edges $E_i \cup F_i$ with lengths $\frac{|x_j|}{||B_j||} \cdot |e|_{T_2}$ if $e \in B_j$ for $1 \leq j \leq i$ and $\frac{|x_j|}{||A_j||} \cdot |e|_{T_1}$ if $e \in A_j$ for $i < j \leq k$. 

13
Notice that if $T' \in Q' \cap \mathcal{O}_i \cap \mathcal{O}_{i+1}$, then $h_i(T') = h_{i+1}(T')$, since the lengths of all the edges in $A_{i+1}$ and $B_{i+1}$ are 0. Therefore, define $h : Q' \to V(\mathbb{R}^k)$ to be $h(T') = h_i(T')$ if $T' \in \mathcal{O}_i \cap Q'$, which is well-defined. Define $g : V(\mathbb{R}^k) \to Q'$ by setting $g(-x_1, \ldots, -x_i, x_{i+1}, \ldots, x_k) = g_i(-x_1, \ldots, -x_i, x_{i+1}, \ldots, x_k)$, for all $1 \leq i \leq k$ and for all $x_j \geq 0$ for all $1 \leq j \leq k$. Then $g$ is also well-defined and the inverse of $h$.

For any geodesic $q$ in $Q'$, map it into $V(\mathbb{R}^k)$ by applying $h$ to each point on $q$ to get path $p$. Notice that since both $h_i$ and $g_i$ are distance preserving, $p$ is the same length as $q$. We claim $p$ is a geodesic in $V(\mathbb{R}^k)$. To prove this, suppose not. Let $p'$ be the geodesic in $V(\mathbb{R}^k)$ between the same endpoints as path $p$. Then $p'$ is strictly shorter than $p$. Use $g$ to map $p'$ back to $Q'$ to get $q'$. Again distance is preserved, so $q'$ is strictly shorter than $q$. But $q$ was a geodesic, and hence the shortest path between those two endpoints in $Q'$, so we have a contradiction. Therefore, the geodesic between $T_1$ and $T_2$ in $Q$ is isometric to the geodesic between $A = (||A_1||, \ldots, ||A_k||)$ and $B = (-||B_1||, \ldots, -||B_k||)$ in $V(\mathbb{R}^k)$.

Thus, finding the shortest path between two trees through a $(k + 1)$-orthant path space is equivalent to finding the shortest path between a point $A$ in the positive orthant and a point $B$ in the negative orthant of $V(\mathbb{R}^k)$. This problem can be transformed into an obstacle-avoiding Euclidean shortest path problem by letting $A$ and $B$ be points in $\mathbb{R}^k$, and letting the orthants which are not in $V(\mathbb{R}^k)$ be obstacles. We now formulate this problem as a touring problem. Let $P_i$ be the boundary between the $i$-th and $(i + 1)$-st orthants in $V(\mathbb{R}^k)$, for all $1 \leq i \leq k$. That is,

$$P_i = \{(x_1, \ldots, x_k) \in \mathbb{R}^k : x_j \leq 0 \text{ if } j < i; x_j = 0 \text{ if } j = i; x_j \geq 0 \text{ if } j > i\}.$$ 

Then our problem is equivalent to finding the shortest path between $A$ and $B$ in $\mathbb{R}^k$ that intersects $P_1, P_2, \ldots, P_k$ in that order.

In dimensions 3 and higher, the Euclidean shortest path problem with obstacles is NP-hard in general [6], including when the obstacles are disjoint axis-aligned boxes [8]. The touring problem can be solved in polynomial time as a second order cone problem when the regions are polyhedra [20]. In the special case of the above touring problem, we find a simple linear algorithm.

### 4.2 Touring Problem Solution

First, Lemma 4.5 establishes when $\overline{AB}$ is the solution to our touring problem. Next we introduce the idea of a locally shortest, ordered path, and prove two conditions that all such paths must satisfy in Lemmas 4.8 and 4.9. Theorem 4.10 shows that repeatedly applying the second condition gives the linear algorithm for finding the shortest, ordered path from $A$ to $B$. Throughout this section $A = (a_1, a_2, \ldots, a_k)$ and $B = (-b_1, -b_2, \ldots, -b_k)$ will be points in $\mathbb{R}^k$ with $a_i, b_i \geq 0$ for all $1 \leq i \leq k$.

**Lemma 4.5.** The line $\overline{AB}$ passes through the regions $P_1, P_2, \ldots, P_k$ in that order and has distance $\overline{AB} = \sqrt{\sum_{i=1}^{k} (a_i + b_i)^2}$ if and only if $\frac{a_1}{b_1} \leq \frac{a_2}{b_2} \leq \ldots \leq \frac{a_k}{b_k}$.

**Proof.** Parametrize the line $\overline{AB}$ with respect to the variable $t$, so that $t = 0$ at $A$ and $t = 1$ at $B$, to get $(x_1, \ldots, x_k) = (a_1, \ldots, a_k) + t(-a_1 - b_1, \ldots, -a_k - b_k)$. Let $t_i$ be the value of $t$ at the intersection of $\overline{AB}$ and $P_i$. Setting $x_i = 0$, and solving for $t$ gives $t_i = \frac{a_i}{a_i + b_i}$. For $\overline{AB}$ to cross $P_1, P_2, \ldots, P_k$ in that order, we need $t_1 \leq t_2 \leq \ldots \leq t_k$ or $\frac{a_1}{a_1 + b_1} \leq \frac{a_2}{a_2 + b_2} \leq \ldots \leq \frac{a_k}{a_k + b_k}$. Since for any $1 \leq i, j \leq k$, $\frac{a_i}{a_i + b_i} \leq \frac{a_j}{a_j + b_j}$ is equivalent to $\frac{a_i}{a_i + b_i} \leq \frac{a_j}{b_j}$ by cross multiplication, we get the desired condition. By the Euclidean distance formula, $\overline{AB} = \sqrt{\sum_{i=1}^{k} (a_i + b_i)^2}$. 

\[\square\]
Corollary 4.6. Let \( A = (a_1, ..., a_k) \) and \( B = (-b_1, ..., -b_k) \) be points in \( \mathbb{R}^k \) with \( a_i, b_i \geq 0 \) for all \( 1 \leq i \leq k \). Then \( \frac{a_i}{b_i} = \frac{a_{i+1}}{b_{i+1}} \) if and only if \( AB \) intersects \( P_i \cap P_{i+1} \).

Proof. This follows directly from the proof of Lemma 4.5.

