The space of ultrametric phylogenetic trees

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Abstract

We introduce two metric spaces on ultrametric phylogenetic trees and compare them with existing models of tree space. We formulate several formal requirements that a metric space on phylogenetic trees must possess in order to be a satisfactory space for statistical analysis, and justify them. We show that only a few known constructions of the space of phylogenetic trees satisfy these requirements. However, our results suggest that these basic requirements are not enough to distinguish between the two metric spaces we introduce and that the choice between metric spaces requires additional properties to be considered.

This paper lies in the broad scope of research on the following two phylogenetic problems, which are also of more general interest, as we demonstrate in this work. First is the problem of introducing a satisfactory parameterisation of phylogenetic trees for statistical analysis of tree space. The space of phylogenetic trees encapsulates the structure of a manifold as well as the combinatorially complicated discrete structure of trees (Semple and Steel 2003). This mix of a continuous and a discrete component is what makes statistical analysis of the space complicated. The second problem is the problem of summarising a finite set of phylogenetic trees (Heled and Bouckaert 2013; Hillis, Heath and John 2005; Huggins et al. 2011). This problem arises in different settings of phylogenetic analysis, the most important of which

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is the problem of computing a statistically consistent summary of a sample from the posterior probability distribution over trees (Bouckaert et al. 2014; Drummond and Rambaut 2007).

A quite extensive amount of research has been done on the space of phylogenetic trees in the general setting when the phylogenetic distance between taxa is given by arbitrary lengths of the edges of the tree (Billera, Holmes and Vogtmann 2001; Semple and Steel 2003). As we demonstrate in this paper, this general setting sometimes leads to computationally intractable models when applied to the space of ultrametric trees (a special case of time-trees). Ultrametric trees are the only satisfactory model for a great body of research in phylogenetics and epidemiology, especially when divergence time dating is the objective, and the taxa are all contemporaneous. In this case the time-tree is ultrametric, and is considered separately to the rates of evolution across lineages, which may vary from one branch to the next.

The aim of this paper is to introduce a mathematically satisfactory model of the space of equidistant phylogenetic trees. The notion of a ‘mathematically satisfactory model’ will be clarified and made exact later in the paper with an eye towards the two general problems described above. Our work is inspired by that of Billera, Holmes and Vogtmann (2001), and is similar to it in the sense that we use polyhedral complexes to define a metric space. The investigation of the tree space from a geometric point of view was initiated by their work (Billera, Holmes and Vogtmann 2001) with the introduction of a parameterisation that later became known as BHV. Due to several nice geometric and algorithmic properties, it was recently suggested (Benner, Bačák and Bourguignon 2014) that BHV is the space for statistical, and particularly MCMC, analysis of phylogenetic trees. Our results presented in this paper show how crucial the way a tree is parameterised can be for geometric, algorithmic, and statistical properties of the space. Particularly, we demonstrate that the summary tree that is suggested in (Benner, Bačák and Bourguignon 2014) will be different for different parameterisations of the tree space. Our results leaves open the question of which parameterisation should be chosen.

We call the same type of trees ‘ultrametric’ in the title of the paper and ‘equidistant’ in the previous paragraph. The reason for this ambiguity is the following. The type of object we consider in this paper is commonly known to evolutionary biologists as an ultrametric tree, while for mathematical biologists, this term is not appropriate for the following reasons:

(1) The popular handbook of a mathematical biologist (Semple and Steel 2003) calls these trees equidistant.
(2) An equidistant tree gives rise to a metric on the taxa. This metric is always an ultrametric, which is a standard notion of geometry.

(3) Every finite ultrametric space $X$ can be presented by a unique equidistant phylogenetic tree on $X$ as taxa.

(4) There are non-equidistant phylogenetic trees that give rise to an ultrametric space on the taxa.

Hence, we have used the term ‘ultrametric’ in the title and abstract of this paper, to make the topic of this paper clear for both communities, and we use the term ‘equidistant’ from now on for reasons (1) and (4) above.

Unless otherwise explicit, by a tree we mean an equidistant phylogenetic tree, that is, a binary rooted tree with distinguished tips and branch lengths such that the distance from the root is the same to every tip.

We follow books (Semple and Steel 2003) for phylogenetics and (Bridson and Haefliger 1999; Thomas 2006) for geometric combinatorics terminology. The structure of our paper is the following. In Section 1. Introduction, we describe the state of the art. Particularly, we present the metric spaces with which we will be comparing our spaces. We note that all the metric spaces, apart from BHV, are not actually used as geometries but as a way of measuring errors instead (Heled and Bouckaert 2013; Huggins et al. 2011). Indeed, some of those characteristics are not even metrics, they are more general geometric objects called dissimilarity maps. In this section, we establish some geometric properties of described spaces (that theoretically justify their sometimes poor fit for both statistical analysis and summarising the posterior). We also describe a way of adapting the BHV space for the space of equidistant trees. Section 2. $\tau$-space is one of the main contributions of the paper. Here we introduce the space and establish its geometric properties that make $\tau$-space attractive for modelling equidistant phylogenetic trees. We also describe effectiveness properties of the space. Section 3. $t$-space is where we describe the $t$-space, establish its geometric properties and compare $\tau$- and $t$-spaces. The seemingly inessential difference between the two spaces of how a tree is parameterised results in a large impact on geometric and algorithmic properties of the space, as we demonstrate in this section, which is one of the main contributions of the paper.

1. Introduction

Although the space of equidistant phylogenetic trees is well understood by biologists, mathematicians, and statisticians, there are a large number of
ways to define this space formally. As a well-chosen formal definition is the main and crucial step for various types of analyses of the space, including mathematical, statistical, and computational, it is important to carefully address the balance between the generality of the definition, its mathematical clarity, and its applicability in analyses of real evolutionary processes. Formal definitions become especially important in modern research because of the massive use of computational tools, for which equivalent definitions can change the complexity of a problem from incomputable on any type of abstract digital computer to rapidly computable on available machines. In this paper, we consider several approaches to defining the space of equidistant phylogenetic trees and compare their mathematical, computational, and statistical tractability.

It is a standard practice in evolutionary biology to model real biological processes by mathematical abstractions (Semple and Steel 2003). Particularly, as biologists are often interested in comparing different hypotheses about an evolutionary process modelled by phylogenetic trees, it is natural to work within the space of such trees. It is also a common practice to introduce different types of measures on the space of trees as a formal way of comparing them. One of the most general and commonly used ways of measuring the similarity between two trees is given by the notion of distance, or metric as it is widely known in mathematics. In order to measure the distance between trees, the tree space has to be parameterised, that is, some real-valued parameters have to be assigned to trees.

Formally, this scenario can be described as follows. Let $T$ be the space of phylogenetic trees on $n$ taxa. A parameterisation of the space $T$ is an embedding $p: T \to M$ of the tree space $T$ to a metric space $M$, which we call a model metric space. By embedding here, we mean a function that maps different trees to different points of the metric space $M$. The embedding $p$ plays the role of the assignment of parameters (points of the space $M$, which could be tuples of real numbers, for example). The existence of such an embedding makes the space $T$ itself a metric space. Indeed, the distance between two trees $T$ and $R$ is given by the distance between their images under the embedding $p$, that is, $d_T(T, R)$ is defined to be $d_M(p(T), p(R))$. We say in this case that the metric $d_T$ is induced by the parameterisation $p$.

As is known (Heled and Bouckaert 2013; Hillis, Heath and John 2005; Huggins et al. 2011), the existence of a parameterisation alone is already a fruitful property of the space of phylogenies, as it allows to test hypotheses such as how far are two trees from each other? How far is an estimate from the true tree? Given two algorithms, which one produces trees that are closer to

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1 We use $n$ to denote the number of taxa throughout the paper.
the true tree? Sometimes it is even possible to extract an objective function minimisation that leads to a practical way of summarising posteriors (Heled and Bouckaert 2013). We will present some of these parameterisations later in this section.

Often biologists and especially phylogeneticists are interested in more subtle properties of the space of trees, such as what tree is in the middle between two given trees\(^2\)? What is the path from one tree to another? What is the mean and the variance of a set of (sampled) trees? The last question is of prominent importance, as this is the very basic question for statistical analysis of data that produces a set of phylogenetic trees. Furthermore, this question is important in testing whether two probability distributions on tree space are the same, a task common in statistical model selection. More sophisticated questions include, for example, how standard phylogenetic models such as coalescent and birth-death can be described under a given parameterisation? Can more efficient proposal mechanisms, such as Hamiltonian Monte Carlo, be employed in Bayesian analysis of phylogenetic data?

A more detailed mathematical analysis is needed in order to approach questions such as these. In what follows, we summarise several basic properties of parameterisations, which we suggest are desirable to advance research on the problems mentioned.

