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Arboreal networks and ultrametrics

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Ultrametrics are an important class of distances used in applications such as phylogenetics, clustering and classification theory. Ultrametrics are distances that can be represented by an edge-weighted rooted tree so that all of the distances in the tree from the root to any leaf of the tree are equal. In this paper, we introduce a generalization of ultrametrics called *arboreal ultrametrics* which have applications in phylogenetics and also arise in the theory of distance-hereditary graphs. These are partial distances that can be represented by an *ultrametric arboreal network*, that is, an edge-weighted rooted network whose underlying graph is a tree. As with ultrametrics, all of the distances in an ultrametric arboreal network from any root to any leaf below it are equal but, in contrast, the network may have more than one root. In our two main results we characterize when a partial distance is an arboreal ultrametric as well as proving that, somewhat surprisingly, given any unrooted edge-weighted phylogenetic tree there is a necessarily unique way to insert roots into this tree so as to obtain an arboreal ultrametric.

Keywords: Ultrametric, symbolic ultrametric, phylogenetic tree, ultrametric network, arboreal ultrametric

1 Introduction

An *arboreal network on* X is a digraph whose underlying graph is an undirected or *unrooted* phylogenetic tree, and whose leaf set is X. Note that such a network can have more than one root, and that if the network has precisely one root then it is commonly known as a *rooted (phylogenetic) tree* Semple and Steel (2003). Arboreal networks have applications in evolutionary biology, where the leaf set X usually corresponds to a set of species and the network represents historical evolutionary relationships between the species Huber et al. (2022). Indeed, there has been growing interest in using networks with multiple roots to represent evolutionary histories since they can, for example, be used to model evolutionary processes such as introgression Scholz et al. (2019) or gene fusion Coleman et al. (2015); Haggerty et al. (2014) where the assumption of a single root can be misleading.

Despite this interest, the mathematical theory surrounding arboreal networks is still in its infancy. This holds in particular with regards to our understanding of arc-weighted arboreal networks, that is, arboreal networks N in which every arc in N is assigned a non-negative real number called the *weight* of that arc. An example of such a network is depicted in Figure 1(i) where $X = \{a, \ldots, f\}$. By taking as distance $\tilde{D}(x, y)$ between any two distinct leaves $x, y \in X$ to be the length of the shortest path joining x and y in

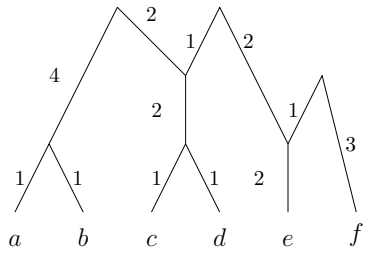
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the underlying tree of an arboreal network N on X in case they are below the same root of N and setting that distance to ∞ in case they are not.

Clearly an arboreal network induces a special kind of distance on X called a *partial distance* – see Figure 1(ii) for an example. Formally, such a distance is a symmetric map $\tilde{D} : X \times X \to \mathbb{R}_{>0} \cup \{\infty\}$. In phylogenetics, partial distances arise when the distance between two taxa is considered irrelevant, or non-existent. In the former case (irrelevance), one can consider, given a distance D on X and a threshold $\tau > 0$, the partial distance D_τ on X defined, for all $x, y \in X$ distinct, as $D_\tau(x, y) = D(x, y)$ if $D(x, y) \leq \tau$, and $D_\tau(x, y) = \infty$ otherwise. In the latter case (non-existence), one can assign distance ∞ between two taxa that are identified as being unrelated, for example in case of overlapping sets of taxa. We emphasize that, in this context, the equality $\tilde{D}(x, y) = \infty$ does not necessarily indicate that the distance between x and y is unknown. Indeed, $\tilde{D}(x, y) = \infty$ is an information about the lack of relation between x and y, and thus, shall not be treated as missing information. This is in contrast to distances which have genuinely missing entries which have been studied in e.g. Huang and Knowles (2016); Kettleborough et al. (2015).

In some cases the partial distances between the elements on X induced by an arc-weighted arboreal network N on X are such that for any root ρ in N all paths from ρ to any leaf in X have the same length, where the length of a path is simply the sum of the weights of the arcs in the path (see e.g. Figure 1(i)). Arc-weighted arboreal networks that enjoy this property are in the center of this paper. To emphasise this, we call such a network an *ultrametric arboreal network (on X)* and remark in passing that in case the network has a single root, N is also called an *equidistant weighted* or *ultrametric* tree. Ultrametric *trees* are commonly used in evolutionary biology to represent the evolution of taxa where the length of any path from the root to a leaf is assumed to be proportional to the time that has passed for the root species to evolve to the leaf species (Felsenstein, 2004, Chapter 9).



(i)

	a	b	c	d	e	f
a	0	2	10	10	∞	∞
b	2	0	10	10	∞	∞
c	10	10	0	2	8	∞
d	10	10	2	0	8	∞
e	∞	∞	8	8	0	6
f	∞	∞	∞	∞	6	0

(ii)

Fig. 1: (i) An ultrametric arboreal network with leaf set $X = \{a, b, \ldots, f\}$ and (ii) its associated partial distance, where all arcs are directed downwards towards the leaves in X. For example, the distance from a to d is 10, which is length of the shortest path from a to d that goes via the root that lies above them both, whereas the distance from a to f is ∞ since there is no root that lies above a and f.

We define an *arboreal ultrametric on X* to be a partial distance on X if it can be obtained as the partial

distance underlying some ultrametric arboreal network. Note that the arboreal ultrametric $\tilde{D}$ induced by an ultrametric arboreal network N is an ultrametric if and only if N has a single root. In addition, as we shall see in Section 4, arboreal ultrametrics are special examples of *symbolic arboreal maps* introduced in Huber et al. (2024). These maps have close connections with the well-known classes of distance-hereditary graphs Scholz (2025) and Ptolemaic graphs Huber et al. (2024). As we shall see in Theorem 4.1, the latter are precisely the graphs that arise from considering pairs of leaves in arboreal networks that have a common ancestor.

We now give an overview of the main results in this paper. One strategy to build ultrametric phylogenetic trees is as follows. First, construct an unrooted, edge-weighted phylogenetic tree and then, after this, try to insert a root into the tree so as to create an ultrametric tree (or one close to being ultrametric) using, for example, methods such as the *mid-point method* or the *Farris transform* (see e.g. Dress et al. (2007); Kinene et al. (2016)). One issue with this strategy is that it is not always possible to find such a root. In our first main result we shall show that, in contrast, given any phylogenetic tree it is possible to insert roots into the tree so as to create an ultrametric arboreal network. Moreover, we show that the choice of where to insert the roots is necessarily unique (see Proposition 3.3 and Theorem 3.5).

We then turn our attention to characterizing when a partial distance is an arboreal ultrametric. It is well-known (see e.g. (Semple and Steel, 2003, Chapter 7)) that a distance D on a set X is an ultrametric if and only if it satisfies the following strengthening of the metric triangle equality

$$D(x, y) \leq \max\{D(x, z), D(y, z)\} \text{ for all distinct } x, y, z \in X.$$

In our second main result, we shall give a similar characterization for characterizing arboreal ultrametrics. To decide whether or not a partial distance $\tilde{D}$ on X is an arboreal ultrametric, it is important to handle the pairs in X for which $\tilde{D}$ is infinity. To do this, we consider the graph $G_{\tilde{D}}$ that has vertex set X in which two distinct vertices x and y are joined by an edge if $\tilde{D}(x, y) < \infty$. We then prove in Theorem 4.3 that a partial distance $\tilde{D}$ is an arboreal ultrametric if and only if (i) $G_{\tilde{D}}$ is a connected, chordal graph, (ii) $\tilde{D}$ satisfies the above 3-point ultrametric condition in case $\tilde{D}$ is defined for all pairs in the triple, and (iii) $\tilde{D}$ satisfies an additional 4-point condition. The 4-point condition is given in full in Theorem 4.3.

The rest of this paper is organized as follows. In Section 2, we present some preliminaries. Then in Section 3 we prove the aforementioned result about rooting trees to obtain ultrametric arboreal networks (Theorem 3.5). In Section 4 we present our characterization for arboreal ultrametrics (Theorem 4.3), before concluding with a brief discussion of some future directions in Section 5.