In general, we will not have \( \frac{a_1}{b_1} \leq \frac{a_2}{b_2} \leq ... \leq \frac{a_k}{b_k} \), and hence the shortest path is not a straight line. We now show how to find where a path bends, using the idea of locally shortest, ordered paths. These bends can be straightened by isometrically mapping the problem to a lower dimensional space, until Lemma 4.5 applies.

An \( \epsilon \)-neighbourhood of a path is all points in \( \mathbb{R}^k \) within \( \epsilon > 0 \) of at least one point on that path. A locally shortest, ordered path, \( q \), is a path from \( A \) to \( B \) which passes through \( P_1, ..., P_k \) in that order, and for which there exists some \( \epsilon > 0 \) such that there is no shorter path \( q' \) from \( A \) to \( B \) contained in the \( \epsilon \)-neighbourhood of \( q \) that also passes through \( P_1, ..., P_k \) in that order. For all \( i \), let \( p_i \) be the first point at which the locally shortest, ordered path under consideration intersects \( P_i \). Then it is easy to show that for all \( 1 \leq i \leq k-1 \), any locally shortest, ordered path \( q \) is a straight line, possibly of length 0, between \( p_i \) and \( p_{i+1} \), and \( q \) intersects each \( P_i \) at exactly one point, \( p_i \).

The following corollary of Theorem 4.4 explains when a touring problem can be isometrically mapped to a lower dimension.

Corollary 4.7. Consider a locally shortest, ordered path from \( A = (a_1, a_2, ..., a_k) \) to \( B = (-b_1, -b_2, ..., -b_k) \) through \( P_1, ..., P_k \). Let \( \{M_j\}_{j=1}^m \) be any ordered partition of \( \{1, 2, ..., k\} \) such that \( i, l \in M_j \) implies \( p_i = p_l \). Then this path is contained in a region of \( \mathbb{R}^k \) isometric to \( V(\mathbb{R}^m) \).

Proof. Suppose \( i, i+1 \) are in the same block in \( \{M_j\}_{j=1}^m \). Then \( p_i = p_{i+1} \), and travelling along the pre-image of the path in tree space, the tree loses splits \( E_{i-1} \setminus E_i \) and \( E_i \setminus E_{i+1} \) simultaneously, and gains splits \( F_i \setminus F_{i-1} \) and \( F_{i+1} \setminus F_i \) simultaneously. Hence, this path is in the path space \( O_0 \cup (\bigcup_{j=1}^{m}O((\cap_{i \in M_j}E_i) \cup (\cup_{i \in M_j}F_i))) \). Apply Theorem 4.4 to get the desired result.

Notice that under the mapping to \( V(\mathbb{R}^m) \) described in the above proof, \( A \) is mapped to \( \tilde{A} = (\sqrt{\sum_{i \in M_1} a_i^2}, \sqrt{\sum_{i \in M_2} a_i^2}, ..., \sqrt{\sum_{i \in M_m} a_i^2}) \) and \( B \) is mapped to \( \tilde{B} = (\sqrt{\sum_{i \in M_1} b_i^2}, \sqrt{\sum_{i \in M_2} b_i^2}, ..., \sqrt{\sum_{i \in M_m} b_i^2}) \).

The following two lemmas give simple constraints on locally shortest, ordered paths.

Lemma 4.8. Let \( q \) be a locally shortest path from \( A \) to \( B \) that passes through \( P_1, P_2, ..., P_k \) in that order. Let \( p_j \) be the intersection of \( q \) and \( P_j \) for each \( 1 \leq j \leq k \). If \( \frac{a_i}{b_j} \leq \frac{a_{i+1}}{b_{j+1}} \leq ... \leq \frac{a_k}{b_k} \), for some \( 1 \leq J < i < k \), \( q \) is a straight line until it bends at \( p_j = p_{j+1} = ... = p_i \), and \( p_{j-1} \neq p_j \), then \( p_i = p_{i+1} \).

Proof. This proof is by contradiction, so assume that \( p_i \neq p_{i+1} \). By properties of locally shortest, ordered paths, \( q \) is a straight line from \( p_i \) to \( p_{i+1} \). Let \( Y = (-y_1, ..., -y_J, y_{J+1}, ..., y_k) \), where \( y_j \geq 0 \) for all \( 1 \leq j \leq k \), be a point on the line \( p_ip_{i+1} \), \( \epsilon > 0 \) past \( p_i \). We will now show that \( \tilde{AY} \) intersects \( P_1, P_2, ..., P_i \) in that order.

Parametrize the paths \( q \) and \( \tilde{AY} \) with respect to time \( t \), so that \( t = 0 \) at \( A \) and \( t = 1 \) at \( Y \). The \( j \)-th coordinate, for \( 1 \leq j \leq J - 1 \), decreases linearly from \( a_j \) to \( -y_j \) in both \( q \) and \( \tilde{AY} \), and thus become 0 at the same time in both paths. This implies that since \( q \) crosses \( P_1, ..., P_{J-1} \) in that order, \( \tilde{AY} \) also crosses \( P_1, ..., P_{J-1} \) in that order.

Let \( t_j \) be the time at which \( \tilde{AY} \) intersects \( P_j \), for \( 1 \leq j \leq i \). Then \( 0 = a_j + t_j(-y_j - a_j) \) or \( t_j = \frac{a_j}{y_j + a_j} \). In \( q \), each coordinate between \( J \) and \( i \) becomes 0 at the same time. These coordinates then decrease linearly, so the ratio between any two consecutive coordinates remains constant as
time increases. This implies \( \frac{y_j}{y_{j+1}} = \frac{b_j}{b_{j+1}} \) for each \( J \leq j < i \). Since \( \frac{a_j}{b_j} \leq \frac{a_{j+1}}{b_{j+1}} \leq \ldots \leq \frac{a_i}{b_i} \) by the hypothesis, then \( \frac{a_j}{y_j} \leq \frac{a_{j+1}}{y_{j+1}} \leq \ldots \leq \frac{a_i}{y_i} \). This implies \( \frac{a_j}{a_j + y_j} \leq \frac{a_{j+1}}{a_{j+1} + y_{j+1}} \leq \ldots \leq \frac{a_i}{a_i + y_i} \), or \( t_j \leq t_{j+1} \leq \ldots \leq t_i \). Thus \( \overline{A} \overline{V} \) intersects \( P_J, P_{J+1}, \ldots, P_t \) in that order.