It is often the case that the metric space \(\mathcal{M}\) that is used to parameterise tree space \(\mathcal{T}\) is greatly different from the metric space \(\mathcal{T}\) with the induced metric \(d_T\). The key reason for this is the nature of the parameterisation \(p\). As we will see later in the paper, some parameterisations \(p\) induce metrics that share almost no geometric properties in common with the original metric space \(\mathcal{M}\) that was used in the parameterisation \(p\). Particularly, those parameterisations are far from being bijective, that is, being able to recover a tree given an arbitrary point from the space \(\mathcal{M}\). The lack of this property can lead to situations where, for example, there are infinitely many trees all of which minimise the total square distance to a given set of trees (Heled and Bouckaert 2013). A sphere, for example, has such a property, where there are infinitely many points minimising the total square distance to two antipodal points. Furthermore, there are two points \(a\) and \(b\) both of which minimise this distance, but the distance between \(a\) and \(b\) is as large as possible.

Although the parameterisations we introduce in Sections 2 and 3 of this paper are bijective, the requirement of being bijective is somewhat strong in the sense that many desirable properties can be achieved without the parameterisation being bijective. We continue with introducing formal re-

\(^2\)Since we are aimed at a metric space that mirrors the prior or the posterior and preferably both, this question is important for us.
quirements that allow to carry the analysis of the space $\mathcal{M}$ over to the space of trees $\mathcal{T}$.

For the statistical analysis of a space, one needs to define probability distributions over the space, e.g. for Bayesian analysis the first step is to define a prior distribution. A continuous probability distribution defined on the metric space $\mathcal{M}$ has to remain the same\(^3\) continuous distribution when pulled back to the space of trees $\mathcal{T}$ under the parameterisation $p$. In order to achieve this, one has to be able to continuously move from one tree to another by a path that stays within the tree space. In other words, any two trees have to be connected by a path.

Formally, a metric space $X$ is called *path-connected* if for each pair of points $x, y$ in the space, there exists a continuous map $\gamma$ (with respect to the standard topologies generated by balls) from the unit real segment $[0, 1]$ to the space $X$ such that $\gamma(0) = x$ and $\gamma(1) = y$.

Thus, the first property a satisfactory parameterisation of the tree space must satisfy is:

\[\text{Image}(p)\text{ is path-connected in } \mathcal{M}.\]  

(P1)

The existence of paths between any two points alone is not necessarily enough to convert paths between points in the space $\mathcal{M}$ into paths between trees in $\mathcal{T}$, because it could be that the pre-image of a path in $\mathcal{M}$ is not a path in $\mathcal{T}$. Hence, we would like to have an easy way of testing what paths in $\mathcal{M}$ remain paths when pulled back to $\mathcal{T}$. Furthermore, it could be that shortest paths in the tree space are not unique even when the model metric space $\mathcal{M}$ has unique shortest paths. The uniqueness of shortest paths is often desirable, as spaces with unique shortest paths possess the uniqueness of several important summary characteristics such as means and barycentres. Requirements of this sort can be fulfilled by the convexity of Image($p$) in $\mathcal{M}$, which means that every shortest path between every two points of Image($p$) stays within Image($p$).

Formally, a subspace $X$ of a space $Y$ is called *convex* if for every pair of points $x, y \in X$, every shortest path $\gamma$ between $x$ and $y$, and every real number $s \in [0, 1]$, it follows that $\gamma(s) \in X$.

Hence, our second property is:

\[\text{Image}(p)\text{ is convex in } \mathcal{M}.\]  

(P2)

Suppose one has a probability distribution $D$ over the metric space $\mathcal{M}$ with parameterisation $p$ and one wants to define the probability distribution $D$ on the tree space $\mathcal{T}$ by pulling $D$ back to $\mathcal{T}$. In this case, the image

\(^3\)In the sense that all statistics, e.g. $k$-th moments, are preserved.
Image(\(p\)) has to be a non-trivial part of \(\mathcal{M}\), particularly it has to accumulate non-zero probability mass. Since a subspace of strictly smaller dimension than the dimension\(^4\) of the space has measure zero, our next requirement is:

\[
\text{Image}(p) \text{ has the same dimension as } \mathcal{M}. \quad \text{(P3)}
\]

Requirements P1–P3 guarantee that desirable geometric properties of the space \(\mathcal{M}\) will be inherited by the induced metric space on trees \(\mathcal{T}\), but none of the requirements causes those properties to exist. They have to be postulated. Hence, we now go on to the properties of the space \(\mathcal{M}\). It is important to note that the following properties only make sense if the requirement P1–P3 are fulfilled.

The notion of convexity refers to a shortest path between two points. This is because it could be that the shortest path is not unique. The uniqueness of shortest paths implies the uniqueness of several types of means, the soundness of the notion of a variance, and the existence and uniqueness of summary trees obtained by minimising an objective function of square distance. Hence, our next property is the following.

We say that a metric space possesses unique geodesics if there exists a unique shortest path between every two points in the space. This shortest path is called a geodesic\(^5\).

\[
\text{Metric space } \mathcal{M} \text{ possesses unique geodesics.} \quad \text{(P4)}
\]

Although for theoretical investigations it is convenient to assume property P4 to be satisfied globally, for practical applications it is almost always enough to assume this property to be satisfied almost surely. Intuitively this means that with probability one the shortest path is unique between two points drawn at random. Formally, we assume that the metric space \(\mathcal{M}\) is equipped with a probability measure \(\mu\) and say that a property \(P(\cdot)\) is satisfied almost surely if \(\mu^*\{x \in \mathcal{M} \mid P(x)\} = 1\), where \(\mu^*\) is the product measure if property \(P\) is defined on tuples. In this case the relaxed requirement is:

\[
\text{Metric space } \mathcal{M} \text{ possesses unique geodesics almost surely.} \quad \text{(P4')}\]

To distinguish Properties P4 and P4', let us consider the following example. Let \(C\) be the surface of a three-dimensional sphere with the standard

\[^4\text{By dimension here we mean the Hausdorff–Besicovitch dimension of the metric space.}\]

\[^5\text{It is worth noting here that our notion of geodesic is somewhat different from the one that is commonly used in differential geometry. We call a path geodesic only if the path is \textit{globally} shortest. For example, the great circle of a sphere with a small interval removed is \textit{not} a geodesic in our sense.}\]
spherical distance and uniform probability measure $\nu$. Space $C$ does not satisfy P4 as any pair of great circles gives an example of four geodesics between the two points at which the circles intersect. However, if we fix a point $x$ on sphere $C$ then the geodesic between $x$ and $y$ is unique for all but one point $y$ on $C$. This implies that $\nu^*\{(x, y) \mid \text{the geodesic between } x \text{ and } y \text{ is unique}\} = 1$, and Property P4$'$ is satisfied.

In some cases even both the existence and the uniqueness of geodesics are not enough for the comprehensive analysis of real data sets, because the geodesics are incomputable for some metric spaces$^6$. Hence our next property of the model space $\mathcal{M}$ is:

Geodesics in metric space $\mathcal{M}$ are computable. \hfill (P5)

The requirement for geodesics to be computable is reasonable for theoretical investigations of presentations of the tree space, but could be still insufficient for the analysis to be carried out on a real computer. Hence if one has an appropriate notion of ‘efficiently computable’, then property P5 can be strengthened to:

Geodesics in metric space $\mathcal{M}$ are efficiently computable. \hfill (P5$'$)

Statisticians and biologists are normally interested in the efficient computability$^7$ of various characteristics of a data set such as its mean, variance, diversity, confidence regions, and so on, rather than the geodesics themselves, but the computational complexity of most of the algorithms for computing these types of characteristics is bounded from below by the complexity of computing the geodesics. In other words, computing the geodesic is an unavoidable step of the algorithms (Bačák 2012; Billera, Holmes and Vogtmann 2001; Owen and Provan 2011).

Our work is motivated by the lack of parameterisations in the literature that enjoy all properties P1–P5. Indeed, all known summary tree estimators operate in spaces larger than the space of equidistant rooted binary trees, hence breaking requirement P3. For instance, Heled and Bouckaert (2013) and Huggins et al. (2011) use the so-called Rooted Branch Score metric (RBS) space for producing a summary tree given a sample of trees from the posterior distribution. The idea of the RBS space is to encode a tree on $n$
taxa by a \((2^n - 1)\)-dimensional real vector, find an optimum in the \((2^n - 1)\)-dimensional Euclidean space, and find the nearest point in the Euclidean space that can be pulled back to the tree space. Although this approach proved to be fruitful in several applied scenarios (Heled and Bouckaert 2013), it lacks properties P1–P3. Moreover, a tree that minimises the RBS distance to a (finite) set of trees is not unique—indeed there could be infinitely many such trees. This optimisation problem is computationally intractable even for moderate values of \(n\). In implementations of this method, the inefficiency is overcome by restricting the search only to tree topologies that are present in the posterior sample, that is, in the given set of trees. Furthermore, the tree topologies and the branch lengths have to be summarised separately in order to make the model computationally tractable (Heled and Bouckaert 2013).

Other metrics used by Huggins et al. (2011) employ projections to smaller dimension spaces to overcome the absence of properties P1–P3. Those metrics share the same pathologies as RBS. Moreover, the use of projections for estimating means can lead to unbounded errors as witnessed by the following proposition that claims that the projection of the mean can be as far from the mean of the projections as possible.