2 Preliminaries

We shall assume throughout the paper that X is a finite set for which $|X| \geq 2$ holds.

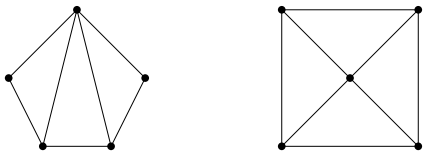
Graphs

A graph G is an ordered pair (V, E), where $V = V(G)$ is a finite set of elements, called *vertices* (of G), and $E = E(G)$ is a set of pairs of distinct elements of V. If the pairs in E are not ordered, we call them *edges*, and we say that G is *undirected*. We denote an edge between two vertices u and v by $\{u, v\}$. If the pairs in E are ordered, we call them *arcs*, and we say that G is *directed*. For two vertices u and v of V we denote the arc from u to v by (u, v). For an arc (u, v) of a directed graph G, we say that u is a *parent* of v, and v is a *child* of u.

A *path* in an undirected (*resp.* directed) graph G is a sequence $x_1, \ldots, x_k$, $k \geq 1$ of pairwise distinct elements of X such that for all $i \in \{1, \ldots, k-1\}$, $\{x_i, x_{i+1}\}$ is an edge of G (*resp.* (x_i, x_{i+1}) is an arc of G). The *length* of a path is the number of its edges (*resp.* arcs). More specifically, a path $x_1, \ldots, x_k$, $k \geq 1$ has length $k-1$. A *cycle* is a sequence $x_1, \ldots, x_k$, $k \geq 3$ of elements of G such that $x_1, \ldots, x_k$ is a path of G, and in addition, $\{x_k, x_1\}$ is an edge of G (*resp.* (x_k, x_1) is an arc of G). As in the case of paths, the *size* of a cycle is the number of edges (*resp.* arcs) it contains. A graph that does not contain any cycle is called *acyclic*. In the undirected case, we also sometimes refer to connected acyclic graphs as *trees*.

We say that two undirected graphs $G = (V, E)$ and $G' = (V', E')$ are *isomorphic* if there exists a bijection $\phi : V \to V'$ such that $\{u, v\} \in E$ if and only if $\{\phi(u), \phi(v)\} \in E'$. This definition naturally extends to directed graphs.

Given an undirected graph $G = (V, E)$ and a non-empty subset $Y \subseteq V$, the *subgraph of G induced by* Y, denoted by $G[Y]$, is the graph with vertex set Y, and with edge set the set $\{\{u, v\} \in E : u, v \in Y\}$. We say that an undirected graph G is *chordal* if it does not contain a cycle of size 4 or more as an induced subgraph. Among the undirected graphs of interest to us are the *gem* which is a path P of length 3 together with a further vertex x not on P that is adjacent to all vertices of P (see Figure 2(i)), and the *wheel* W_k, $k \geq 4$, which is a cycle C of length $k-1$ together with a vertex x adjacent to all vertices of C (see Figure 2(ii) for the wheel W_5) . We say that a graph G is *Ptolemaic* Howorka (1981) if G is chordal and does not contain the gem as an induced subgraph.



(i) (ii)

Fig. 2: (i) The gem is an example of a chordal graph on 5 vertices, and it is the only chordal forbidden induced subgraphs for Ptolemaic graphs. (ii) The wheel W_5 is a non-chordal graph that is obtained from the gem by adding a single edge.

Three key operations on graphs will be of interest to us throughout this contribution. Let $G = (V, E)$ be an undirected graph, v a vertex of G of degree 2, and let u and w be the vertices adjacent to v in G. Then, the first operation is the *suppressing* of v operation which consists of removing v and the edges $\{u, v\}$ and $\{v, w\}$ from G, and adding the edge $\{u, w\}$. If G is directed, and v is a vertex of G with a unique parent u and a unique child w, then *suppressing* of v is the operation that consists of removing v and the arcs (u, v) and (v, w) from G, and adding the arc (u, w).

The second operation is an operation that reverses the suppressing operation. More precisely, given an edge $\{u, w\}$ of an undirected graph G, then *subdividing* of $\{u, w\}$ consists of removing the edge $\{u, w\}$ from G, adding a new vertex v, and adding the edges $\{u, v\}$ and $\{v, w\}$. If G is directed and (u, w) is an arc of G, then the *subdividing* of (u, w) operation consists of removing the arc (u, w) from G, adding a new vertex v, and adding the arcs (u, v) and (v, w). In either case, we call such a vertex v a *subdivision vertex*.

Our final operation is the *contracting* of an edge $\{u, v\}$ operation which in an undirected graph G consists of removing v from G, and replacing all edges $\{v, w\}$, $w \neq u$ of G with the edge $\{u, w\}$. If G is a directed graph, then the *contracting* of an arc (u, v) operation consists of removing v from G, replacing all arcs (v, w) of G with the arc (u, w), and replacing all arcs (w, v), $w \neq u$ of G with the arc (w, u).

Networks

A *network N (on X)* is a connected directed acyclic graph with leaf set X such that all vertices of indegree 0 have outdegree at least 2, all vertices of outdegree 0 have indegree 1, and no vertices have indegree and outdegree equal to 1. We call the vertices of indegree 0 the *roots* of a network and the vertices with outdegree 0 its *leaves*. We denote by $L(N)$ the set of leaves of N and by $R(N)$ the set of roots of N. Also, we put $r(N) = |R(N)|$. Note that we must have $r(N) \geq 1$. A network with a single root is commonly called a *rooted phylogenetic network*. In this case, if the undirected graph obtained by ignoring directions in the network is a tree, it is called a *rooted phylogenetic tree* (see e.g. Steel (2016) for more details on such networks). We say that two networks N, N' on X are *isomorphic* if there exists a digraph isomorphism ϕ from the vertex set $V(N)$ of N to the vertex set $V(N')$ of N' that is the identity on X.

Assume for the remainder of this section that N is a network on X. For u, v two vertices of N, we say that u is an *ancestor* of v if there is a path from u to v in N. In this case, we also refer to v as a *descendant* of u. If in addition, $u \neq v$, then we say that u is a *proper ancestor* of v and that v a *proper descendant of* u.

For v a vertex of N, we denote by $C_N(v)$ the set of all leaves of N that are a descendant of v. We say that two distinct leaves $x, y \in X$ *share an ancestor* in N if there exists a vertex v of N such that $x, y \in C_N(v)$. This notion allows us to define the *shared-ancestry graph* $\mathcal{A}(N)$ of N as follows. The vertex set of $\mathcal{A}(N)$ is X, and two distinct elements $x, y \in X$ are joined by an edge if and only if x and y share an ancestor in N. As an example, for N the network on $X = \{a, b, c, d, e, f, g\}$ depicted in Figure 3(i), we present the shared-ancestry graph $\mathcal{A}(N)$ of N in Figure 3(ii).

If two distinct leaves $x, y \in X$ share an ancestor in N, we say that a vertex v is a *lowest common ancestor* of x and y if v is an ancestor of both x and y, and no child of v is also an ancestor of both x and y. By definition, two vertices sharing an ancestor in N have at least one lowest common ancestor. However, that ancestor may not be unique. If two leaves x and y of N do have a unique lowest common ancestor, then we denote it by $\mathrm{lca}_N(x, y)$.

Let $R_2(N)$ be the set of roots of N with outdegree 2. We define the *underlying graph* $\overline{N}$ of N as the undirected graph with vertex set $V(\overline{N}) = V(N) \setminus R_2(N)$, and with edge set those pairs $\{u, v\}$ of vertices in $V(\overline{N})$ such that one of the following holds:

- One of (u, v) or (v, u) is an arc of N.
- There exists a root $r \in R_2(N)$ such that (r, u) and (r, v) are arcs of N.

In other words, $\overline{N}$ is the undirected graph obtained from N by suppressing the direction of the arcs and suppressing resulting vertices of degree 2. In particular, the leaf set of $\overline{N}$ is X. As an example, for N the network depicted in Figure 3(i), the underlying undirected graph $\overline{N}$ of N is depicted in Figure 3(iii).