It remains to show that \( \overline{A} \overline{V} \) intersects \( P_{j-1} \) before \( P_j \), which we do by contradiction. So assume that \( t_j < t_{j-1} \). Let \( r_j \) and \( r_{j-1} \) be the points of intersection of \( \overline{A} \overline{V} \) with \( P_{j-1} \) and \( P_j \), respectively. By the hypotheses and assumption, \( r_j \) and \( P_j \) are contained in \( P_j \setminus P_{j-1} \). Since \( P_{j-1} \) and \( P_j \) are convex, \( \overline{r_{j-1}P_{j-1}} \) and \( \overline{r_jP_j} \) are contained in \( P_{j-1} \) and \( P_j \), respectively. Now \( \overline{r_{j-1}P_{j-1}} \) intersects \( \overline{r_jP_j} \) inside the triangle \( \overline{A} \overline{V} \). This implies that \( \overline{r_{j-1}P_{j-1}} \) passes from \( P_j \setminus P_{j-1} \) into \( P_{j-1} \cap P_j \), on the boundary of \( P_j \), and back into \( P_j \setminus P_{j-1} \). But this contradicts the convexity of \( P_j \). Thus \( t_{j-1} \leq t_j \), and \( \overline{A} \overline{V} \) passes through \( P_1, P_2, \ldots, P_t \) in that order.

By the triangle inequality, \( \overline{A} \overline{V} \) is shorter than the section of \( q \) from \( A \) to \( Y \). This contradicts \( q \) being a locally shortest, ordered path, and thus \( p_i = p_{i+1} \).

**Lemma 4.9.** For any locally shortest paths from \( A \) to \( B \) that pass through \( P_1, P_2, \ldots, P_k \) in that order, if \( \frac{a_1}{b_1} \leq \frac{a_2}{b_2} \leq \ldots \leq \frac{a_{k+1}}{b_{k+1}} \), then any such path intersects \( P_i \cap P_{i+1} \).

**Proof.** Suppose that \( \frac{a_1}{b_1} \leq \frac{a_2}{b_2} \leq \ldots \leq \frac{a_{k+1}}{b_{k+1}} \) and consider some locally shortest path, \( q \), such that \( p_i \neq p_{i+1} \). Parametrize \( q \) with respect to the variable \( t \), so that the path starts at \( A \) when \( t = 0 \), ends at \( B \) when \( t = 1 \), and passes through \( P_j \) at point \( p_j = (p_{j,1}, p_{j,2}, \ldots, p_{j,k}) \) when \( t = t_j \), for all \( 1 \leq j \leq k \). If \( p_j = p_{j+1} \) for some \( 1 \leq j < i \) and \( q \) bends at this point, then by repeated applications of Lemma 4.8, it also passes through \( P_i \cap P_{i+1} \) and we are done. So assume that \( q \) is a straight line from \( A \) to \( p_{i+1} \). Thus, the \( i \)-th coordinate changes linearly from \( a_i \) to \( -b_i \), and from the parametrization of this, we get \( t_{i+1} = \frac{a_i - p_{i+1} - 1}{a_i + b_i} \).

Case 1: \( p_{i+1,i+2} \neq 0 \) (That is, the locally shortest ordered path does not bend at \( p_{i+1} \).)

In this case, \( p_{i+1,i+1} = 0 = a_{i+1} + t_{i+1}(-b_{i+1} - a_{i+1}) \), which implies \( t_{i+1} = \frac{a_{i+1}}{a_{i+1} + b_{i+1}} \). Equate this value of \( t_{i+1} \) with the one found above, and rearrange to get \( p_{i+1,i} = a_i - \frac{a_{i+1}}{a_{i+1} + b_{i+1}}(a_i + b_i) \). The definition of \( P_{i+1} \) and the assumption \( p_i \neq p_{i+1} \) implies that \( p_{i+1,i} < 0 \). Hence, \( a_i < \frac{a_{i+1}}{a_{i+1} + b_{i+1}}(a_i + b_i) \), which can be rearranged to \( \frac{a_i}{b_i} < \frac{a_{i+1}}{b_{i+1}}(a_i + b_i) \), a contradiction.

Case 2: \( p_{i+1,i+2} = 0 \) (That is, the locally shortest ordered path bends at \( p_{i+1} \), and \( p_{i+1} = p_{i+2} \).)

Let \( J \geq 2 \) be the largest integer such that \( p_{i+J} = p_{i+1} \), but \( p_{i+J+1} \neq p_{i+1} \). Apply Corollary 4.7 using the partition \{1\}, \{2\}, \ldots, \{i\}, \{i+1\}, \{i+2, \ldots, i+J\}, \{i+J+1\}, \ldots, \{k\} to reduce the space by \( J - 2 \) dimensions. \( A \) and \( B \) are mapped to \( \overline{A} = (\overline{a}_1, \ldots, \overline{a}_{k-(J-2)}) \) and \( \overline{B} = (-\overline{b}_1, \ldots, -\overline{b}_{k-(J-2)}) \), respectively, in the lower dimension space, where:

\[
\overline{a}_j = \begin{cases} a_j & \text{if } j \leq i + 1 \\ \sqrt{\sum_{l=2}^{j} a_{i+1}^2} & \text{if } j = i + 2 \\ a_{j+J-2} & \text{if } j > i + 2 \end{cases}
\]

and \( \overline{b}_j = \begin{cases} b_j & \text{if } j \leq i + 1 \\ \sqrt{\sum_{l=2}^{j} b_{i+1}^2} & \text{if } j = i + 2 \\ b_{j+J-2} & \text{if } j > i + 2 \end{cases} \)

Let \( \overline{k} = k - (J-2) \). Let \( \overline{p}_j \) be the image of \( p_j \) in \( \mathbb{R}^{\overline{k}} \) under the above mapping if \( j \leq i+2 \) and the image of \( p_{j+J-2} \) if \( j > i+2 \). Let \( \overline{P}_j = \{(x_1, \ldots, x_{\overline{k}}) \in \mathbb{R}^{\overline{k}} : x_l \leq 0 \text{ if } l < j; x_1 = 0 \text{ if } l = j; x_l \geq 0 \text{ if } l > j \} \).

So \( \overline{P}_j \) is the boundary between the \( j \)-th and \((j+1)\)-st orthants in the lower dimension space \( \mathbb{R}^{\overline{k}} \). Let \( \overline{q} \) be the image of \( q \).