**Proposition 1.** Let \(N\) be a (arbitrarily large) real number, \(E\) a Euclidean space of dimension \(k > 1\), and \(x_1, \ldots, x_s\) a set of points in \(E\). Then there exists a subspace \(D\) of \(E\) such that

\[
d_E(\text{pr}_D(\text{mean}_E(x_1, \ldots, x_s)), \text{mean}_D(\text{pr}_D(x_1), \ldots, \text{pr}_D(x_s))) \geq N,
\]

where \(d_E\) is the Euclidean distance, \(\text{pr}_D(x)\) is the projection of the point \(x \in E\) onto \(D\), and \(\text{mean}_X(x_1, \ldots, x_s)\) is the Fréchet mean of \(x_1, \ldots, x_s\) in the space \(X\).

**Proof.** We prove the proposition for \(k = s = 2\). An arbitrary case is analogous. Let \(\ell\) be the line through \(x_1\) and \(x_2\) in \(E\) and \(\ell_0\) be a line parallel to \(\ell\) at a distance \(M\) from \(\ell\). Consider a parabola \(D\) which has its vertex on the line \(\ell_0\) and crosses the line \(\ell\) at some points \(a\) and \(b\) both of which are between \(x_1\) and \(x_2\). It is not hard to see that for large enough \(M\), we get \(d_E(\text{pr}_D(\text{mean}_E(x_1, x_2)), \text{mean}_D(\text{pr}_D(x_1), \text{pr}_D(x_2))) \geq N\).

It might appear that the construction used in the proof is slightly artificial, but this is actually very similar to what is happening in such parameterisations as RBS and dissimilarity map distance (Huggins et al. 2011), where the conditions on the set of points that correspond to trees are nontrivial (Cardona et al. 2010). The dissimilarity map distance (Huggins et
al. 2011) between two trees is defined as the distance between the distance matrices of the trees, in the space of square matrices. That is, the parameterisation \( p \) maps a tree to its distance matrix, and the model metric space \( \mathcal{M} \) is the space of \( n \times n \) matrices with the pointwise distance. This space is geometrically similar to RBS in the way that none of properties P1–P3 are satisfied. Cardona et al. (2010) characterise \( \text{Image}(p) \) for the case when the trees are not necessarily equidistant. This characterisation fulfils the requirements P1–P3. An attempt to carry this characterisation over to the space of equidistant trees has the same complication as the BHV space, which we discuss below.

The most geometrically attractive parameterisation of non-equidistant tree space is the BHV space (Billera, Holmes and Vogtmann 2001). This is the only parameterisation we are aware of that fulfils all the properties P1–P5’ (Billera, Holmes and Vogtmann 2001; Owen and Provan 2011). This parameterisation employs a \((2n-2)\)-dimensional cubical complex with unique geodesics as the model metric space \( \mathcal{M} \), then a bijective correspondence between the space of all phylogenetic trees and the complex \( \mathcal{M} \) is established. Trees of fixed topology are parameterised by a \((2n-2)\)-dimensional vector given by the lengths of the branches, and correspond to a cube. The adjacent cubes of the complex correspond to NNI-adjacent trees. Although it took ten years to establish property P5’ for the parameterisation, the polynomial algorithm designed by Owen and Provan (2011) appears to be quite practical.

As we demonstrate in the rest of this section, it is somewhat involved to apply the BHV model to the space of equidistant trees. A possible (naive) approach could be to simply restrict the BHV space to the set of equidistant trees. Unfortunately, this simple adaptation lacks all properties P1–P3, so the algorithms developed by Owen and Provan (2011) become inapplicable.

Another (less naive) approach is to make the edge lengths dependent and demand that given the lengths of all internal edges and the shortest pendant edge, the lengths of the rest of pendant edges are computed so that the resulting tree is equidistant. This ‘less naive adaptation’ of the BHV space is similar to the ‘bounded BHV’ adaptation, which we consider in the end of this section.

A fundamental issue of all BHV-like spaces is that the subspaces corresponding to different ranked tree topologies have different volumes, which results in complications for statistical analysis of the space, particularly, for introducing prior probability distributions over the space.

In the rest of this section, we model the space of trees by a set of bounded polyhedral complexes indexed by the set of positive reals. We assume here that the reader is familiar with BHV space (Billera, Holmes and Vogtmann 2001). Otherwise, the rest of this section (excluding the next paragraph) can
be skipped, as the following sections of the paper are self-containing.

Since the complexity of presentations is not the matter of this paper, we shall make no distinction between the tree space $\mathcal{T}$ and the model metric space $\mathcal{M}$ used in the parameterisation $p$ of $\mathcal{T}$, in the case when $p$ is a bijection. For instance, when $\mathcal{M}$ has unique geodesics and $p$ is a bijection, we shall simply say that $\mathcal{T}$ has unique geodesics (under this parameterisation). A parameterisation $p$ is called strict if $p$ is a bijection.

Consider the space $\text{BHV}^\circ$, which is the BHV space where pendant branches are ignored. The orthants in $\text{BHV}^\circ$ are unbounded and the space is a polyhedral complex of dimension $n - 2$, where $n$ is the number of taxa. If each axis of each orthant was bounded by the same number, the complex would be cubical and would have identical geometric properties as the original BHV space. We restrict each orthant of the space $\text{BHV}^\circ$ to the set $\{T \mid T \text{ has height at most } H\}$, where $H$ is a fixed real number, and denote thus obtained space by $\text{BHV}^\circ \upharpoonright H$. The space $\text{BHV}^\circ \upharpoonright H$ can be seen as the space of trees of height $H$, because every tree from $\text{BHV}^\circ \upharpoonright H$ can be extended in a unique way to a tree of height $H$ by attaching the pendant edges of appropriate lengths to the places where they were in the original BHV space. Thus, the polyhedral complex $\text{BHV}^\circ \upharpoonright H$ is a strict parameterisation of the space of equidistant trees of height $H$. By varying $H$ over the set of positive reals, we get a strict parameterisation of the tree space as a set of bounded polyhedral complexes indexed by positive reals. We call this space bounded BHV space.

Although the space $\text{BHV}^\circ \upharpoonright H$ is not a cubical complex, it is geometrically and algorithmically similar to the BHV space. Indeed, since in a neighbourhood of the origin the space $\text{BHV}^\circ \upharpoonright H$ is a cubical complex, it possesses efficiently computable unique geodesics in the same way as BHV does. This can be seen by noticing the following. Suppose $\mathcal{C}$ is a cubical complex with unique geodesics such that each cube is given by inequalities $x_i \leq K$. Let $\mathcal{S}$ be a polyhedral complex obtained from $\mathcal{C}$ by replacing the inequalities $x_i \leq K$ by $\sum x_i \leq K$. Then $\mathcal{S}$ has unique geodesics. Furthermore, if geodesics in $\mathcal{C}$ are efficiently\textsuperscript{8} computable then so are geodesics in $\mathcal{S}$. Both of the statements are not hard to prove, but this goes beyond the scope of this paper.

The first and most obvious complication of this parameterisation is the lack of independence between coordinates. The last coordinate, the length of the tree, cannot be smaller than the sum of coordinates corresponding to the internal edges. This results in technicalities in the study of the geometry of

\textsuperscript{8}By ‘efficiently computable’ here and in the rest of the paper we mean computable in (low degree) polynomial (in the number $n$ of taxa) time.
the space, and more problems in implementing algorithms. Another feature of this space is that a change of the length of only one internal branch causes a change of the length of all pendant edges. Hence, if the edge length is interpreted as time, which is the case for many phylogenetic applications, then a change of an older divergence time impacts the times of most recent divergence events for each taxon.

Although these technical issues are not very pleasant to deal with, they can be overcome. There are issues with parameterising the tree space using the bounded BHV that are more fundamental. If, for instance, one wants to bound the lengths of some internal edges using, for example, confidence intervals for those lengths, and perform the analysis under the assumption that these lengths vary only within the intervals, it will result in non-trivial boundary conditions on the lengths of the other internal edges as well as on the last parameter $H$. Another issue, which we mentioned before, is a non-uniform distribution of the volume among different ranked tree topologies.

To overcome these and similar issues is the goal of the further sections of our paper.

We note that although we exclusively consider equidistant trees in this paper, both parameterisations we introduce, $\tau$-space and $t$-space, can be generalised to the class of all time-trees as well as to the even more general class of all sampled ancestor trees (Gavryushkina, Welch and Drummond 2013; Gavryushkina, Welch, Stadler et al. 2014). This generalisation is the subject of a future paper.

2. $\tau$-space

In this section, we model the space of equidistant trees by a cubical complex, which we call $\tau$-space, with efficiently computable unique geodesics and establish several geometric and algorithmic properties of the space.
2.1. Construction of the space

Figure 1: Parameterisation of a tree from $T_5$.

Those readers who are familiar with BHV space will probably not need much extra explanation other than Figures 1 and 2. Figure 1 depicts a tree from 5-dimensional $\tau$-space $T_5$ and shows how the tree is parameterised. Figure 2 depicts one third of 4-dimensional $\tau$-space $T_4$, where each orthant is projected onto the subspace with the first coordinate $\tau_1$ fixed. Although this projected space cannot be embedded into 3-dimensional Euclidean space, it can be visualised by imagining the other two thirds of the space. The figure is also helpful in understanding the fact that the Cartan–Alexandrov–Toponogov axiom (for $k = 0$), which we explain in Definition 4, holds for the space, that is, triangles are thin.
We now give a formal construction of the space to complement the figure. Since one of the main reasons for our interest in equidistant trees is that they allow accurate modelling of evolutionary processes, and in most of those models the height of a node is interpreted as time, we will be using words ‘height’ and ‘time’ interchangeably.