Following Huber et al. (2022), we say that a network N on X is *arboreal* if its underlying graph $\overline{N}$ is a *phylogenetic tree (on X)*, that is, an unrooted tree which does not have any vertices of degree two and whose leaf set is X. Note that the network N depicted in Figure 3(i) is arboreal, since the underlying graph $\overline{N}$ of N, depicted in Figure 3(iii), is a phylogenetic tree on $L(N)$. Note that a network N is arboreal

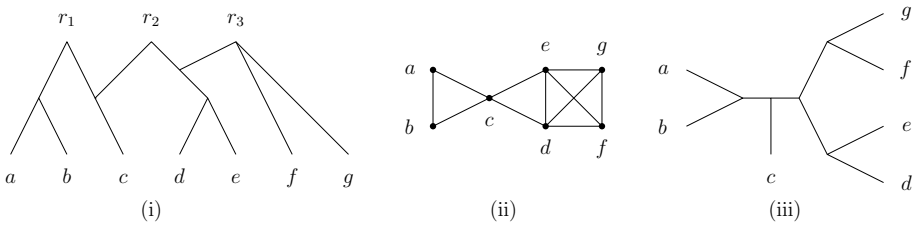


Fig. 3: (i) An arboreal network N on $X = \{a, b, c, d, e, f, g\}$, with three roots r_1, r_2 and r_3. (ii) The shared ancestry graph $\mathcal{A}(N)$ of N. (iii) The underlying graph $\overline{N}$ of N.

if and only if for all arcs a of N, the removal of a from N disconnects N. Also, note that the least common ancestor of a pair of leaves in an arboreal network, if it exists, is necessarily unique (Huber et al., 2024, Proposition 7.1), and that the shared-ancestry graph of an arboreal network is always Ptolemaic (Huber et al., 2024, Proposition 6.3).

For T a phylogenetic tree on X, an arboreal network N such that $\overline{N}$ and T are isomorphic can be obtained by subdividing some of the edges of T, and assigning directions to the edges of the resulting graph in such a way that all subdivision vertices have indegree 0, and a vertex v has outdegree 0 if and only if it is a leaf of T. Note that in view of the first requirement, an edge of T cannot be subdivided more than once in this process. Note also that a non-leaf vertex that is not a subdivision vertex is allowed to have indegree 0. We call a network obtained this way an *uprooting* of T. It is straight-forward to check that, although the underlying tree of an arboreal network is uniquely defined, there may in general be several non-isomorphic uprootings of a given phylogenetic tree.

Distances and weighted networks

Let G be an undirected graph. A *weighting* of G is a map $\lambda : E(G) \to \mathbb{R}_{>0}$ that assigns to each edge of G a positive value. We call the pair (G, λ) a *weighted graph*. For $e \in E(G)$, we call $\lambda(e)$ the *length* of e. We extend this definition to directed graphs in the obvious way, and will tend to use the symbol ω instead of λ to designate weightings in such graphs. In addition, the notion of isomorphism can be generalized to weighted graphs as follows. We say that two weighted graphs (G, λ) and (G', λ') are *isomorphic* if G and G' are isomorphic via a map $\phi : V(G) \to V(G')$, and the bijection ϕ satisfies $\lambda(\{u, v\}) = \lambda'(\{\phi(u), \phi(v)\})$ for all edges $\{u, v\}$ of G. Again, this definition extends naturally to directed graphs.

Let (T, λ) be a weighted phylogenetic tree on X. Since T is a tree, then for any pair u, v of vertices of T, there exists a unique path $P_T(u, v)$ between u and v in T. The *distance* $l_{(T,\lambda)}(u, v)$ between u and v in (T, λ) is defined as the sum of the lengths of all edges lying on $P_T(u, v)$. In particular, $l_{(T,\lambda)}(u, v) \geq 0$ always holds, with equality holding if and only if $u = v$. Viewing $l_{(T,\lambda)}$ as a map from $V(T) \times V(T)$ into the non-negative reals, then the restriction of the map $l_{(T,\lambda)}$ to $X \times X$ induces a map $D_{(T,\lambda)} : X \times X \to \mathbb{R}_{\geq 0}$ defined by putting $D_{(T,\lambda)}(x, y) = l_{(T,\lambda)}(x, y)$, for all $x, y \in X$.

Now, consider an arbitrary distance D on X, that is, a map $D : X \times X \to \mathbb{R}_{\geq 0}$, that is, a map such that D is *symmetric* (i.e. $D(x, y) = D(y, x)$ for all $x, y \in X$), and D vanishes precisely on the diagonal (i.e. $D(x, y) = 0$ if and only if $x = y$). We say that D is *tree-like* if there exists a weighted phylogenetic tree (T, λ) on X such that $D = D_{(T,\lambda)}$. In that case, we say that (T, λ) *represents* D. As is well-known

(Buneman (1971), see also (Semple and Steel, 2003, Section 7.1)), we have:

Theorem 2.1. *Let D be a distance on X. Then D is tree-like if and only if D satisfies the* four-point condition*, that is, for all (not necessarily distinct) $x, y, z, u \in X$, $D(x, y) + D(z, u) \leq \max\{D(x, z) + D(y, u), D(x, u) + D(y, z)\}$ holds. Moreover, if D is tree-like, then there exists a unique (up to isomorphism) phylogenetic tree T and a unique weighting λ of T such that $D = D_{(T,\lambda)}$.*

Consider now a weighted arboreal network (N, ω). The *weighted underlying phylogenetic tree* of (N, ω) is the weighted phylogenetic tree $(\overline{N}, \overline{\omega})$, where $\overline{\omega}$ is defined, for all edges $\{u, v\}$ of $\overline{N}$, as:

- $\overline{\omega}(\{u, v\}) = \omega((u, v))$ (*resp.* $\omega((v, u))$) if (u, v) (*resp.* (v, u)) is an arc of N.
- $\overline{\omega}(\{u, v\}) = \omega((r, u)) + \omega((r, v))$ if u and v are children of some $r \in R_2(N)$ in N.

Note that $(\overline{N}, \overline{\omega})$ is uniquely determined by (N, ω). In view of this, and since $\overline{N}$ is a phylogenetic tree, we define $D_{(N,\omega)} := D_{(\overline{N},\overline{\omega})}$, and we call $D_{(N,\omega)}$ the *distance induced by* (N, ω).

We now define the concept of an ultrametric arboreal network, a concept that generalises the definition of an ultrametric tree. To do this, we require further notation. Let (N, ω) be a weighted arboreal network on X. For u, v two vertices of N such that u is an ancestor of v in N, there is a unique directed path $P_N(u, v)$ from u to v in N (see e.g. (Scholz, 2025, Lemma 3)). We denote the sum of the lengths of all arcs of $P_N(u, v)$ by $l_{(N,\omega)}(u, v)$. Note that if $u \notin R_2(N)$, then by definition u and v are vertices of $\overline{N}$, so $l_{(N,\omega)}(u, v) = l_{(\overline{N},\overline{\omega})}(u, v)$ holds. We say that a weighted arboreal network (N, ω) is *ultrametric* if for all vertices u of N, and all leaves $x, y \in C_N(u)$, we have $l_{(N,\omega)}(u, x) = l_{(N,\omega)}(u, y)$. This definition generalises the notion of an *ultrametric tree* (sometimes also known as an *equidistant tree*, see e.g. (Semple and Steel, 2003, Section 7.2)) which, in our terminology, is simply an ultrametric arboreal network N with a single root.