Then \( \overline{q} \) is a straight line from \( \overline{A} \) to \( \overline{p}_{i+1} \), and \( \overline{p}_{i+1} = \overline{p}_{i+2} \neq \overline{p}_{i+3} \), so \( \overline{q} \) bends in \( \overline{P}_{i+1} \cap \overline{P}_{i+2} \). Since \( \overline{q} \) does not intersect \( \overline{P}_{i+2} \cap \overline{P}_{i+3} \), by the contrapositive of Lemma 4.8, \( \frac{a_{i+1}}{b_{i+1}} > \frac{a_{i+2}}{b_{i+2}} \). In \( \mathbb{R}^{\overline{k}}, \)
this translates into the condition that \( a_{i+1}b_{i+1} > \frac{\sqrt{\sum_{j=2}^{l-1} a_j^2}}{\sqrt{\sum_{j=2}^{l-1} b_j^2}} \). Cross-multiply, square each side, add

\[ a_{i+1}b_{i+1}, \text{ and rearrange to get } a_{i+1} > \frac{\sqrt{\sum_{j=2}^{l-1} a_j^2}}{\sqrt{\sum_{j=2}^{l-1} b_j^2}}. \]

The analysis of the space is in \( \mathbb{R}^k \). If the locally shortest, ordered path is a straight line through \( p_{i+1} \), then we make the same argument as in Case 1. Otherwise, since the path does not bend at \( p_i \), the \( i \)-th coordinate changes linearly from \( a_i \) to \( -b_i \). We use this parametrization to find

\[ t_{i+2} = t_{i+1} = \frac{a_i-p_{i+1,i}}{a_i+b_i}. \]

Furthermore, the \((i+1)\)-st to \((i+J)\)-th coordinates decrease at the same rate from \( A \) to \( p_{i+1} \) and at the same, but possibly different than the first, rate from \( p_{i+1} \) to \( B \). Therefore, we can apply Corollary 4.7 to the partition \( \{1\}, \{2\}, \ldots, \{i\}, \{i+1, i+2, \ldots, i+J\}, \{i+J+1\}, \ldots, \{k\} \) to isometrically map the locally shortest, ordered path into \( \mathbb{R}^{m-(J-1)} \). Let \( \tilde{a} = \sqrt{\sum_{l=1}^{J} a_l^2} \), and let

\[ \tilde{b} = \sqrt{\sum_{l=1}^{J} (-b_l)^2}. \]

Then in \( \mathbb{R}^{m-(J-1)} \), the \((i+1)\)-st coordinate of the locally shortest ordered path changes at a constant rate from \( \tilde{a} \) to \( -\tilde{b} \). This implies \( 0 = \tilde{a} + t_{i+1}(-\tilde{b} - \tilde{a}) \), or \( t_{i+1} = \frac{\tilde{a}}{\tilde{a} + \tilde{b}} \). Equate the two expressions for \( t_{i+1} \) to get \( p_{i+1,i} = a_i - \frac{(a_i+b_i)\tilde{a}}{\tilde{a} + \tilde{b}} \). By definition of \( p_{i+1} \), \( p_{i+1,i} < 0 \). This implies \( \frac{a_i}{b_i} < \frac{-\tilde{a}}{-\tilde{b}} = \frac{\sqrt{\sum_{l=1}^{J} a_l^2}}{\sqrt{\sum_{l=1}^{J} (-b_l)^2}}. \) But we showed that \( \frac{\sqrt{\sum_{l=1}^{J} a_l^2}}{\sqrt{\sum_{l=1}^{J} (-b_l)^2}} < \frac{a_{i+1}}{b_{i+1}} \), so \( \frac{a_i}{b_i} < \frac{a_{i+1}}{b_{i+1}} \), which is also a contradiction.

By repeatedly applying this lemma, we find the lower dimensional space that all the locally shortest, ordered paths lie in. In this space, the ratios derived from the coordinates of the images of \( A \) and \( B \) form a non-descending sequence. The following theorem gives the shortest path through \( V(\mathbb{R}^k) \) from a point in the positive orthant to a point in the negative orthant, or equivalently, the shortest tour that passes through \( P_1, \ldots, P_m \) in \( \mathbb{R}^k \).

**Theorem 4.10.** Let \( A = (a_1, a_2, \ldots, a_k) \) and \( B = (-b_1, -b_2, \ldots, -b_k) \) with \( a_i, b_i \geq 0 \) for all \( 1 \leq i \leq k \) be points in \( \mathbb{R}^k \). Alternate between applying Lemma 4.9 and Corollary 4.7 until there is a non-descending sequence of ratios \( \frac{a_1}{b_1} \leq \frac{a_2}{b_2} \leq \ldots \leq \frac{a_m}{b_m} \), where \( a_i \) and \( b_i \) are the coordinates in the lower dimensional space. There is a unique shortest path between \( \tilde{A} = (a_1, \ldots, a_m) \) and \( \tilde{B} = (-b_1, \ldots, -b_m) \) in \( V(\mathbb{R}^m) \), with distance \( \sqrt{\sum_{i=1}^{m} (\tilde{a}_i + \tilde{b}_i)^2} \). This is the length of the shortest ordered path between \( A \) and \( B \) in \( V(\mathbb{R}^k) \).

**Proof.** For the smallest \( i \) such that \( \frac{a_i}{b_i} > \frac{a_{i+1}}{b_{i+1}} \), Lemma 4.9 implies that \( p_i = p_{i+1} \) in all locally shortest, ordered paths in \( \mathbb{R}^k \). Thus, we can apply Corollary 4.7 using the partition \( \{1\}, \{2\}, \ldots, \{i-1\}, \{i,i+1\}, \{i+2\}, \ldots, \{m\} \) to reduce the space containing all locally shortest, ordered paths by one dimension. Repeat the previous two steps until the ratio sequence in the lower dimensional space is non-descending. Let \( \frac{a_1}{b_1} \leq \frac{a_2}{b_2} \leq \ldots \leq \frac{a_m}{b_m} \) be this ratio sequence. By Lemma 4.5 the geodesic between \( \tilde{A} \) and \( \tilde{B} \) is a straight line, and hence unique. Furthermore, its length is \( \sqrt{\sum_{i=1}^{m} (\tilde{a}_i + \tilde{b}_i)^2} \). Since we mapped from \( V(\mathbb{R}^k) \) to \( V(\mathbb{R}^m) \) by repeated isometries, both the length of the path and the order it passes through \( P_1, \ldots, P_m \), or their images, remain the same. The straight line is the only locally shortest, ordered path in \( \mathbb{R}^m \), so its pre-image is the only locally shortest, ordered path in \( \mathbb{R}^k \) and thus must be the globally shortest path. \( \Box \)
4.2.1 PathSpaceGeo: A Linear Algorithm for Computing Path Space Geodesics

Theorem 4.10 can be translated into a linear algorithm called PathSpaceGeo, for computing the path space geodesic between $T_1$ and $T_2$ through some path space $S = \bigcup_{i=0}^{k} O_i$. For all $1 \leq i \leq k$, let $A_i = E_{i-1} \setminus E_i$ and let $B_i = F_i \setminus F_{i-1}$. Let $a_i = \|A_i\|$ and $b_i = \|B_i\|$, for all $1 \leq i \leq k$.