Let $T$ be an equidistant tree on $n$ taxa with times assigned to its nodes. Assuming that the times of all internal nodes are pairwise distinct, we denote the set of such trees by $T_n$. We parameterise the tree $T$ by a pair that consists of the ranked topology of the tree and the differences between the times of the tree’s consecutive nodes. We proceed by defining this parameterisation formally. Let us order the internal nodes of $T$ according to their times: $v_2, \ldots, v_n$. Note that the node $v_n$ must be the root in this case. Denote the difference between the time of node $v_{i+1}$ and the time of node $v_i$ by $\tau_i$ for all $i \in \{2, \ldots, n - 1\}$. We call $\tau_i$ the coordinate of node $v_i$. Since the tree is equidistant, the differences between the time of $v_2$ and the times of external nodes are all the same. Denote this difference by $\tau_1$. The coordinates of the tree $T$ are given by the $n$-tuple $(\text{rt}(T), \bar{\tau})$, where $\text{rt}(T)$ is the ranked topology of tree $T$ and $\bar{\tau}$ is the tuple $(\tau_1, \ldots, \tau_{n-1})$ from $\mathbb{R}_0^{n-1}$ that consists of the
coordinates of the nodes of $T$. By $\mathbb{R}_0^{n-1}$ we denote the $(n - 1)$-dimensional non-negative orthant $\{(r_1, \ldots, r_{n-1}) \mid r_i \in \mathbb{R} \& r_i \geq 0\}$, where $\mathbb{R}$ is the set of reals. Figure 1 depicts an example of $\tau$-parameterisation of a tree from $\mathcal{T}_5$.

Consider now the set $\mathcal{RT}_n$ of all ranked topologies on $n$ taxa such that all internal nodes have different ranks. We recall that there are $\frac{(n-1)! \cdot n!}{2^{n-1}}$ many such topologies (Semple and Steel 2003), and we denote this number by $m$ throughout the paper.

Thus, we have constructed a disjoint union of $m$ $(n - 1)$-dimensional polyhedra $S = \{\text{rt}(T), \vec{\tau} \mid T \in \mathcal{T}_n, \vec{\tau} \in \mathbb{R}_0^{n-1}\}$. Specifically, the polyhedra are orthants indexed by tree topologies. It is clear that the set $\mathcal{T}_n$ is in a bijective correspondence with the interior of $S$. It is also obvious how to establish a bijection between the faces of the polyhedra in $S$ and the set of ranked (multifurcating) tree topologies on $n$ taxa which have at least two internal nodes of the same rank. Indeed, if we consider such a tree, the coordinates $\tau_i$ that are between two nodes of the same rank have to be 0, and the faces of the polyhedra in $S$ are precisely the tuples $(\text{rt}(T), \vec{\tau})$ where some of the coordinates $\tau_i$ are 0. It remains to note that faces for which $\tau_1 = 0$ (may be with some $\tau_2, \ldots, \tau_i$ also 0) will correspond to the trees where the most recent divergence event (may be with second, $\ldots$, $i^{th}$ most recent divergence events) occurs at the origin of time.

We now want to create a polyhedral complex in the obvious way, that is, by gluing the faces that correspond to same ranked (not necessarily fully resolved) tree topologies together. We proceed formally as follows. We define an equivalence relation $\sim$ on the set of faces of polyhedra in $S$. We say that two faces $F$ and $G$ are equivalent, written $F \sim G$, if they correspond to the same ranked tree topology. Now, consider the set $S'$ that consists of the union of the set $S$ and the set of all faces of elements from $S$. The polyhedral complex is then the quotient set $S'/\sim$.

Since trees are in a bijective correspondence with this complex, the parameterisation is strict and we shall refer to the space of trees $\mathcal{T}_n$ as to a polyhedral complex slightly abusing the notation.

Polyhedral complexes where the polyhedra are orthants share the same local geometric properties as cubical complexes. By ‘local properties’ here we mean those that can be observed at a finite distance from the origin, rather than the properties that arise at infinity. Hence, one can always assume that

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9This situation does not make sense in most of biological applications, but considering these faces in our parameterisation is an avoidable technicality, since every facet $F$ in which $\tau_1 = 0$ is the facet of a unique orthant $O_F$.

10We note that we abuse the notation here not only because we make no distinction between the space of trees and the polyhedral complex, but also because the multifurcating trees are present in the complex and absent from the tree space $\mathcal{T}_n$ we initially considered.
all coordinates of the orthants are bounded by a (large enough) constant. This boundary makes the polyhedral complex $T_n$ a cubical complex, which is standard and well-studied object of geometric combinatorics (Bridson and Haefliger 1999; Thomas 2006). This does not imply that unbounded polyhedra are of smaller interest. For example, Gromov’s influential programme on large scale geometry (Gromov 1992) focuses on investigating geometric asymptotic properties at infinity. We make this restriction because for our goals cubical complexes are a more appropriate object to model the space of trees because only local properties are at question. All of the results contained in this paper remain true in the unbounded case.

An interesting example where asymptotic properties of tree space at infinity are treated differently is so-called ‘orange geometry’ (Kim 2000), where polyhedra are ‘glued’ together at infinity. That geometric framework encodes not only phylogenies but also data sets, evolution models, and estimation methods.

From now on we can think of the tree space $T_n$ as of a cubical complex. This in particular implies that the space $T_n$ is a metric space with geodesics. It is easy to construct an example of a cubical complex where geodesics are not unique. Hence, the immediate question is whether geodesics are unique in $\tau$-space $T_n$. They are, and we prove this, but before that let us consider some geometric properties of the space and compare them with those of BHV space.

It is convenient to think of $\tau$-space as a set of points (trees) that freely move within orthants without leaving them as long as all the coordinates $\tau_i$ are strictly positive. This movement results in changes in branch lengths (time between divergence events) but the ranked tree topology remains the same. When one of the $\tau_i$ becomes 0, the point (tree) is on the boundary of one smaller dimension. The point now can either move along the boundary by varying the other $\tau_i$, or it can leave the boundary by increasing the $\tau_i$ that became 0. The boundary corresponds to a facet $F$ and there could be several orthants that share this facet $F$. It is not hard to understand that the possible numbers of orthants which share a common facet are one, two, and three. Indeed, we have seen an example of a polyhedron and its facet that is not a face of any other polyhedron, i.e. when $\tau_1 = 0$. If a facet does not correspond to a multifurcation (see the facet between polyhedra corresponding to trees $T$ and $E$ in Figure 2), there are precisely two orthants that share the facet. If it does (as the other facet of the orthant corresponding

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11By a facet of a polyhedron here and throughout the paper, we mean a face the dimension of which is one smaller than the dimension of the polyhedron, that is, a face of codimension one.
to the tree $T$ in Figure 2), then the number is three.

2.2. Some geometric properties

At first glance it might seem that the BHV and $\tau$-space are very similar$^{12}$. It might even appear that they are the same space. The graph on Figure 3 depicts the link of the origin of $\mathcal{T}_4$ space. The link is similar to that of BHV space on four taxa indeed, but it already suggests several differences that we would like to investigate.

Figure 3: Link of the origin of $\mathcal{T}_4$.

In this subsection, we establish several geometric properties of the two spaces to better understand the differences and similarities between them in order to answer the question of whether the algorithms developed for BHV space (Owen and Provan 2011) are applicable in $\tau$-space. The first property we want to point out is the following. For every tree topology, the

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$^{12}$This subsection can be skipped by those who are not familiar with BHV space, as the rest of the paper does not depend on this subsection.
dimensions of corresponding orthants in \( \text{BHV}_n \) and \( \mathcal{T}_n \) are different. This is because pendant edges add \( n \) to the dimension of the BHV-orthant and add 1 to the dimension of the \( \tau \)-orthant. One might suggest that the spaces \( \text{BHV}_n^\circ \) and \( \mathcal{T}_n^\circ \), which are the corresponding spaces where all pendant edges are omitted, are geometrically similar. They are indeed, they share a number of geometric properties. However, some dissimilarities between them become clear if one attempts to uniformly map one distance to the other. If such a mapping existed, all geometric and algorithmic results for BHV could be directly applied to \( \tau \)-space. We formalise this assertion in the following two propositions.

**Proposition 2.** Spaces \( \text{BHV}_n^\circ \) and \( \mathcal{T}_n^\circ \) are not isometric.

**Proof.** This follows from the fact that isometries preserve angles. Indeed, let us fix a non-caterpillar tree topology and consider the corresponding orthants in \( \text{BHV}_n^\circ \) and \( \mathcal{T}_n^\circ \). We may notice that there are several orthants corresponding to the tree topology in \( \mathcal{T}_n^\circ \) and only one orthant in \( \text{BHV}_n^\circ \) space. One can use an appropriate number of hyperplanes to partition the \( \text{BHV}_n^\circ \)-orthant in a way that every member of the partition corresponds to the trees in precisely one \( \mathcal{T}_n^\circ \)-orthant. Clearly, no embedding between these subspaces preserves angles.