We conclude this section by recalling the concept of an ultrametric. We say that a distance $D : X \times X \to \mathbb{R}_{\geq 0}$ is an *ultrametric* if $D = D_{(T,\omega)}$ for (T, ω) an ultrametric tree. In this case, we say that (T, ω) *represents* D. Similar to the case of tree-like distances, ultrametrics can be characterized in terms of the following 3-point condition (see e.g. (Semple and Steel, 2003, Theorem 7.2.5)):

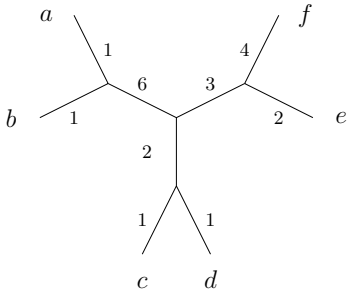
Theorem 2.2. *Let D be a distance on X. Then D is an ultrametric if and only if $|X| \leq 2$ or, for all $x, y, z \in X$ distinct, $D(x, y) \leq \max\{D(x, z), D(y, z)\}$. Moreover, if this holds, then there exists a unique (up to isomorphism) ultrametric tree (T, ω) such that $D = D_{(T,\omega)}$.*

3 Ultrametric uprootings

Often in phylogenetics, biologists first compute a weighted phylogenetic tree (T, λ) for their data and then insert a root into this tree to obtain a rooted phylogenetic tree in which the root represents the last common ancestor of all of the leaves. For most data sets it is not possible to do this in such a way that the resulting rooted tree is an ultrametric tree, since this would be equivalent to $D_{(T,\lambda)}$ being an an ultrametric, which is often not the case. For example, for (T, λ) the weighted phylogenetic tree depicted in Figure 4(i), the distance $D := D_{(T,\lambda)}$ (Figure 4(ii)) is not an ultrametric, since we have $D(a, e) = 12 > 10 = \max\{D(a, c), D(c, e)\}$.

Even so, if one were trying to build an arboreal network instead of a rooted tree, it could still be of interest to understand whether more roots might be inserted into a weighted phylogenetic tree order to obtain an ultrametric arboreal network even if no ultrametric rooting of the tree were possible. In

this section, we shall show that it is in fact *always* possible to insert some roots into a given weighted phylogenetic tree to obtain such a network and, in fact, for any given weighted phylogenetic tree there is only one way to do this (Theorem 3.5).



(i)

	a	b	c	d	e	f
a	0	2	10	10	12	14
b	2	0	10	10	12	14
c	10	10	0	2	8	10
d	10	10	2	0	8	10
e	12	12	8	8	0	6
f	14	14	10	10	6	0

(ii)

Fig. 4: (i) A weighted phylogenetic tree (T, λ) that admits the ultrametric network in Figure 1 as an ultrametric uprooting. (ii) The distance $D_{(T,\lambda)}$.

Definitions

For (T, λ) a weighted phylogenetic tree with leaf set X, we say that a weighted arboreal network (N, ω) on X is a *weight-preserving uprooting* of (T, λ) if (T, λ) is isomorphic to the underlying weighted graph $(\overline{N}, \overline{\omega})$ of N. In addition, we say that (N, ω) is an *ultrametric uprooting* of (T, λ) if (N, ω) is a weight-preserving uprooting of (T, λ), which, in addition, is ultrametric. For example, the ultrametric network depicted in Figure 1(i) is an ultrametric uprooting of the weighted phylogenetic tree depicted in Figure 4(i).

Note that, as we have seen above, there exists in general more than one uprooting of a phylogenetic tree T. Similarly, for a given uprooting N of T, there are infinitely many edge-weightings ω of N such that $\lambda = \overline{\omega}$. To see this, let (N, ω) be a weight-preserving uprooting of (T, λ). By definition, $\omega((u, v)) = \lambda(\{u, v\})$ for all arcs (u, v) of N for which $u \notin R_2(N)$. However, if $u \in R_2(N)$, the only requirement on $\omega((u, v))$ is that the equality $\omega((u, v)) + \omega((u, v')) = \lambda(\{v, v'\})$ holds for v' the second child of u in v.

We start with proving that any weighted phylogenetic tree admits an ultrametric uprooting (Proposition 3.1). Since our proof is constructive we shall present an algorithm called ULTRAMETRIC UPROOTING in Algorithm 1 and prove that it always produces such an uprooting (Proposition 3.1). We first introduce some additional notation concerning phylogenetic trees.

Let T be a phylogenetic tree on X. Given a subset $Y \subseteq X$, we denote by $T|_Y$ the phylogenetic tree obtained from T by removing all leaves in $X \setminus Y$ as well as all new leaves created in the process, and suppressing all resulting vertices of degree 2. Note that all edges $e = \{u, v\}$ in $T|_Y$ coincide with the path $P_T(u, v)$ between u and v in T. In view of this, if T is equipped with a weighting λ, we define the weight $\lambda|_Y(e)$ of an edge e of $T|_Y$ as the sum of the weights (under λ) of the edges in $P_T(u, v)$. In addition, we

say that a leaf x of T is *in a cherry* if the (necessarily unique) vertex v adjacent to x in T is adjacent to a leaf $y \in X$ that is distinct from x. If in addition, T is equipped with a weighting λ, and $x \in X$ is such that $\lambda(\{v, x\}) \geq \lambda(\{v, y\})$ for all leaves $y \in X$ adjacent to v in T, then we say that x is a *long-end of a cherry* in T.

We say that an ordering $x_1, \ldots, x_n$, $n = |X|$ of the elements of X is a *cherry-picking sequence* Humphries et al. (2013)[(i)] (or *cps* for short) if, for all $i \in \{3, \ldots, n\}$, x_i is part of a cherry in $T|_{\{x_1,\ldots,x_i\}}$. If T is equipped with a weighting λ, we call a cherry-picking sequence $x_1, \ldots, x_n$ a *weighted cherry-picking sequence* (or *wcps* for short) if, for all $i \in \{3, \ldots, n\}$, x_i is the long end of a cherry in $T|_{\{x_1,\ldots,x_i\}}$. As an example, consider the weighted phylogenetic tree (T, λ) on $X = \{a, b, c, d, e\}$ depicted in Figure 5(i). Then, the sequences a, b, c, d, e and e, d, c, b, a are both cherry picking sequences. However, only the former is a weighted cherry picking sequence. Indeed, to see that e, d, c, b, a is not a wcps, we remark that, even though c is part of a cherry in $T|_{\{e,d,c\}}$, it is not the long-end of a cherry, as the (unique) long-end of that cherry is e. Note that the same also holds for b in $T|_{\{e,d,c,b\}}$.

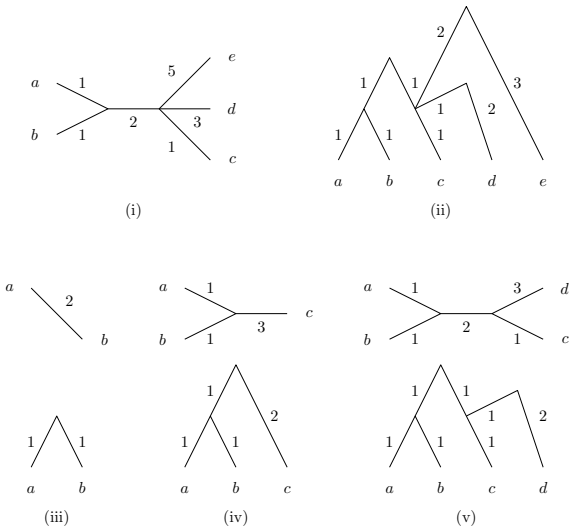


Fig. 5: (i) A weighted phylogenetic tree (T, λ) on $X = \{a, b, c, d, e\}$. (ii) the output of Algorithm 1 applied on (T, λ) and the wcps a, b, c, d, e. (iii), (iv) and (v) Top, the trees $T|_{\{a,b\}}$, $T|_{\{a,b,c\}}$ and $T|_{\{a,b,c,d\}}$, respectively. Bottom, the intermediate steps of the algorithm. See text for details.

As remarked in Döcker et al. (2019), all phylogenetic trees T on X admit a cps, which can be computed as follows. Put $n = |X|$. First, consider a non-leaf vertex v of T adjacent to at least two leaves. Note that in a phylogenetic tree, such a vertex always exists. Then choose x_n as one of the leaves adjacent to v in T, and repeat this process with T replaced by $T|_{X\setminus\{x_n\}}$. After $n - 2$ instances, we are left with a tree that has two leaves x and x', which can be independently defined as x_1 and x_2. Unsurprisingly, this approach can also be used to compute a wcps for some weighted phylogenetic tree (T, λ). Indeed, after

[(i)] Note that, in Humphries et al. (2013) a cherry picking sequence is defined on a set S of rooted phylogenetic trees. Here, we restrict to the case $|S| = 1$.

choosing a non-leaf vertex v of T adjacent to at least two leaves, one can pick a leaf x adjacent to v such that $\lambda(\{v,x\}) \geq \lambda(\{v,x'\})$ for all leaves x' adjacent to v. By definition, this results in a wcps.