Let $1 \leq i < k$ be the least integer such that $\frac{a_i}{b_i} > \frac{a_{i+1}}{b_{i+1}}$. Then by Theorem 4.10 to find the path space geodesic through $S$, we should apply Lemma 4.9 and Corollary 4.7 to the ratio sequence $\frac{a_1}{b_1}, \frac{a_2}{b_2}, \ldots, \frac{a_k}{b_k}$, to map the problem to $V(\mathbb{R}^{k-1})$, where the ratio sequence becomes $\frac{a_1}{b_1}, \frac{a_2}{b_2}, \sqrt{\frac{a_1^2 + a_2^2}{b_1^2 + b_2^2}}, \frac{a_3}{b_3}, \ldots, \frac{a_k}{b_k}$. Repeat this process until the ratio sequence is non-descending.

Unfortunately, this process is not deterministic, in that different non-descending ratio sequences can be found for the same geodesic, depending on the starting path space. This occurs, because by Corollary 4.6, two equal ratios can be combined to give a ratio sequence corresponding to a path with the same length. However, if we modify the algorithm to also combine equal ratios, the output ascending ratio sequence will be unique for a given geodesic.

Alternatively, define the carrier of the path space geodesic through $S$ between $T_1$ and $T_2$ to be the path space $Q = \bigcup_{i=0}^{l} O_{c(i)} \subseteq S$ such that the path space geodesic through $S$ traverses the relative interiors of $O_{c(0)}, O_{c(1)}, \ldots, O_{c(l)}$, where the function $c : \{0, 1, \ldots, l\} \rightarrow \{0, \ldots, k\}$ takes $i$ to the $i$-th orthant in $Q$ is the $c(i)$-th orthant in $S$. If a path space geodesic is the geodesic, we just write carrier of the geodesic. The carrier of the path space geodesic is the path space whose corresponding ratio sequence is the unique ascending ratio sequence for the path space geodesic.

We now explicitly describe the algorithm for computing the ascending ratio sequence corresponding to the path space geodesic, PathSpaceGeo, and prove it has linear runtime.

PathSpaceGeo

**Input:** Path space $S$ or its corresponding ratio sequence $R = \frac{a_1}{b_1}, \frac{a_2}{b_2}, \ldots, \frac{a_k}{b_k}$

**Output:** The path space geodesic, represented as an ascending ratio sequence, which is understood to be the partition of $R$ where the ratio $\frac{\sqrt{\sum_{j=0}^{l} a_{i+j}^2}}{\sqrt{\sum_{j=0}^{l} b_{i+j}^2}}$ corresponds to the block $\{ \frac{a_i}{b_i}, \frac{a_{i+1}}{b_{i+1}}, \ldots, \frac{a_{i+j}}{b_{i+j}} \}$.

**Algorithm:** Starting with the ratio pair $\{ \frac{a_1}{b_1}, \frac{a_2}{b_2} \}$, PathSpaceGeo compares consecutive ratios. If for the $i$-th pair, we have $\frac{a_i}{b_i} \geq \frac{a_{i+1}}{b_{i+1}}$, then combine the two ratios by replacing them by $\frac{\sqrt{a_i^2 + a_{i+1}^2}}{\sqrt{b_i^2 + b_{i+1}^2}}$ in the ratio sequence. Compare this new, combined ratio with the previous ratio in the sequence, and combine these two ratios if they are not ascending. Again the newly combined ratio must be compared with the ratio before it in the sequence, and so on. Once the last combined ratio is strict greater then the previous one in the sequence, we again start moving forward through the ratio sequence, comparing consecutive ratios. The algorithm ends when it reaches the end of the ratio sequence, and the ratios form an ascending ratio sequence.

**Theorem 4.11.** PathSpaceGeo has complexity $\Theta(k)$, where $k + 1$ is the number of orthants in the path space between $T_1$ and $T_2$.

**Proof.** We first show the complexity is $O(k)$. Combining two ratios reduces the number of ratios by 1, so this operation is done at most $k - 1 = O(k)$ times. It remains to count the number of comparisons between ratios. Each ratio is involved in a comparison when it is first encountered in the sequence. There are $k - 1$ such comparisons. All other comparisons occur after ratios are combined, so there are at most $k - 1$ of these comparisons. Therefore, PathSpaceGeo has complexity $O(k)$. Any algorithm must make $k - 1$ comparisons to ensure the ratios are in ascending order, so the complexity is $\Omega(k)$, and thus this bound is tight.
We use \texttt{PathSpaceGeo(S)} = \texttt{PathSpaceGeo} \left( \frac{a_1}{b_1}, \frac{a_2}{b_2}, ..., \frac{a_k}{b_k} \right) \) to represent the ascending ratio sequence output by running \texttt{PathSpaceGeo} with input \( S \). When \texttt{PathSpaceGeo} is run with an ascending ratio sequence as input, the output is the same sequence. Thus

\[
\text{PathSpaceGeo} \left( \text{PathSpaceGeo} \left( \frac{a_1}{b_1}, \frac{a_j}{b_j}, ..., \frac{a_{j+1}}{b_{j+1}}, ..., \frac{a_k}{b_k} \right) \right) \\
= \text{PathSpaceGeo} \left( \frac{a_1}{b_1}, \frac{a_2}{b_2}, ..., \frac{a_k}{b_k} \right).
\]

\text{PathSpaceGeo} lets us quickly calculate the shortest path through a maximal path space.

## 5 Algorithms

In this section, we show in Theorem 5.1 how to compute the geodesic distance between two trees \( T_1 \) and \( T_2 \) by computing the geodesic between certain smaller, related trees. This allows us to use the results from Sections 3 and 4, as well as either dynamic programming or divide and conquer techniques, to devise two algorithms for finding the geodesic between two trees with no common splits. Experiments on random trees show these algorithms are exponential, but practical on trees with up to 40 leaves and significantly better than the only other algorithm [15] published, to my knowledge. We also apply these algorithms to some biological data.