The proof above can intuitively be understood by trying to establish an isometry between the orthants that correspond to the trees \( T \) and \( E \) in Figure 2. The corresponding \( \tau \)- and BHV-subspaces can be drawn as Figure 4 (note that the objects depicted are flat).

![Figure 4: BHV are \( \tau \)-space are not isometric.](image)

One might still wonder in what way the distances are related. It might even appear that the BHV-distance majorates the \( \tau \)-distance, that is, \( d_\tau(T, R) \leq d_{\text{BHV}}(T, R) \) for all trees \( T \) and \( R \). Although it is obvious that the BHV- and the \( \tau \)-coordinates are easily computable from each other\(^{13}\),

\(^{13}\)It is important to note that the claim is about *coordinates* rather than *distances*. Computing the \( \tau \)-distance given the BHV-distance, or vice versa, could be somewhat involved in general.
the following proposition is true.

**Proposition 3.** None of the BHV- and $\tau$-metrics majorates the other.

It is important to note that since the dimensions of $\text{BHV}_n$ and $\tau_n$ are different, we are ignoring the external branches here and considering $\text{BHV}_n^\circ$ and $\tau_n^\circ$.

**Proof.** Consider trees $T$, $R$, and $E$ depicted in Figure 2. We finish the proof of the lemma by setting

1. All sigmas, mus, and taus to 1. In this case:
   \[ d_{\tau}(T, R) = 2 < \sqrt{5} = d_{\text{BHV}}(T, R) \]
   \[ d_{\tau}(T, E) = 2 > \sqrt{2} = d_{\text{BHV}}(T, E) \]

   One might hypothesise that an inequality of the second type can only be obtained in the quadrants that present in $\tau$-space but not in BHV space. Although it is not necessary for the proof, we demonstrate that this hypothesis can be refuted by setting
   2. $\tau_2 = 1$, $\tau_3 = 2$, $\mu_2 = 3$, $\mu_3 = 4$. In this case:
      \[ d_{\tau}(T, R) = \sqrt{40} > 6 = d_{\text{BHV}}(T, R). \]

2.3. Uniqueness and efficiency of geodesics

The geometric property of main interest to us in this paper is the uniqueness of geodesics. We are aimed at efficient procedures for computing several geometric characteristics such as Fréchet mean, standard deviation, and convex hulls, for which the uniqueness of geodesics is important. Although most of the properties of the space, including the uniqueness of geodesics, can be shown directly, we will establish those properties in this section using Gromov’s CAT theory (Gromov 1987). Our main motivation for doing this is that this way is more elegant, to our taste, than the one that uses a direct construction of geodesics.

We recall that a metric space $X$ is called geodesic if every pair of points from $X$ is connected by a shortest path. A geodesic metric space has unique geodesics if the geodesic is unique between every two points from $X$.

**Definition 4.** A geodesic metric space $X$ is said to satisfy Cartan–Alexandrov–Toponogov axiom, or be CAT(0), if the following property holds.

For all triples $x_1, x_2, x_3 \in X$ and all points $y$ on a geodesic from $x_1$ to $x_2$, the inequality $d_X(x_3, y) \leq d_E(x'_3, y')$ holds, where $x'_1, x'_2, x'_3$ are three points on the Euclidean plane such that $d_E(x'_i, x'_j) = d_X(x_i, x_j)$ for all $1 \leq i < j \leq 3$, $y'$ is the point on the segment $[x'_1, x'_2]$ such that $d_E(x'_1, y') = d_X(x_1, y)$, and $d_E$ is the Euclidean distance.
In other words, a metric space $X$ is CAT(0) if no triangle $\Delta$ in $X$ is thicker than a Euclidean triangle $\Delta_E$ of the same size as $\Delta$.

It follows from the definition of a CAT(0) metric space that it has unique geodesics. Indeed, let $X$ be a CAT(0) space and $a, b$ two points from $X$. Consider a point $x$ on a geodesic $\gamma$ from $a$ to $b$ and consider a degenerate Euclidean triangle $a', x', b'$ where $x'$ lies on the segment $[a', b']$ at the same distance from $a'$ as $x$ is from $a$ in $X$. The axiom CAT(0) implies then that $d_X(x, y) \leq d_E(x', x')$, where $y$ is a point on any geodesic from $a$ to $b$ at the same distance from $a$ as $x$. Since $d_E(x', x') = 0$, $d_X(x, y) = 0$ and every geodesic from $a$ to $b$ coincides with $\gamma$ because we have chosen $x$ arbitrarily.

Due to this observation, the fact that $\tau$-space has unique geodesics is derived from the following theorem.

**Theorem 5** (Gromov 1987). A cubical complex $C$ with the intrinsic $l_2$-metric is CAT(0) if and only if $C$ is connected, simply connected, and for all natural numbers $k$, if three $(k + 2)$-cubes of $C$ share a common $k$-cube and pairwise share common different $(k+1)$-cubes, then they are contained in a $(k+3)$-cube of $C$.

Clearly $\tau$-space is a cubical complex which is connected and simply connected (follows from Lemma 7 below). For the last requirement of the theorem we note that the $(k + 2)$-cubes cannot be of the highest possible dimension, otherwise the $(k + 1)$-cubes would result in a cycle of length 3 in the link of the origin of $\tau$-space. Hence, we can assume that there exists a unique\(^\text{14}\) $\tau_i$ such that the first $(k + 2)$-cube $C_1$ has $\tau_i = 0$ and has the rest of $\tau$-coordinates strictly positive. Similarly, the second $(k + 2)$-cube $C_2$ has a unique $\tau_j = 0$ and $C_3$ has $\tau_r = 0$.

Case 0. $i = j = r$. This case results in a cycle of length 3 in the link of the origin of a smaller dimensional $\tau$-space, which is impossible.

Case 1. $i \neq j = r$. Since $C_2$ and $C_3$ share a $(k + 1)$-cube, they both must have a coordinate $\tau_s$ such that $\tau_s > 0$ and if we put $\tau_s = 0$ in both $C_2$ and $C_3$ then the resulting cubes will coincide. We note that $s \neq i$ because the $(k + 1)$-cubes must be pairwise different. Then the only way for $C_1$ and $C_2$ to share a $(k + 1)$-cube is via setting both $\tau_i$ and $\tau_j$ to zero (this is because $i \neq j$). Hence $\tau_s$ is resolved in the same way in $C_1$ and $C_2$. By the same reason, $\tau_s$ is resolved in the same way in $C_1$ and $C_3$. This implies that $C_2$ and $C_3$ coincide, so the case is impossible.

\(^{14}\)The uniqueness is assumed for the sake of clarity. The proof can straightforwardly be modified to the case when there are several non-resolved $\tau$-coordinates.
Case 2. All $i$, $j$, and $r$ are pairwise distinct. Since $C_1$ and $C_2$ share a $(k + 1)$-cube, $\tau_r$ is resolved in the same way in both of these cubes. By a similar reason, $\tau_i$ is resolved in the same way in $C_2$ and $C_3$ and $\tau_j$ in $C_1$ and $C_3$. In this case we construct a $(k + 3)$-cube that contains all $C_1$, $C_2$, and $C_3$ by taking cube $C_1$ and resoling $\tau_i$ in the way it is resolved in $C_2$ and $C_3$.

Thus, we have established the following result.

**Theorem 6.** $\tau$-space has unique geodesics.

This property is fundamental for summarising sets of trees, because the uniqueness of geodesics implies that several geometric centres are unique. For example, such objects as Fréchet mean (Sturm 2002), convex hull, and many other, are well-defined. Furthermore, since the notions of a mean and a variance are well-defined, fundamental theorems of probability theory, such as the Central Limit Theorem, can be applied in tree space.

The immediate question that arises once the existence and uniqueness of the geometric characteristics such as above is established, is the question of effectiveness. Can different types of means, centroids, and hulls be efficiently computed? The answer to this question depends on whether or not geodesics are efficiently computable. Indeed, in most cases non-existence of a polynomial algorithm for computing geodesics implies non-existence of such algorithms for computing various versions of means. Fortunately geodesics are computable in polynomial time in $\tau$-space. A careful consideration of the algorithm in (Owen and Provan 2011) shows that the same algorithm works in $\tau$-space. Indeed, geodesics in $\tau$-space satisfy the Characterisation Theorem (2.3–2.5 in Owen and Provan 2011), so once two $\tau$-trees are converted into an incompatibility graph, (Owen and Provan 2011) gives a polynomial algorithm to find the splits of the set of vertices of the graph corresponding to the geodesic. However, the data structures for the algorithm in $\tau$-space should be different. We have implemented the algorithm in Java and the implementation can be accessed at (Gavryushkin and Drummond 2014) under the GNU General Public Licence. The novel data structures necessary for this implementation are formally introduced later in this paper. The running time of the implementation is similar to that of (Owen and Provan 2011).