Algorithm

We are now ready to present our algorithm, ULTRAMETRIC UPROOTING, for uprooting a weighted phylogenetic tree (Algorithm 1). Before proving that this algorithm is correct, we illustrate its inner-workings using a small example. Consider the weighted phylogenetic tree (T,λ) on $X = \{a,b,c,d\}$ depicted in Figure 5. As remarked above, a,b,c,d,e is a wcps of (T,λ). So assume that a,b,c,d,e is the wcps computed at Line 1.

Algorithm 1 ULTRAMETRIC UPROOTING

Input: A weighted phylogenetic tree (T,λ) with leaf set X
Output: An ultrametric uprooting (N,ω) of (T,λ)

1: Compute a wcps $x_1,\ldots,x_{|X|}$
2: Initialize N as the network with vertex set $\{x_1,x_2,r_2\}$ and arc set $\{(r_2,x_1),(r_2,x_2)\}$
3: Define $\omega((r_2,x_1)) = \omega((r_2,x_2)) = \frac{1}{2}\lambda_2(\{x_1,x_2\})$
4: **for** i from 3 to $|X|$ **do**
5: Put $T_i = T|_{\{x_1,\ldots,x_i\}}$ and $\lambda_i = \lambda|_{\{x_1,\ldots,x_i\}}$
6: Let v_i be the vertex of T_i adjacent to x_i, and let x be a further leaf of T_i adjacent to v_i
7: Let p_x be the parent of x in N
8: **if** $\omega((p_x,x)) > \lambda_i(\{v_i,x\})$ **then**
9: Subdivide (p_x,x) by introducing a new vertex v
10: Define $\omega((v,x)) = \lambda_i(\{v_i,x\})$ and $\omega((p_x,v)) = \omega((p_x,x)) - \lambda_i(\{v_i,x\})$
11: **else if** $\omega((p_x,x)) < \lambda_i(\{v_i,x\})$ **then** ▷ p_x has outdegree 2 (see proof)
12: Let u be the child of p_x distinct from x
13: **if** $\lambda_i(\{v_i,x\}) = \omega((p_x,x)) + \omega((p_x,u))$ **then**
14: Define $v = u$
15: **else**
16: Subdivide (p_x,u) by introducing a new vertex v
17: Define $\omega((p_x,v)) = \lambda_i(\{v_i,x\}) - \omega((p_x,x))$ and $\omega((v,u)) = \omega((p_x,u)) + \omega((p_x,x)) - \lambda_i(\{v_i,x\})$
18: **else** ▷ $\omega((p_x,x)) = \lambda_i(\{v_i,x\})$
19: Define $v = p_x$
20: **if** $\lambda_i(\{v_i,x_i\}) = l_{(N,\omega)}(v,z)$ for some $z \in C_N(v)$ **then**
21: Add to N the arc (v,x_i)
22: Define $\omega((v,x_i)) = \lambda_i(\{v_i,x_i\})$
23: **else**
24: Add to N a new vertex r and the arcs (r,v) and (r,x_i)
25: Define $\omega((r,v)) = \frac{1}{2}(\lambda_i(\{v_i,x_i\}) - l_{(N,\omega)}(v,z))$ and $\omega((r,x_i)) = \frac{1}{2}(\lambda_i(\{v_i,x_i\}) + l_{(N,\omega)}(v,z))$
26: **return** (N,ω)

First, we initialize N as the network with a single root and two leaves a and b (Line 2). Since

$\lambda_2(\{a,b\}) = 2$, we assign length $\lambda_2(\{a,b\})/2 = 1$ to both arcs of N (Line 3). This results in the network depicted in Figure 5(iii), bottom, which is an ultrametric uprooting of the weighted phylogenetic tree depicted in Figure 5(iii), top. Next, we enter the loop at Line 4.

In the first instance of the loop, we consider the leaf $x_3 = c$ of $T|_{\{a,b,c\}}$ (Figure 5(iv), top). The vertex v_3 adjacent to c in $T|_{\{a,b,c\}}$ is adjacent to both a and b, so we can independently choose $x = a$ or $x = b$ at Line 6. Suppose we choose $x = a$. We have $\lambda_3(\{v_3, a\}) = 1$ and $\omega((p_a, a)) = 1$, so $\omega((p_a, a)) = \lambda_3(\{v_i, a\})$, and neither of the conditions at Lines 8 and 11 ar satisfied. Hence we enter the subcase at Line 18, and we put $v = p_a$ (Line 19). Next, we have $\lambda_3(\{v_3, c\}) = 3$ and $l_{(N,\omega)}(v, a) = 1$. Since $a \in C_N(v)$, we are in the situation of Line 23. Following Lines 24 and 25, we therefore add a new vertex r and the arcs (r, c) and (r, v), and we put $\omega((r, v)) = \frac{1}{2}(\lambda_3(\{v_3, c\}) - l_{(N,\omega)}(v, a)) = 1$ and $\omega((r, c)) = \frac{1}{2}(\lambda_3(\{v_3, c\}) + l_{(N,\omega)}(v, a)) = 2$. This results in the network depicted in Figure 5(iv), bottom, which is an ultrametric uprooting of the weighted phylogenetic tree depicted in Figure 5(iv), top.

In the second instance of the loop, we consider the leaf $x_4 = d$ of $T|_{\{a,b,c,d\}}$ (Figure 5(v), top). The vertex v_4 adjacent to d in $T|_{\{a,b,c,d\}}$ is adjacent to c only, so we must choose $x = c$ at Line 6. We have $\lambda_4(\{v_4, c\}) = 1$ and $\omega((p_c, c)) = 2$, so $\omega((p_c, c)) > \lambda_4(\{v_4, c\})$. Hence, the condition of Line 8 holds. We then subdivide the arc (p_c, c) by introducing a new vertex v(Line 9), and we put $\omega((v, c)) = \lambda_4(\{v_4, c\}) = 1$ and $\omega((p_c, v)) = \omega((p_c, c)) - \lambda_4(\{v_4, c\}) = 1$ (Line 10). Next, we have $\lambda_4(\{v_4, d\}) = 3$ and $l_{(N,\omega)}(v, c) = 1$. Since $c \in C_N(v)$, we are in the situation of Line 23. Following Lines 24 and 25, we therefore add a new vertex r and the arcs (r, d) and (r, v), and we put $\omega((r, v)) = \frac{1}{2}(\lambda_4(\{v_4, d\}) - l_{(N,\omega)}(v, c)) = 1$ and $\omega((r, d)) = \frac{1}{2}(\lambda_4(\{v_4, d\}) + l_{(N,\omega)}(v, c)) = 2$. This gives rise to the network depicted in Figure 5(v), bottom, which is an ultrametric uprooting of the weighted phylogenetic tree depicted in Figure 5(v), top.

In the third and last instance of the loop, we consider the leaf $x_5 = e$ of $T|_{\{a,b,c,d,e\}} = T$ (Figure 5(i)). The vertex v_5 adjacent to e in T is adjacent to both c and d, so we can independently choose $x = c$ or $x = d$ at Line 6. Suppose we choose $x = c$. We have $\lambda_5(\{v_5, c\}) = 1$ and $\omega((p_c, c)) = 1$, so $\omega((p_c, c)) = \lambda(\{v_5, c\})$, and neither of the conditions at Lines 8 and 11 ar satisfied. Hence, we enter the subcase at Line 18, and we put $v = p_c$ (Line 19). Next, we have $\lambda_5(\{v_5, e\}) = 5$ and $l_{(N,\omega)}(v, c) = 1$. Since $c \in C_N(v)$, we are in the situation of Line 23. Following Lines 24 and 25, we therefore add a new vertex r and the arcs (r, e) and (r, v), and we put $\omega((r, v)) = \frac{1}{2}(\lambda_5(\{v_5, e\}) - l_{(N,\omega)}(v, c)) = 2$ and $\omega((r, e)) = \frac{1}{2}(\lambda_5(\{v_5, e\}) + l_{(N,\omega)}(v, c)) = 3$. This gives rise to the network depicted in Figure 5(ii), right, which is an ultrametric uprooting of the weighted phylogenetic tree depicted in Figure 5(i).