### 5.1 A Relation between Geodesics

Let \( T_1 \) and \( T_2 \) be two trees in \( T_n \) with no common splits. The following theorem shows that there exists a maximal path space \( M \) containing the geodesic between \( T_1 \) and \( T_2 \) such that a certain subspace of it contains the geodesic between two smaller, related trees, \( T_1' \) and \( T_2' \). As \( T_1' \) and \( T_2' \) have fewer splits than \( T_1 \) and \( T_2 \), it is easier to compute this geodesic. Therefore, we can find the geodesic between \( T_1 \) and \( T_2 \), by finding the geodesic between all such \( T_1' \) and \( T_2' \).

**Theorem 5.1.** Let \( T_1 \) and \( T_2 \) be two trees in \( T_n \) with no common splits. Then there exist a maximal path space \( M = \bigcup_{i=0}^{k-1} O_i = \bigcup_{i=0}^{k-1} O(E_i \cup F_i) \) between \( T_1 \) and \( T_2 \) and a maximal path space \( M' = \bigcup_{i=0}^{k-1} O_i' = \bigcup_{i=0}^{k-1} O(E_i \cup E_{k-1} \cup F_i) \) between \( T_1' = T(E_{k-1} \setminus F_{k-1}) \) and \( T_2' = T(F_{k-1}) \), such that \( M \) contains the geodesic between \( T_1 \) and \( T_2 \) and \( M' \) contains the geodesic between \( T_1' \) and \( T_2' \).

To prove this theorem, we first prove two lemmas which hold for any maximal path space \( M = \bigcup_{i=0}^{k-1} O_i = \bigcup_{i=0}^{k-1} O(E_i \cup F_i) \) between \( T_1 \) and \( T_2 \). In this context, let \( T_1' = T(E_{k-1} \setminus F_{k-1}) \) and \( T_2' = T(F_{k-1}) \). That is, \( T_1' \) and \( T_2' \) are exactly the trees \( T_1 \) and \( T_2 \) with the edges \( E_{k-1} \) and \( F_{k-1} \) contracted. Let \( M' = \bigcup_{i=0}^{k-1} O_i' = \bigcup_{i=0}^{k-1} O(E_i \cup E_{k-1} \cup F_i) \) be the path space containing exactly the trees in \( M \), with the edges \( E_{k-1} \) and \( F_{k-1} \) contracted.

**Lemma 5.2** shows that the carrier of the path space geodesic through \( M \) is contained in the orhants corresponding to the carrier of the path space geodesic through \( M' \). **Lemma 5.3** shows that if \( M' \) does not contain the geodesic between \( T_1' \) and \( T_2' \), and hence we can find another path space \( P' \) containing a shorter path space geodesic, then the corresponding path space \( P \) between \( T_1 \) and \( T_2 \) contains a path space geodesic at least as short as that through \( M \).

**Lemma 5.2.** Let \( T_1, T_2, T_1', T_2', M \) and \( M' \) be as described above. Let \( Q' = \bigcup_{i=0}^{k-1} O'_c(i) \) be the carrier of the path space geodesic through \( M' \). Let \( Q = (Q' \oplus O(E_{k-1})) \cup O_{k-1} \). Then \( d_Q(T_1, T_2) = d_M(T_1, T_2) \).
Proof. We want to show that PathSpaceGeo\( (Q) = \text{PathSpaceGeo} (M) \).

By properties of PathSpaceGeo,
\[
\text{PathSpaceGeo} (Q) = \text{PathSpaceGeo} \left( \text{PathSpaceGeo} (Q'), \frac{\|E_{k-1} \setminus E_k\|}{\|F_k \setminus F_{k-1}\|} \right).
\]

Similarly, \( \text{PathSpaceGeo} (M) = \text{PathSpaceGeo} \left( \text{PathSpaceGeo} (M'), \frac{\|E_{k-1} \setminus E_k\|}{\|F_k \setminus F_{k-1}\|} \right) \). But \( \text{PathSpaceGeo} (M') = \text{PathSpaceGeo} (Q') \) by definition of the carrier of the path space geodesic, and thus \( \text{PathSpaceGeo} (Q) = \text{PathSpaceGeo} (M) \).

Lemma 5.3. Let \( T_1, T_2, T_1', T_2', M \) and \( M' \) be as described above. If \( M' \) does not contain the geodesic between \( T_1 \) and \( T_2 \) in \( T_n \), then there exists a path space \( P' \) between \( T_1' \) and \( T_2' \) such that \( d_{P'} (T_1', T_2') < d_M (T_1, T_2) \) and \( d_P (T_1, T_2) \leq d_M (T_1, T_2) \), where \( P = (P' \oplus \mathcal{O}(E_{k-1})) \cup \mathcal{O}_k \).

Proof. Let \( Q' = \bigcup_{i=0}^\infty \mathcal{O}'_{c(i)} \) be the carrier of the path space geodesic through \( M' \). Let \( q \) be the path space geodesic through \( Q' \) between \( T_1' \) and \( T_2' \), and let \( q_i = \mathcal{O}'_{c(i-1)} \cap \mathcal{O}'_{c(i)} \cap q \) for every \( 1 \leq i \leq l \). Since \( q \) is not the geodesic from \( T_1' \) to \( T_2' \), \( q \) cannot be locally shortest in \( T_n \). By Proposition 4.1, for all \( 1 \leq i \leq l-1 \), the part of \( q \) between \( q_i \) and \( q_{i+1} \) is a line, and cannot be made shorter in \( T_n \). Thus we can only find a locally shortest path in \( T_n \) by varying \( q \) is the neighbourhood of some \( q_j \). In particular, there exists some \( \varepsilon \) such that if \( s \) and \( t \) are the points on \( q_i, \varepsilon \) before and after \( q_j \) in the orthants \( \mathcal{O}_{c(j-1)} \) and \( \mathcal{O}_{c(j)} \), respectively, then the geodesic between \( s \) and \( t \) does not follow \( q \). Replace the part of \( q \) between \( s \) and \( t \) with the true geodesic between \( s \) and \( t \) to get a shorter path in \( T_n \), with distance \( d_s \). Let \( \mathcal{O}_{c(j-1)}', \mathcal{O}_1' = \mathcal{O}(E_1' \cup F_1'), \ldots, \mathcal{O}_m' = \mathcal{O}(E_m' \cup F_m'), \mathcal{O}_{c(j)} \) be the sequence of orthants through whose relative interiors the geodesic between \( s \) and \( t \) passes. Note that \( \mathcal{O}_1', \ldots, \mathcal{O}_m' \) are not in \( M' \). These orthants must form a path space, and thus \( P' = Q' \cup (\bigcup_{i=0}^m \mathcal{O}'_m) \) is a path space. Since the path space geodesic is the shortest path through a path space, \( d_{P'} (T_1', T_2') \leq d_s < d_{Q'} (T_1', T_2') \). In \( T_n \).