Thus, we suggest that $\tau$-space serves as a tool for statistical analysis of sets of trees. Particularly, for computing the summary tree of a posterior sample obtained using, for example, MCMC.
3. t-space

A natural question one could ask is why we take the time differences instead of actual times as coordinates of trees in the orthants of $\tau$-space. One of the reasons for this is that $\tau$-coordinates are independent as opposed to $t$-coordinates—the times of the nodes. The independence of coordinates is a useful property of parameterisations because it avoids constant checking of dependency conditions while performing the analysis (both geometric and algorithmic) of the space. We have seen in previous sections an example of a parameterisation where coordinates are dependent in a way which causes complications. Another reason is that the $\tau$-parameterisation is used in several phylogenetic models e.g. in coalescent theory.

In some cases boundary conditions are unavoidable. For example, some boundary conditions present implicitly in $\tau$-space—we require the coordinates to be positive and bound the first coordinate to the set of topologies of trees. The boundary condition that makes orthants cubes is explicit. Since these conditions are easily satisfiable and checkable, they do not cause any serious complication as we have seen in Section 2. Furthermore, as absolute divergence times are often the object of interest, the parameterisation of trees using the times of their nodes is natural for several phylogenetic modes, e.g. birth-death models (Kendall 1948). As birth-death priors are one of the main classes of priors used in Bayesian inference, we address this parameterisation in more detail.

The purpose of this section is twofold. First, as we mentioned, we would like to study geometric and efficiency properties of one of the prominent parameterisations in evolutionary biology. Secondly, we demonstrate how radically these properties can change after a seemingly negligible change in parameterisation. Namely, converting $\tau$-coordinates to their initial sums, that is, to the times of divergence events, makes fundamental results from combinatorial geometry such as Gromov’s theorem used to prove Theorem 6 inapplicable, along with the algorithmic results from (Owen and Provan 2011) and (Owen 2011).

We note that Ardila and Klivans (2006) considered branch lengths and a tree height to parameterise the space of ultrametric trees and prove that equidistant trees are in one-to-one correspondence with the Bergman fans of complete graphs (for details see Ardila and Klivans 2006). As explained in the introduction, this parameterisation is not convenient for our purposes. However, the results in (Ardila and Klivans 2006) imply that t-space is in one-to-one correspondence with the Bergman fans of complete graphs, so our results on t-space are applicable to the corresponding fans.
We proceed with a formal introduction of the space, which we call the t-space. Let us consider an equidistant tree $T$ with ranked topology $rt(T)$ with no pair of nodes of the same rank. For each node $v_i$ from $T$, let $t_i$ be the distance from $v_i$ to the nearest taxon. In this way, we assign times to all nodes of $T$, with all taxa being of time 0. Let us order all internal vertices of $T$ according to their times: $v_1, \ldots, v_{n-1}$ (the ordering is the same as the ordering according to their ranks). Then the coordinates of the tree $T$ in t-space is a tuple $(rt(T), t_1, \ldots, t_{n-1})$.

We note that if we vary the times of the nodes of $T$ while keeping the ranked topology preserved, we get a simplex $\{(t_1, \ldots, t_{n-1}) \mid 0 \leq t_1 \leq \ldots \leq t_{n-1} \leq H\}$, where the upper bound on the height of the tree $H$ is introduced by the same reason it was introduced in $\tau$-space. Figure 5 depicts one such simplex.

![Figure 5: One simplex of t-space.](image)

We create a simplicial complex out of $\frac{(n-1)! \cdot n!}{2^{n-1}}$ such simplices corresponding to different ranked topologies on $n$ taxa in a similar way the complexes are created in BHV and $\tau$-spaces, namely, we identify faces of simplices corresponding to same tree topology. The metric is defined in the same way as in $\tau$-space to be the standard piecewise Euclidean distance. The first substantial difference is that the edge of the complex that is shared by all the simplices is not an axes, it is rather the line $t_1 = \ldots = t_{n-1}$. Furthermore, the faces are defined by some of the coordinates being equal, $t_i = t_k$, rather
than some of the coordinates being 0. We denote the $t$-space on $n$ taxa by $T_n$.

Figure 6 depicts space $T_3$ in full.

In this figure, three coloured triangles of the simplicial complex correspond to the three depicted topologies. The triangles share a line that corresponds to the unresolved tree on three taxa. The upper bound of the triangles is the artificial bound $H$.

The following Figure 7 depicts a part of the $t$-space $T_4$. Unlike Figure 2, we do not project the simplices onto a 2-dimensional subspace and draw them as 3-dimensional pyramids. Three such pyramids are depicted in Figure 7 in white, blue, and grey. The white pyramid shares a facet with both grey and blue pyramids. The grey and blue pyramids share the edge $t_1 = t_2 = t_3$ of the complex only. This is one-sixth of the space $T_4$ corresponding to the topologies depicted.
The following lemma is an important property that connects BHV space, \( \tau \)-space, and t-space. This lemma has already been used to prove that \( \tau \)-space is CAT(0).

**Lemma 7.** BHV space, \( \tau \)-space, and t-space are pairwise homeomorphic.

**Proof.** The homeomorphisms are induced by parameterisations \( p_{\text{BHV}} \), \( p_{\tau} \), and \( p_{t} \) used to construct the corresponding spaces. \( \square \)

In particular this lemma implies that both \( \tau \)-space and t-space are connected and simply connected.

Our next step is naturally to ask whether t-space has unique geodesics. This question cannot be answered in the same way as it is done for BHV and \( \tau \)-space using Gromov’s characterisation of CAT(0) cubical complexes, because t-space is not a cubical complex. It is reasonable to expect that there exists a result similar to Gromov’s theorem for simplicial complexes. There is one indeed. A simplicial complex is called \( k \)-large if every cycle in the link of every vertex, such that no two consecutive edges of the cycle are contained in a 2-simplex of the complex, has length at least \( k \). As noted in (Januszkiewicz and Świątkowski 2006), although no combinatorial formulation of the CAT(0) property of the standard piecewise Euclidean metric on a simplicial complex is known, the following theorem holds.

**Theorem 8** (Januszkiewicz and Świątkowski 2006). If \( k \geq \frac{7\pi\sqrt{2}}{2} n + 2 \), then every connected simply connected \( k \)-large simplicial complex of dimension\(^{15} \)

\(^{15}\)By dimension here the simplicial dimension of a simplicial complex is meant, that is, the greatest dimension of a simplex in the complex. For example, the simplicial dimension of the t-space on \( n \)-taxa is \( n - 1 \).
at most $n$ is $\text{CAT}(0)$ with respect to standard piecewise Euclidean metric.

It is not hard to see that t-space $\mathbb{T}_n$ is 6-large and not 7-large when $n \geq 4$, hence the theorem above is not applicable. Simplicial complexes that are connected, simply connected, and 6-large are called systolic. Systolic complexes have extensively been studied (Zimmer, Farb and Fisher 2011) and it was shown that in dimension\textsuperscript{15} two, a simplicial complex is systolic exactly when the standard piecewise Euclidean metric is $\text{CAT}(0)$, while in higher dimensions being systolic is neither stronger nor weaker than the standard piecewise Euclidean metric being $\text{CAT}(0)$. Hence for t-space, being systolic does not necessarily imply having unique geodesics.

However, t-space possesses unique geodesics, as we show below. This fact makes t-space an example of a non-trivial simplicial complex which is $\text{CAT}(0)$. Indeed, t-space is an example of a $\text{CAT}(0)$ simplicial complex for which the $\text{CAT}(0)$ axiom cannot be established using Theorem 8.

**Theorem 9.** t-space has unique geodesics.

**Proof.** We start with the following lemma, which is an important ingredient of the proof.

**Lemma 10.** Let $S$ be a simplex in $\mathbb{T}_n$ and $\angle$ be an angle between a pair of facets in $S$. Then $\angle \leq \pi/3$.

**Proof.** First scale the simplex $S$ so that the height of the trees corresponding to $S$ is bounded by 1. Then the set of vertices $V$ of simplex $S$ is

$$\{(0, \ldots, 0, 1, \ldots, 1) \mid i \leq n\}.$$  

The set of facets of simplex $S$ is then given by the set of all $(n-2)$-element subsets of $V$. Note that there are exactly two facets of $S$ which are not shared by any other simplex in $\mathbb{T}_n$. Indeed, every facet of every simplex in $\mathbb{T}_n$ contains both points $(0, \ldots, 0)$ and $(1, \ldots, 1)$. Hence the shared facets of $S$ are precisely those that contain both $(0, \ldots, 0)$ and $(1, \ldots, 1)$. For example, the grey and the red facets of the simplex on Figure 5 are not shared by any other simplex, while the blue and the invisible facets are shared with other simplices.

For every pair of shared facets of $S$, we now find the angle between the facets. To do so we first need to find the normal vectors of all shared facets. Every shared facet $F_i$, $0 \leq i \leq n-2$, of $S$ can be represented as an $(n-1) \times n$
matrix $j$-th row of which is
\[
\begin{cases}
(1, \ldots, 1, 0, \ldots, 0) & \text{if } 0 \leq j \leq i, \\
(1, \ldots, 1, 0, \ldots, 0) & \text{if } i + 1 \leq j \leq n - 2.
\end{cases}
\]

Normal vectors $f_i$ of facet $F_i$ are then given by the null spaces of these matrices. For every $i$ such that $0 \leq i \leq n - 2$, we fix one such vector $f_i$ to be $(0, \ldots, 0, (-1)^i, (-1)^{i+1}, 0, \ldots, 0)$.