We now state the aforementioned result that any weighted phylogenetic tree admits an ultrametric uprooting. As the proof is quite long and technical, we present it in the Appendix

Proposition 3.1. *Given a weighted phylogenetic tree (T, λ) on X, the output (N, ω) of Algorithm* ULTRAMETRIC UPROOTING *is an ultrametric uprooting (N, ω) of (T, λ). In particular, all weighted phylogenetic trees admit an ultrametric uprooting.*

We now turn our attention to the problem of proving that the ultrametric uprooting for a weighted phylogenetic tree (T, λ) constructed by Algorithm 1 is in fact the only possibly uprooting of (T, λ) up to isomorphism. To do this, we first introduce some additional terminology.

Let T be a phylogenetic tree with leaf set X, and let N be an uprooting of T. As mentioned in the previous section, for all vertices u, v of T, there is a unique path $P_T(u, v)$ in T between u and v. We say that a vertex w of $P_T(u, v)$ distinct from u and v is a *low point* of $P_T(u, v)$ (in N) if no proper descendant of w in N is a vertex of $P_T(u, v)$. In particular, a low point of $P_T(u, v)$ must have indegree 2 or more in

N. Indeed, since w is distinct from u and v, there exists two distinct vertices w_1, w_2 of T that are adjacent to w in $P_T(u,v)$. Since w is a low point, neither w_1 nor w_2 is a child of w in N. It follows that w has two distinct parents p_1, p_2 in N, where for $i \in \{1,2\}$, p_i is either w_i, or a root of $R_2(N)$ whose children are w and w_i. Note however that not all vertices of $P_T(u,v)$ that have indegree 2 or more in N are low points. Moreover, $P_T(u,v)$ does not have any low point if and only if x and y share an ancestor in N.

Before proving our aforementioned uniqueness result, we present a useful lemma. For v a vertex of T, we define $cl_T(v)$ as the set of leaves of T that are closest to v in (T,λ) with regards to λ, that is, $cl_T(v) = cl_{(T,\lambda)}(v) = \operatorname{argmin}_{x\in X}\{l_{(T,\lambda)}(v,x)\}$.

Lemma 3.2. *Let (T,λ) be a weighted phylogenetic tree on X, and let (N,ω) be an ultrametric uprooting of (T,λ). Then for all vertices v of T, we have $C_N(v) = cl_T(v)$.*

Proof: To ease notation, we put $l = l_{(T,\lambda)}$ and $D = D_{(T,\lambda)}$. Recall that if u, v are two vertices of T such that u is an ancestor of v in N, then $l(u,v) = l_{(N,\omega)}(u,v)$.

We first remark that, since (N,ω) is ultrametric, $l(v,x) = l(v,x')$ holds for all $x, x' \in C_N(v)$. Hence, to show that $C_N(v) = \operatorname{argmin}_{x\in X}\{l_{(T,\lambda)}(v,x)\}$ holds, it suffices to show that for all pairs $x, y \in X$ such that $x \in C_N(v)$, $y \notin C_N(v)$, we have that $l(v,x) < l(v,y)$. So, let x, y be such a pair. We show that $l(v,x) < l(v,y)$ holds by induction on the number of low points of $P_T(x,y)$.

To see the base case, suppose that $P_T(x,y)$ does not have any low point. Then, x and y share and ancestor in N. Let $w = \operatorname{lca}_N(x,y)$. Since $y \notin C_N(v)$, w is not a descendant of v in N.

If w is an ancestor of v, we have $l(v,y) = l_{(N,\omega)}(w,y) + l_{(N,\omega)}(w,v)$. Moreover, (N,ω) is ultrametric, and so $l_{(N,\omega)}(w,y) = l_{(N,\omega)}(w,x) = l_{(N,\omega)}(w,v) + l_{(N,\omega)}(v,x)$. Combining these two equalities together, we obtain $l(v,y) = 2l_{(N,\omega)}(w,v) + l_{(N,\omega)}(v,x) = 2l(w,v) + l(v,x)$. Hence, $l(v,y) > l(v,x)$ holds in this case.

If otherwise, w is not an ancestor of v, we denote by h the first vertex of N that is common to the paths from v to x and from w to x in N. Then we have $l(v,y) = l_{(N,\omega)}(w,y) + l_{(N,\omega)}(w,h) + l_{(N,\omega)}(v,h)$. Moreover, (N,ω) is ultrametric, so $l_{(N,\omega)}(w,y) = l_{(N,\omega)}(w,x) = l_{(N,\omega)}(w,h) + l_{(N,\omega)}(h,x)$. Putting these two equalities together, we obtain $l(v,y) = 2l_{(N,\omega)}(w,h) + l_{(N,\omega)}(v,h) + l_{(N,\omega)}(h,x) = 2l(w,h) + l(v,x)$. Hence, $l(v,y) > l(v,x)$ also holds in this case.

Now, suppose that $P_T(x,y)$ contains $h \geq 1$ low points, and that for all $y' \in X$ such that $y' \notin C_N(v)$ and $P_T(x,y')$ has $h' < h$ low points, we have that $l(v,x) < l(v,y')$. In addition, let u be a low point of $P_T(x,y)$ such that u and y share an ancestor in N, and let z be a descendant of u in N.

Clearly, u is a vertex of both $P_T(z,v)$ and $P_T(y,v)$. In particular, we have $l(v,y) = l(y,u) + l(u,v) = l(y,z) + l(z,v) - 2l(u,z)$. Moreover, $l(y,z) = D(y,z) = 2l_{(N,\omega)}(w,z)$, where $w = \operatorname{lca}(y,z)$, so the previous equality can be written $l(v,y) = 2l_{(N,\omega)}(w,z) + l(z,v) - 2l_{(N,\omega)}(u,z)$. Since u is not an ancestor of y, but shares an ancestor with y, it follows that w is a proper ancestor of u in N. Hence, $l_{(N,\omega)}(w,z) > l_{(N,\omega)}(u,z)$. It follows that $l(v,y) > l(v,z)$. By choice of z, the path $P_T(x,z)$ has $h-1$ low points. By our induction hypothesis, $l(v,z) > l(v,x)$ follows, so $l(v,y) > l(v,x)$ holds as desired. □

We are now ready to prove our uniqueness result.

Proposition 3.3. *Let (T,λ) be a weighted phylogenetic tree on X. Then up to isomorphism, there exists a unique ultrametric uprooting of (T,λ).*

Proof: Let (N,ω) be an ultrametric uprooting of (T,λ). For $\{u,v\}$ an edge of T, exactly one of the following must hold: (u,v) is an arc of N, (v,u) is an arc of N, or there exists a root $r \in R_2(N)$ such

that u and v are the children of r in N. To show that N is uniquely determined by (T, λ), we show that for all edges of N, the choice between the aforementioned three possibilities is uniquely determined by (T, λ).

So, let $\{u, v\}$ be an edge of T. By Lemma 3.2, all leaves $x \in cl_T(v)$ are descendants of v in N. In particular, if there exists some $x \in cl_T(v)$ such that u is a vertex of $P_T(v, x)$, then (v, u) must be an arc in N. By symmetry, if there exists $y \in cl_T(u)$ such that v is a vertex of $P_T(u, y)$, then (u, v) must be an arc in N. Note that these two situations cannot happen simultaneously. Indeed, suppose for contradiction that there exist x and y as specified. Then, we have $l_{(T,\lambda)}(v, x) = l_{(T,\lambda)}(u, x) + \lambda(\{u, v\}) > l_{(T,\lambda)}(u, x)$ and $l_{(T,\lambda)}(u, y) = l_{(T,\lambda)}(v, y) + \lambda(\{u, v\}) > l_{(T,\lambda)}(v, y)$. Since $x \in cl_T(v)$ and $y \in cl_T(u)$, we also have $l_{(T,\lambda)}(v, x) \leq l_{(T,\lambda)}(v, y)$ and $l_{(T,\lambda)}(u, y) \leq l_{(T,\lambda)}(u, x)$. Taken together, these four inequalities yield a contradiction.