By definition of \( Q' \), \( d_{Q'} (T_1', T_2') = d_M (T_1', T_2') \), and hence \( d_{P'} (T_1', T_2') < d_M (T_1', T_2') \), as desired.

We will now show that \( d_P (T_1, T_2) \leq d_M (T_1, T_2) \). Let \( Q = (Q' \oplus \mathcal{O}(E_{k-1})) \cup \mathcal{O}_k \). Then \( Q \subset P \), which implies \( d_P (T_1, T_2) \leq d_Q (T_1, T_2) \). By Lemma 5.2 \( d_Q (T_1, T_2) = d_M (T_1, T_2) \), and so \( P' \) is the desired path space.

We use Lemma 5.3 to prove Theorem 5.4.

Proof of Theorem 5.4. Let \( S \) be any maximal path space containing the geodesic between \( T_1 \) and \( T_2 \). Suppose \( S \) consists of \( l+1 \) orthants, and let \( E \) be the set of edges dropped at the transition to the \( (l+1) \)-st orthant \( \mathcal{O}_l \). Let \( S' \) be defined by \( (S' \oplus \mathcal{O}(E)) \cup \mathcal{O}_l = S \). Then \( S' \) is a maximal path space between \( T_1' \) and \( T_2' \), as the conditions in Theorem 3.4 still hold.

If \( S' \) contains the geodesic between \( T_1' \) and \( T_2' \), then we are done. If not, then by Lemma 5.3, there exists another path space \( P \) from \( T_1 \) to \( T_2 \), with \( d_P (T_1, T_2) \leq d_S (T_1, T_2) \) and \( d_P (T_1, T_2) < d_{S'} (T_1', T_2') \). If \( P' \) does not contain the geodesic between \( T_1' \) and \( T_2' \), then we can keep applying Lemma 5.3 to a maximal path space containing it, until it does. As this process produces a path space containing a strictly shorter path space geodesic at each iteration, and there are only a finite number of path spaces between \( T_1' \) and \( T_2' \), it eventually finds the path space \( Q' \), containing the geodesic from \( T_1' \) to \( T_2' \). Furthermore, letting \( Q = (Q' \oplus \mathcal{O}(E)) \cup \mathcal{O}_l \), Lemma 5.3 implies that \( d_Q (T_1, T_2) \leq d_S (T_1, T_2) \). But \( S \) contains the geodesic between \( T_1 \) and \( T_2 \), so \( d_S (T_1, T_2) \leq d_Q (T_1, T_2) \), and hence \( d_Q (T_1, T_2) = d_S (T_1, T_2) \). Let \( M' = \bigcup_{i=0}^{k-1} \mathcal{O}_i' \) be a maximal path space between \( T_1' \) and \( T_2' \) containing \( Q' \). Then \( M = (M' \oplus \mathcal{O}(E)) \cup \mathcal{O}_l \) contains \( Q \) and is a maximal path space between \( T_1 \) and \( T_2 \) with the required properties.
We will now present two specific algorithms for computing geodesics. Each of these algorithms uses Theorem 5.1 to avoid computing the path space geodesic for each maximal path space between \( T_1 \) and \( T_2 \). This significantly decreases the run time. We call these algorithms GEODEMAPS, which stands for GEodesic DistancE via MAXimal Path Spaces. The first algorithm uses dynamic programming techniques, and is denoted GEODEMAPS-DYNAMIC, while the second uses a divide and conquer strategy, and is denoted GEODEMAPS-DIVIDE.

5.2 GeodeMaps-Dynamic: a Dynamic Programming Algorithm

Theorem 5.1 implies that for any element \( A \) in \( K(T_1, T_2) \), we can find the geodesic between \( T(X_{T_1}(A)) \) and \( T(A) \) by only considering the maximal path spaces that contain a geodesic between \( T(X_{T_1}(B)) \) and \( T(B) \) for some \( B \) covered by \( A \). Furthermore, since given a geodesic \( g_B \) between \( T(X_{T_1}(B)) \) and \( T(B) \) for some \( B \) covered by \( A \), the candidate for the geodesic between \( T(X_{T_1}(A)) \) and \( T(A) \) is computed using only the carrier of \( g_B \), which is independent of the choice of maximal path space containing \( g_B \).

This suggests that we can compute the geodesic distance by doing a breath-first search on the Hasse diagram of \( K(T_1, T_2) \). As we visit each node \( A \) in \( K(T_1, T_2) \), we construct the geodesic between \( T(X_{T_1}(A)) \) and \( T(A) \) using the geodesics between \( T(X_{T_1}(B)) \) and \( T(B) \) for each node \( B \) covered by \( A \), which we have already visited. As we showed in Section 3, there can be an exponential number of elements in the path poset, so this algorithm is exponential in the worst case. However, this is a significant improvement over considering each maximal path space.

**Example 5.4.** Consider the trees \( T_1 \) and \( T_2 \), their incompatibility poset \( P(T_1, T_2) \), and their path poset \( K(T_1, T_2) \) in Figure 4. Assume the splits in \( T_1 \) and \( T_2 \) have lengths, and label each edge in the Hasse diagram of \( K(T_1, T_2) \) with the ratio of the length of the split dropped to the length of the split added during the corresponding orthant transition, as shown in Figure 7(a). The sequence of ratios along a maximal chain is the ratio sequence passed to PathSpaceGeo to find the path space geodesic corresponding to that chain. We first find the geodesic from \( T(\{e_1, e_4\}) \) in \( O_{\varnothing} \) to \( T(\{f_1, f_4\}) \) in \( O_{\frac{f_4}{f_1}} \), by passing the ratio sequences \( \frac{0.83}{0.7} \frac{0.88}{0.15} \frac{0.83}{0.7} \) and \( \frac{0.88}{0.15} \frac{0.83}{0.7} \) to PathSpaceGeo, which returns the distances 1.84 and 1.95, respectively (Figure 7(b)). This and Theorem 5.1 imply that if the geodesic from \( T_1 \) to \( T_2 \) travels through \( O_{\frac{f_4}{f_1}} \), then it travels through \( O_{\frac{f_3}{f_1}} \). We next calculate the geodesic between \( T(\{e_1, e_3, e_4\}) \) in \( O_{\varnothing} \) and \( T(\{f_1, f_2, f_4\}) \) in \( O_{\frac{f_4}{f_2}} \). There are three maximal chains between \( \varnothing \) and \( f_1, f_2 \). However, we ignore \( \varnothing < f_1 \) \( f_2 \) \( f_1, f_2 \), because we just showed that if the geodesic intersects \( O_{\frac{f_4}{f_1}} \), then it intersects \( O_{\frac{f_3}{f_1}} \). Applying PathSpaceGeo to the ratio sequences \( \frac{0.83}{0.7} \frac{0.88}{0.15} \frac{0.83}{0.7} \) \( \frac{0.88}{0.15} \frac{0.83}{0.7} \) \( \frac{0.88}{0.15} \frac{0.83}{0.7} \) gives distances 2.4244 and 2.4243, respectively. Thus, by Theorem 5.1, if the geodesic between \( T_1 \) and \( T_2 \) intersects \( O_{\frac{f_4}{f_2}} \), then it also intersects \( O_{\frac{f_3}{f_2}} \), \( O_{\frac{f_4}{f_1}} \), and \( O_{\varnothing} \). But this is the case, and hence we have found the maximal path space containing the geodesic, as shown in Figure 7(d). The length of the geodesic is 2.65.