Since the inner product of these vectors is either 0 or 1, the smallest possible angle between the facets is $\pi/3$, which proves the lemma.

We now note the following property. For every positive real number $\varepsilon$, the $\varepsilon$-neighbourhood of the origin of $T_n$—point $(0, \ldots, 0)$ in terms of the proof of previous lemma—contains a simplicial complex similar to $T_n$. This property follows by scaling $T_n$ with small enough scaling factor. Hence, to establish the claim of the theorem it is enough to show that the space is locally CAT(0). To prove this, we apply the following result:

**Theorem 11** (Gromov 1987, see Bridson and Haefliger 1999, 5.2 on p. 206).

A finite simplicial complex is locally CAT(0) if and only if the link of every vertex of the complex is a CAT(1) space.

Hence, to finish the proof of Theorem 9, we need to show that the link of every vertex of $T_n$ is a CAT(1) complex. By Theorem 5.4(7) in (Bridson and Haefliger 1999, p. 206), it is enough to show that $T_n$ contains no isometrically embedded circles of length less than $2\pi$. That means the following. Let $C$ be a geodesic curve in (the link of a vertex of) $T_n$ of length $\ell$ which is isometric to a Euclidean circle $C_E$. If we scale the space so that $C_E$ is a unit circle then $\ell \geq 2\pi$.

This last property follows from Lemma 10 for space $T_n$. Let $T_1, \ldots, T_k$ be completely resolved ranked tree topologies with the property that if $C$ intersects a simplex corresponding to tree topology $T$ then there is an $i$ such that $T = T_i$. We claim that $k \geq 6$. Indeed, $k$ is bounded from below by the length of a shortest cycle in the link of the origin of $T_n$, and we have seen above that the length of such a cycle is 6. The length $\ell$ of $C$ satisfies $\ell \geq k \angle$ where $\angle$ is the smallest angle between facets of the simplex corresponding to a $T_i$. It follows from Lemma 10 that $\ell \geq k \pi/3$ and since $k \geq 6$, we have $\ell \geq 2\pi$ as desired.
The change in the parameterisation of trees results not only in the question of uniqueness becoming more complicated. What is more important is that the algorithms used for computing geodesics in BHV and \( \tau \)-space cannot directly be applied in \( t \)-space. Moreover, their existence has to be questioned. Hence we propose the following question, on which we make some progress below, but do not obtain a complete answer.

**Problem 1.** What is the complexity of computing geodesics in \( t \)-space?

First we would like to develop some intuition of why \( t \)-space is so different from both BHV and \( \tau \)-space. The key property for this difference is that the cone path is rarely a geodesic in \( t \)-space. Indeed, in both BHV and \( \tau \)-space the position of two cubes can result in a cone path being the geodesic between any pair of trees from those cubes. Particularly, the (uniform) measure of the set of pairs of trees between which the cone path is a geodesic is positive. For example, if two trees \( T \) and \( R \) have topologies with no compatible splits, then the geodesic between \( T \) and \( R \) is a cone path (Billera, Holmes and Vogtmann 2001). \( t \)-space does not have this property. It will follow from observations below that the set of pairs of trees between which the geodesic is a cone path in \( t \)-space has measure \( 0 \). Let us illustrate this effect by the following example. Consider trees \( T \) and \( R \) depicted in Figure 8. Since the trees do not have compatible splits, the geodesic is a cone path in both BHV and \( \tau \)-space. It is not hard to see that the shortest cone path in \( t \)-space passes through the star-tree of height 6 and has length \( 2\sqrt{38} > 12.3 \), while the path that goes through \(((1, 2) : 4, 3, 4) : 8, ((1, 3, 2) : 6, 4) : 8, \) and \(((1, 3) : 4, 2, 4) : 7 has length \( \sqrt{10} + \sqrt{8} + \sqrt{6} + \sqrt{14} < 12.2 \) and is hence shorter than any cone path.

This example demonstrates another important property that distinguish \( \tau \)-space and \( t \)-space. Every tree on the geodesic between two trees in \( \tau \)-space contains only splits that present in the origin tree or in the destination tree (or both). Not so in \( t \)-space. Split \((123 \mid 4)\) does not present in either tree on Figure 8 but present in an intermediate tree on the \( t \)-geodesic.
We now develop a formalism that is convenient for the study of computational content of \( t \)-space. This formalism can be used for \( \tau \)-space as well and is actually the data structure that we use in our implementation of geodesic algorithms for \( \tau \)-space (Gavryushkin and Drummond 2014). The formalism is motivated by and consistent with the treatment of ranked tree topologies in (Semple and Steel 2003).

By a partition with attached time-coordinate, we mean an object of the form \((N_1 \mid \ldots \mid N_q): t\), where \(N_1 \mid \ldots \mid N_q\) is a partition of taxa that can be obtained by cutting the tree along the line obtained by fixing the time-coordinate, and \(t\) is the least value of the time-coordinate that produces this partition. For example, the left-hand side tree on Figure 8 is defined by the set of partitions

\[\{(12 \mid 3 \mid 4): 1, \ (12 \mid 34): 8, \ (1234): 9\},\]

while the right-hand side tree—by

\[\{(13 \mid 2 \mid 4): 1, \ (13 \mid 24): 8, \ (1234): 9\}.
\]

Removing one or more partitions from a set of partitions that defines a completely resolved tree gives rise to a non-resolved tree or a tree with two or more internal nodes of the same rank. For example, if we remove partition \((12 \mid 3 \mid 4)\) from the left-hand side tree on Figure 8 then we get the tree \(((1, 2), (3, 4))\) of height 9 with both internal nodes being of height 8.

We note here that as we consider only trees with all taxa being at time 0, the partition \((1 \mid 2 \mid \ldots \mid n): 0\) is assumed to be (invisibly) present everywhere\(^\text{16}\). Clearly, a tree is unambiguously defined by its set of partitions with attached time-coordinates, and a set of partitions defines a tree if and only if

\(^{16}\)This assumption cannot be made, for example, in the general setting of time-trees or even more general setting of sampled ancestor trees (Gavryushkina, Welch and Drummond 2013; Gavryushkina, Welch, Stadler et al. 2014).
one member of every pair of partitions from the set refines the other and the
time-coordinates of the partitions are monotonic under those refinements.

It can be shown in the same way as in (Owen 2011) that the coordinates
in t-space change at a fixed rate along geodesics. This justifies the following
definition.

We assume that trees $T$ and $R$ are completely resolved and have all in-
ternal nodes of different ranks, that is, neither of them has t-coordinates $t_i$
and $t_{i+1}$ such that $t_i = t_{i+1}$. We say that the geodesic $\gamma$ between trees $T$
and $R$ is \textit{computable (in polynomial time)} if (a polynomial and) an algorithm
exists that given the t-coordinates of trees $T$ and $R$, outputs (after a number
of steps bounded by the polynomial of $n$) a sequence of sets of partitions
$A_0, \ldots, A_k$ with time-coordinates attached to every partition such that

(1) The set of partitions $A_0$ along with the attached time-coordinates defines
tree $T$.

(2) The set of partitions $A_k$ along with the attached time-coordinates defines
tree $R$.

Let $S_0, \ldots, S_k$ be all the simplices the geodesic $\gamma$ traverses, ordered in
the order they are traversed. Particularly, $S_0$ contains $T$ and $S_k$ contains
$R$.

(3) For every $i$, the pair of sets $A_i, A_{i+1}$ along with the attached time-
coordinates define the trees where geodesic $\gamma$ enters and exits simplex
$S_i$, respectively.

Since tree $T$ is completely resolved, the number of elements of $A_0$ is $n-1$.
In terms of simplices, the number $n - 1 - |A_i|$, where $|A_i|$ is the number of
elements in $A_i$, is the codimension of the face of simplex $S_i$. In terms of trees,
this number is the number of multifurcations plus the number of non-resolved
ranks of internal nodes of the tree corresponding to $S_i$.

Note that the properties above imply that all sets $A_i$ are pairwise different,
all time-coordinates attached to the partitions from the same set are pairwise
different, and the time coordinates attached to the same partition in different
sets may or may not be different. Clearly, every geodesic is unambiguously
defined by a sequence of sets of partition satisfying these properties.

We say that the geodesic $\gamma$ is an \textit{NNI-path}\footnote{The term “NNI-path” is used here because every change of topology along such a path is an NNI-move.} if $n - 1 - |A_i| = 1$ for all $i$ such
that $0 < i < k$. The following proposition, which is interesting on its own,
explains several properties of t-space, particularly, that if we draw a pair of
trees uniformly at random then the probability of the geodesic between them being a cone path is 0.

**Proposition 12.** Let $T$ and $R$ be two trees and $\gamma$ the geodesic in t-space between them. Then there exists a tree $T'$ such that $T'$ and the geodesic $\gamma'$ between $T'$ and $R$ satisfy

1. Trees $T$ and $T'$ have the same ranked topology.
2. Geodesic $\gamma'$ is an NNI-path.
3. Tree $T'$ is computable in polynomial time from $T$ and $\gamma$.
4. The sets of partitions that define geodesic $\gamma'$ is computable in polynomial time from $T$ and $\gamma$.