We next show that if there is no $x \in cl_T(v)$ such that u is a vertex of $P_T(v, x)$ and no $y \in cl_T(u)$ such that v is a vertex of $P_T(u, y)$, then there exists $r \in R_2(N)$ such that u and v are the children of r in N. To see this, suppose for contradiction that one of (u, v) or (v, u), say (v, u), is an arc of N. Then, we have $C_N(u) \subsetneq C_N(v)$. So, let $x \in C_N(u)$. By Lemma 3.2, we have $x \in cl_T(v)$. Moreover, $x \in C_N(u)$ and u is a child of v, so the path from v to x in N contains u. Hence, there is a path in T between v and x that contains u. Such a path being unique, it follows that u is a vertex of $P_T(v, x)$, a contradiction to our assumption that there is no leaf $x \in cl_T(v)$ such that u is a vertex of $P_T(v, x)$.

We have shown that up to isomorphism, N is uniquely determined by (T, λ). It remains to show that the weighting ω is also uniquely determined by (T, λ). Since (N, ω) is a weight-preserving uprooting of (T, λ), $\omega((u, v)) = \lambda(\{u, v\})$ holds by definition for all arcs (u, v) of N such that $u \notin R_2(N)$. Consider a vertex $r \in R_2(N)$ with children u and v. By definition, $\{u, v\}$ is an edge of T, and we have $\omega((r, u)) + \omega((r, v)) = \lambda(\{u, v\})$. Moreover, (N, ω) is an ultrametric arboreal network, so for all $x \in C_N(u)$, $y \in C_N(v)$, $l_{(N,\omega)}(r, x) = l_{(N,\omega)}(r, y)$ holds. Since $l_{(N,\omega)}(r, x) = \omega((r, u)) + l_{(N,\omega)}(u, x)$ and $l_{(N,\omega)}(r, y) = \omega((r, v)) + l_{(N,\omega)}(v, y)$, we have $\omega((r, u)) + l_{(N,\omega)}(u, x) = \omega((r, v)) + l_{(N,\omega)}(v, y)$. Together with the previous equality, it follows that $\omega((r, u)) = \frac{1}{2}(\lambda(\{u, v\}) + l_{(N,\omega)}(v, y) - l_{(N,\omega)}(u, x))$ and $\omega((r, v)) = \frac{1}{2}(\lambda(\{u, v\}) + l_{(N,\omega)}(u, x) - l_{(N,\omega)}(v, y))$. Since the length of the paths from u to x and from v to y are uniquely determined by N and (T, λ), this is also the case of $l_{(N,\omega)}(u, x)$ and $l_{(N,\omega)}(v, y)$. Hence, $\omega((r, u))$ and $\omega((r, v))$ are uniquely determined by (T, λ). This concludes the proof that $\omega(e)$ is uniquely determined by (T, λ) for all arcs e of N. □

An important consequence of Proposition 3.3 is that choices made by algorithm ULTRAMETRIC UPROOTING do not affect its output. More specifically, we have:

Observation 3.4. *The output of Algorithm 1 is independent of the choice of the wcps at Line 1, and of the successive choices of the element x at Line 6.*

Taking Propositions 3.1 and 3.3 together with Theorem 2.1, we immediately obtain the main result of this section:

Theorem 3.5. *Let D be a distance on X. The following are equivalent:*

(i) There exists an ultrametric arboreal network (N, ω) on X such that $D = D_{(N,\omega)}$.

(ii) There exists a weighted phylogenetic tree (T, λ) on X such that $D = D_{(T,\lambda)}$.

(iii) For all $x, y, z, u \in X$,

$$D(x, y) + D(z, u) \leq \max\{D(x, z) + D(y, u), D(x, u) + D(y, z)\}.$$

Moreover, if this holds, then both (T, λ) *and* (N, ω) *are unique up to isomorphism, and* (N, ω) *is an ultrametric uprooting of* (T, λ).

4 Characterizing arboreal ultrametrics

In this section we turn our attention to giving a characterization for when a partial distance is an arboreal ultrametric. We begin with some definitions.

A map $\tilde{D} : X \times X \to \mathbb{R}_{\geq 0} \cup \{\infty\}$ is called a *partial distance (on* X*)* if it is symmetric and vanishes precisely on the diagonal. To any weighted arboreal network (N, ω) on X, we can associate a partial distance $\tilde{D}_{(N,\omega)}$ on X as follows: if $x, y \in X$ share an ancestor in N, we put $\tilde{D}_{(N,\omega)}(x, y) = l_{(N,\omega)}(v, x) + l_{(N,\omega)}(v, y)$, where $v = \mathrm{lca}_N(x, y)$. Note that in this case $\tilde{D}_{(N,\omega)}(x, y) = D_{(N,\omega)}(x, y)$ and, if (N, ω) is ultrametric, then $l_{(N,\omega)}(v, x) = l_{(N,\omega)}(v, y)$, and so $\tilde{D}_{(N,\omega)}(x, y) = 2l_{(N,\omega)}(v, x) = 2l_{(N,\omega)}(v, y)$ also holds. If otherwise, x and y do not share an ancestor in N, we put $\tilde{D}_{(N,\omega)}(x, y) = \infty$. Note that $\tilde{D}_{(N,\omega)}$ is a distance on X if and only if N is a rooted phylogenetic tree, in which case $\tilde{D}_{(N,\omega)}$ is equal to $D_{(N,\omega)}$. We say that a partial distance $\tilde{D}$ on X is *arboreal representable* if there exists an ultrametric arboreal network (N, ω) on X satisfying $\tilde{D}_{(N,\omega)} = \tilde{D}$. In this case, we say that (N, ω) *represents* $\tilde{D}$.

Partial distances induced by weighted arboreal networks are closely related to the symbolic arboreal maps introduced in Huber et al. (2024). For M be a non-empty set of *symbols* and $\odot$ an element that is not in M, a *symbolic map* on X is a map $d : \binom{X}{2} \to M \cup \{\odot\}$. In particular, we shall view a partial distance $\tilde{D}$ on X as a symbolic ultrametric d where $M = \mathbb{R}_{>0}$ and $\odot = \infty$, where the fact that $\tilde{D}$ is symmetric ensures that d is well defined.

In what follows, we will make use of a characterization of symbolic maps that arise from arboreal networks given in Huber et al. (2024), which we now recall for the convenience of the reader. Given an arboreal network N on X, we denote by $V(N)^-$ the set of all vertices of N of outdegree 2 or more. A *labelled arboreal network* is a pair (N, t) where N is an arboreal network and $t : V(N)^- \to M$ is a map assigning an element of M to each vertex of $V(N)^-$. For a symbolic map $d : \binom{X}{2} \to M \cup \{\odot\}$, define the undirected graph G_d to be the graph with vertex set X and edges precisely those $\{x, y\} \in \binom{X}{2}$ such that $d(x, y) \neq \odot$. Then, we say that (N, t) *explains* d if, for all $x, y \in X$ distinct, $d(x, y) = t(\mathrm{lca}_N(x, y))$ if x and y share an ancestor in N, and $d(x, y) = \odot$ otherwise. Symbolic maps that can be explained by labelled arboreal networks, also called as *symbolic arboreal maps*, were characterised in Huber et al. (2024) as follows:

Theorem 4.1 (Huber et al. (2024), Theorem 7.5)**.** *Suppose that* X *is a set with* $|X| \geq 2$ *and that* $d : \binom{X}{2} \to M \cup \{\odot\}$ *is a symbolic map. Then,* d *is a symbolic arboreal map if and only if the following four properties all hold:*

(A1) G_d *is connected and Ptolemaic.*

(A2) No three elements $x, y, z \in X$ *satisfy* $|\{d(x, y), d(x, z), d(y, z)\}| = 3$ *and* $\odot \notin \{d(x, y), d(x, z), d(y, z)\}$.

(A3) No four elements $x, y, z, u \in X$ *satisfy* $d(x, y) = d(y, z) = d(z, y) \neq d(y, u) = d(u, x) = d(x, z)$ *and* $\odot \notin \{d(x, y), d(x, z)\}$.

(A4) For all $x, y, z, u \in X$ *distinct such that* $d(z, u) = \odot$ *and* d *maps all other elements of* $\binom{\{x,y,z,u\}}{2}$ *to an element of* M*, both* $d(x, z) = d(y, z)$ *and* $d(x, u) = d(y, u)$ *hold.*

We now use this result to characterize arboreal-representable partial distances. First, we show that if (N, ω) is an ultrametric arboreal network, then $\tilde{D}_{(N,\omega)}$ is a symbolic arboreal map.