We implemented a more memory-efficient version of this algorithm, called GEODEMAPS-DYNAMIC. This version uses a depth-first search of the Hasse diagram of \( K(T_1, T_2) \). For each element \( A \) in \( K(T_1, T_2) \), it stores the distance of the shortest path space geodesic found so far between \( T(X_{T_1}(A)) \) and \( T(A) \). Thus if GEODEMAPS-DYNAMIC revisits an element by following a chain in \( K(T_1, T_2) \) with a longer path space geodesic, it prunes this branch of the search. GEODEMAPS-DYNAMIC stores the carrier of the shortest path space geodesic found so far between \( T_1 \) and \( T_2 \). As a heuristic improvement, at each step in the depth-first search, GEODEMAPS-DYNAMIC chooses the node with the lowest transition ratio of the nodes not yet visited.
5.3 GeodeMaps-Divide: a Divide And Conquer Algorithm

If $A$ is an element in $K(T_1, T_2)$, then the trees in $\mathcal{O}_A$ share the splits $A$ with $T_2$. This inspires the following algorithm, which we call GeodeMaps-Divide. Choose some minimal element of $P(T_1, T_2)$, and add the splits in this equivalence class to $T_1$ by first dropping the incompatible splits. For example, if we choose to add the split set $F_1$, then we must drop $X_{T_1}(F_1)$. The trees in this orthant $\mathcal{O}_{F_1}$ now have splits $F_1$ in common with $T_2$. Apply Theorem 2.1 to divide the problem into subproblems along these common splits. For each subproblem, recursively call GeodeMaps-Divide. Since some subproblems will be encountered many times, store the geodesics for each solved subproblem using a global hash table.

Example 5.5. Consider the trees $T_1$ and $T_2$ in Figure 8. These trees belong to the family of trees given in Figure 5 which have an exponential number of elements in their path posets. Suppose we first chose the minimal element $f_3$. We drop $e_4$ from $T_1$ and add $f_3$ to get the tree $T$ in Figure 8(c). $T$ and $T_2$ now share the split $f_3$, so we apply Theorem 2.1 to decompose the problem into two subproblems. The incompatibility poset can also be decomposed, as illustrated by Figure 8(e).

Each subproblem corresponds to an element in $K(T_1, T_2)$, and GeodeMaps-Divide is polynomial in the number of subproblems solved. Hence an upper bound on the complexity of GeodeMaps-Divide is the number of elements in $K(T_1, T_2)$. This was shown to be exponential in the number of leaves by the family of trees presented in Figure 5. However, for this particular family of trees, one can show that GeodeMaps-Divide has a polynomial runtime, while GeodeMaps-Dynamic has an exponential runtime. However, there exists a family of trees such that GeodeMaps-Dynamic is exponential. See [19] Section 5.2.2 for details.

5.4 Performance of GeodeMaps-Dynamic and GeodeMaps-Divide

We now compare the runtime performance of GeodeMaps-Dynamic and GeodeMaps-Divide with GeoMeTree [15], the only other geodesic distance algorithm published to our knowledge. For $n = 10, 15, 20, 25, 30, 35, 40, 45$, we generated 200 random rooted trees with $n$ leaves, using a birth-death process. Specifically, we ran Evolver, part of PAML [30] with the parameters estimated for the phylogeny of primates in [31], that is 6.7 for the birth rate ($\lambda$), 2.5 for the death rate ($\mu$), 0.3333 for the sampling rate, and 0.24 for the mutation rate. For each $n$, we divided the 200 trees
into 100 pairs, and computed the geodesic distance between each pair. The average computation times are given in Figure 9. Memory was the limiting factor for all three algorithms, and prevented us from calculating the missing data points.

Both GeodeMaps-Dynamic and GeodeMaps-Divide exhibit exponential runtime, but they are significantly faster than GeoMeTree. Note that as the trees used were random, they have very few common splits. Biologically meaningful trees often have many common splits, resulting in much faster runtimes. For example, for a data set of 31 43-leaved trees representing possible ancestral histories of bacteria and archaea [16], we computed the geodesic distance between each pair of trees. Using GeodeMaps-Dynamic the average computation time was 0.531 s, while using GeodeMaps-Divide the average time was 0.23 s. This contrasts to an average computation time of 22 s by GeodeMaps-Dynamic for two random trees with 40 leaves.

All computations were done on a Dell PowerEdge Quadcore with 4.0 GB memory, and 2.66 GHz x 4 processing speed. The implementation of these algorithms, GeodeMaps 0.2, is available for download from www.cam.cornell.edu/~maowen/geodemaps.html.

6 Conclusion

We have used the combinatorics and geometry of the tree space $T_n$ to develop two algorithms to compute the geodesic distance between two trees in this space. In doing so, we have provided a linear time algorithm for computing the shortest path in the subspace $V(\mathbb{R}^n)$ of $\mathbb{R}^n$, which will help characterize when the general problem of finding the shortest path through $\mathbb{R}^n$ with obstacles is NP-hard. Furthermore, these algorithms are significantly faster than all known algorithms, and the freely available implementation will be of use to any researcher wishing to use the tree space framework in their work with phylogenetic trees. For example, Yap and Pachter [32] and Suchard...
Figure 9: Average runtimes of the three geodesic distance algorithms.

[27] have explicitly mentioned this as a direction for future work.

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