**Proof.** Let $A_0, \ldots, A_k$ be the sequence of sets of partitions that define the geodesic $\gamma$ from $T$ to $R$. We adjust the time-coordinates of $T$ to obtain $T'$ with desired properties. Let $s$ be the least natural number such that $n - 1 - |A_s| > 1$. If such an $s$ does not exist, there is nothing to prove because $\gamma$ is an NNI-path.

Suppose first that $n - 1 - |A_s| = 2$. This implies that $|A_{s-1} \setminus A_s| = 2$. Denote the set $A_{s-1} \setminus A_s$ by $\{q_1, q_2\}$. We can assume that the time-coordinate attached to $q_1$ changes from $t_0$ to $t_1$ when the geodesic traverses the simplex between the trees corresponding to $A_{s-1}$ and $A_s$. Similarly, the time-coordinate attached to $q_2$ changes from $t_0$ to $t_2$. Since the time coordinate changes at a constant rate along the geodesic and the distance function is a continuous function, it is possible to find a positive real number $\varepsilon$ such that if we vary the time-coordinate $t_0$ (or $t_2$) by $\varepsilon$, then there exists a tree $T_1$ with the same ranked topology as $T$ satisfying the following property.

The geodesic from $T_1$ to $R$ has all partitions but those in $A_s$ the same as $\gamma$ and has two sets of partitions $A'_s$ and $A''_s$ instead of $A_s$ such that $n - 1 - |A'_s| = n - 1 - |A''_s| = 1$.

To prove this property, we not the following. Since $s$ is the least number satisfying $n - 1 - |A_s| > 1$, we have that $n - 1 - |A_0| = 0$ and $n - 1 - |A_i| = 1$ for all $i$ such that $0 < i < s$. Hence there exists $\delta$ such that for every $i < s$, the $\delta$-neighbourhood of the tree corresponding to $A_i$ intersects at most one facet of the simplex and intersects no facets if $i = 0$. This last requirement follows because $T$ is a completely resolved tree with no nodes of the same rank. There exists an $\varepsilon$ such that varying $t_0$ (or $t_2$) leaves the geodesic within those $\delta$-neighbourhoods. To finish the proof of the property above, it remains
to note that an arbitrary small change in $t^0_1$ (or $t^0_2$) results in the replacement of $A_s$ by $A'_s$ and $A''_s$ with the desired property.

Informally, this means that we can adjust the time-coordinate of the partitions in $T$ so that instead of passing the face corresponding to $A_s$ of codimension 2, the geodesic passes first the face $A'_s$ of codimension 1 and then another face $A''_s$ of one smaller codimension than $A_s$. This happens because the change of the coordinate $t^0_1$ (or $t^0_2$) results in the geodesic developing faster in the direction of $t^0_1$ (or $t^0_2$), so the geodesic first reaches the face corresponding to $A'_s$ and then the one corresponding to $A''_s$ rather than both $A'_s$ and $A''_s$ simultaneously as geodesic $\gamma$ does.

If $n - 1 - |A_s| > 2$, we repeat the construction above until the set $A_s$ is replaced by several sets corresponding to co-dimension 1 facets.

Clearly, this algorithm of computing $T'$ is polynomially equivalent to the maximum of complexities of $T$ and $\gamma$. It remains to note that on our way of adjusting the time coordinates of tree $T$, we computed all the partitions that define the geodesic $\gamma'$.

We note that it follows from the proof of this proposition that the measure of the set $U$ of pairs of trees with the geodesic being a cone path is zero. Indeed, if we fix a tree $T$ then the set of trees $R$ for which the geodesic from $T$ to $R$ is a cone path has measure 0, according to the proof of the proposition. That is, the measure of the set $\{R \mid (T, R) \in U\}$ is 0 for all $T$. Then it follows from Fubini’s theorem that the (product) measure of the set $U$ is 0.

Thus geodesics in t-space follow NNI-paths almost always. However, they do not necessarily follow shortest NNI-paths. Indeed, it is possible to show that any tree on the geodesic between two caterpillar trees in t-space is a caterpillar tree. This property is violated in NNI space: consider two caterpillar trees $(\ldots(1, 2), 3, \ldots, 10)$ and $(\ldots(1, 4), 5, \ldots, 9, 2, 3, 10)$. It is not hard to see that no tree, apart from these two, is a caterpillar tree on an NNI-geodesic between them. Furthermore, if two trees $T$ and $R$ share a partition of taxa, the partition is shared by all trees along the geodesic between $T$ and $R$ in t-space. However, it is not the case in NNI space. These two properties suggest that t-space might be algorithmically simpler than NNI.

4. Conclusion and further directions

We have considered two standard parameterisations of the space of ultrametric phylogenetic trees: (1) using lengths of coalescent intervals and (2) using
times of divergence events. By considering suitable polyhedral complexes, we have found two possible representations of the space of trees called \( \tau \)-space and \( t \)-space respectively. Despite their similarity, the two parameterisations have significantly different geometric and algorithmic properties. Although it required quite different geometric approaches, we proved that shortest paths are unique in both \( \tau \)- and \( t \)-space. We also proved that shortest paths are efficiently computable in \( \tau \)-space. We have implemented the algorithm for computing exact shortest paths in Java. We also implemented the algorithms for efficiently approximating Fréchet means, standard variances, and some other geometric and statistical characteristics of finite samples of trees. Although the algorithmic complexity of \( t \)-space remains unknown, the space has several properties that are desirable for statistical analysis of tree space. For instance, we proved that the paths that traverse a star tree are often shortest in \( \tau \)-space and are almost never shortest in \( t \)-space. This feature of \( t \)-space is a desirable property for phylogenetic applications, and particularly for summarising posterior samples by a point estimate. Indeed, one of the unpleasant features of BHV space is that parts of the summary tree are often close to the star-tree, when incompatible subtrees are supported by the posterior. As we have demonstrated in this paper, this feature is a consequence of a fundamental geometric property of the space. The property is that the measure (volume) of the set of pairs of trees for which the shortest path traverses a star-tree is positive in \( \tau \) space (and in BHV space (Billera, Holmes and Vogtmann 2001)), while in \( t \)-space the measure of this set is zero. Thus we expect summary trees produced using \( t \)-space to be more informative and realistic.

Although all results in this paper and presented for ultrametric trees, they can straightforwardly be extended to the set of all time trees, as well as to the set of all sampled ancestor trees.

An obvious direction of further research is to test our algorithms on simulated and real data sets, compare them with known algorithms, and suggest what extra formal properties of a parameterisation of the tree space are desirable. As is suggested in our work, there are other possible ways that equidistant tree space can be parameterised. We have considered two obvious parameterisations and established that they are already quite different. One can certainly come up with many other ways to parameterise the space. The question arises:

**Problem 2.** Is there, in some sense, a single optimal parameterisation of the tree space? If not, what is the class of acceptable parameterisations?

Our paper suggests a number of directions for further theoretical investigations. An important statistical question is
**Problem 3.** What parameterisation should be used for coalescent models? Birth-death models? Must the parameterisations used for these two types of models be different?

The first step towards an answer for this question is obviously to consider the coalescent and the birth-death priors in $\tau$- and $t$-spaces. Are these priors continuous in these spaces? Can the distance between two trees be made a (simple) function of their prior probabilities?

Although much work has been done to investigate CAT(0) simplicial complexes, no satisfactory characterisation of the complexes is known (Zimmer, Farb and Fisher 2011). Further research is needed with an eye towards effectiveness properties. The problem in general is expected to be hard because even constructing non-trivial examples of CAT(0) simplicial complexes requires significant effort and only a few such examples are known (Zimmer, Farb and Fisher 2011). In this paper, we have provided such an example—the $t$-space. Hence the following question, which we ask for $t$-space, is also important for CAT(0) simplicial complexes in general.

**Problem 4.** Is there an efficient (in any sense) algorithm for computing shortest paths between trees in $t$-space? If yes, how large a data set can be handled using the algorithm?

As we have established in this paper, the measure (volume) of the set of pairs of trees between which the shortest path traverses a star-tree is 0 in $t$-space and is positive in $\tau$-space. This measure is positive in BHV space (Billera, Holmes and Vogtmann 2001) too. Hence the obvious question to understand the geometry of the space is to find this measure. More precisely:

**Problem 5.** Let $\mu_n$ be the uniform measure of the set of pairs of trees on $n$ taxa between which the geodesic is a cone path\textsuperscript{18}. What is the value of $\mu_n$ for BHV space? For $\tau$-space? Is the sequence $\{\mu_n\}_{n \in \omega}$ convergent? If so, what is the limit $\lim_{n \to \infty} \mu_n$? What is the meaning of this limit?

Clearly, $\mu_3 = 1$ in both BHV and $\tau$-space. To find $\mu_4$ is an entertaining exercise.

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\textsuperscript{18}We denoted this set by $U$ in the paper. Also, we assume that the measure is a probability measure, that is, the measure of the whole space is equal to 1, and that the measures of all cubes are pairwise equal.
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