Lemma 4.2. *Let (N, ω) be an ultrametric arboreal network on X. Then, there exists a labelling map $t : V(N)^- \to \mathbb{R}_{>0}$ such that the labelled network (N, t) explains $\tilde{D}_{(N,\omega)}$. In particular, $\tilde{D}_{(N,\omega)}$ is a symbolic arboreal map on X.*

Proof: To ease notation, we put $\tilde{D} = \tilde{D}_{(N,\omega)}$. As already mentioned, $\tilde{D}$ is a symbolic map on X. To obtain the labelling map t, we put, for all $v \in V(N)^-$, $t(v) = 2l_{(N,\omega)}(v, x)$, where $x \in C_N(v)$. Note that, since (N, ω) is ultrametric, $t(v)$ does not depend on the choice of x in $C_N(v)$.

We now show that (N, t) explains $\tilde{D}$. Let $x, y \in X$ distinct. Since (N, ω) represents $\tilde{D}$, we have $\tilde{D}(x, y) = \infty$ if and only if x and y do not share an ancestor. Suppose now that $\tilde{D}(x, y) \neq \infty$. Then x and y have a common ancestor in N. Let $v = \mathrm{lca}_N(x, y)$. By definition, $\tilde{D}(x, y) = l_{(N,\omega)}(v, x)+l_{(N,\omega)}(v, y)$. Since (N, ω) is ultrametric, we have $l_{(N,\omega)}(v, x) = l_{(N,\omega)}(v, y)$, so $D_{(N,\omega)}(x, y) = 2l_{(N,\omega)}(v, x) = t(v)$. Hence, (N, t) explains $\tilde{D}$. □

We next present a characterization for arboreal representable partial distances.

Theorem 4.3. *Let $\tilde{D} : X \times X \to \mathbb{R}_{>0} \cup \{\infty\}$ be a partial distance on X. Then there exists an ultrametric arboreal network on X representing $\tilde{D}$ if and only if the following three properties hold:*

(U1) $G_{\tilde{D}}$ is connected and chordal.

(U2) If $x, y, z \in X$ are pairwise distinct such that $\infty \notin \{\tilde{D}(x, y), \tilde{D}(x, z), \tilde{D}(y, z)\}$, then $\tilde{D}(x, y) \leq \max\{\tilde{D}(x, z), \tilde{D}(y, z)\}$.

(U3) If $x, y, z, u \in X$ are pairwise distinct such that $\tilde{D}(z, u) = \infty$ and $\tilde{D}$ maps all other elements of $\binom{\{x,y,z,u\}}{2}$ to an element in $\mathbb{R}_{>0}$, then

$$\tilde{D}(x, y) < \min\{\tilde{D}(x, z), \tilde{D}(x, u), \tilde{D}(y, z), \tilde{D}(y, u)\}.$$

The intuition behind Property (U3) is as follows. If N is an ultrametric arboreal network on X and x, y, z and u are as in Property (U3) then if x and y share an ancestor with z and an ancestor with u, but z and u do not share an ancestor, then there must exist a vertex of indegree 2 or more in N that is an ancestor of x and y but not of z and u. As a consequence, x and y are "closer" to each other than they are to z and to u, respectively.

To further illustrate Property (U3), consider the distance $\tilde{D}$ on $X = \{x, y, z, u\}$ defined by $\tilde{D}(x, z) = 1$, $\tilde{D}(y, z) = \tilde{D}(x, y) = 2$, $\tilde{D}(x, u) = \tilde{D}(y, u) = 3$, and $\tilde{D}(z, u) = \infty$. Then it is straight-forward to verify that $\tilde{D}$ satisfies (U1) and (U2), but not (U3). If there existed an ultrametric arboreal network N on X representing $\tilde{D}$, then the restriction of $\tilde{D}$ to $\{x, y, z\}$ implies that the last common ancestor of x and y is an ancestor of the last common ancestor of x and z, and the restriction of $\tilde{D}$ to $\{x, y, u\}$ implies that the last common ancestor of x and u is an ancestor of the last common ancestor of x and y. Taken together, these two observations imply that z and u share an ancestor in N contradicting $\tilde{D}(z, u) = \infty$.

Before proving Theorem 4.3, we make an observation about Property (U3) that will be useful in the proof and in subsequent results.

Observation 4.4. *If $\tilde{D}$ satisfies (U3), then $G_{\tilde{D}}$ is gem-free and W_5-free. In particular, if $\tilde{D}$ satisfies (U1) and (U3), then $G_{\tilde{D}}$ is Ptolemaic.*

Proof: Suppose that $\tilde{D}$ satisfies (U3), and assume for contradiction that there exists pairwise distinct vertices x, y, z, u, v of $G_{\tilde{D}}$ such that the subgraph of $G_{\tilde{D}}$ induced by these five vertices is a gem or a W_5. Then up to a permutation, $G_{\tilde{D}}$ contains the edges $\{x, y\}, \{x, v\}, \{y, z\}, \{y, v\}; \{z, u\}, \{z, v\}$ and $\{u, v\}$, and does not contain the edges $\{x, z\}$ and $\{y, u\}$. Applying (U3) on x, y, z, u, we obtain $\tilde{D}(y, v) < \tilde{D}(z, v)$, and applying (U3) on y, z, u, v, we get $\tilde{D}(z, v) < \tilde{D}(y, v)$. This is impossible, so $G_{\tilde{D}}$ is gem-free and W_5-free. If in addition, $\tilde{D}$ satisfies (U1), then $G_{\tilde{D}}$ is chordal, so $G_{\tilde{D}}$ is Ptolemaic. □

We now proceed with the proof of Theorem 4.3.

Proof: Suppose first that there exists an ultrametric arboreal network (N, ω) on X representing $\tilde{D}$. By Lemma 4.2, $\tilde{D}$ is a symbolic arboreal map, and so it follows by Theorem 4.1 that $\tilde{D}$ satisfies Properties (A1)-(A4). Since a Ptolemaic graph is chordal, (U1) is a weaker version of (A1), so Property (U1) holds.

To see that Property (U2) holds, let $x, y, z \in X$ be three pairwise distinct elements such that $\infty \notin \{\tilde{D}(x, y), \tilde{D}(x, z), \tilde{D}(y, z)\}$. Since (N, ω) represents $\tilde{D}$ and is arboreal, it follows that there exists a root r of N such that $x, y, z \in C_N(r)$. In particular, the restriction of $\tilde{D}$ to $C_N(r)$ is an ultrametric on $C_N(r)$. By Theorem 2.2, $\tilde{D}(x, y) \leq \max\{\tilde{D}(x, z), \tilde{D}(y, z)\}$ follows.

To see that Property (U3) holds, let $x, y, z, u \in X$ be four pairwise distinct elements such that $\tilde{D}(z, u) = \infty$ and $\tilde{D}$ maps all other elements in $\binom{\{x,y,z,u\}}{2}$ to an element in $\mathbb{R}_{>0}$. Since $\tilde{D}$ satisfies Property (A4), we have $\tilde{D}(x, z) = \tilde{D}(y, z)$ and $\tilde{D}(x, u) = \tilde{D}(y, u)$. Moreover, since $\tilde{D}$ satisfies Property (U2) by the previous paragraph, we have $\tilde{D}(x, z) = \tilde{D}(y, z) \geq \tilde{D}(x, y)$ and $\tilde{D}(x, u) = \tilde{D}(y, u) \geq \tilde{D}(x, y)$. It remains to show that these two inequalities are strict.

To see that this is the case, suppose for contradiction that $\tilde{D}(x, z) = \tilde{D}(x, y) = \tilde{D}(y, z)$. Since N is arboreal, and $\omega(a) > 0$ for all arcs a of N, $\mathrm{lca}_N(x, y) = \mathrm{lca}_N(x, z) = \mathrm{lca}_N(y, z)$ must hold. Denote this least common ancestor by v. Since $\tilde{D}(x, u), \tilde{D}(y, u) \in \mathbb{R}_{>0}$, it follows that x, y and u share an ancestor in N. Then, either u is a descendant of v in N, or v is a descendant of $\mathrm{lca}_N(x, u)$. In the first case, v is a common ancestor of z and u, and in the second case, $\mathrm{lca}_N(x, u)$ is a common ancestor of z and u. Both are impossible, since $\tilde{D}(z, u) = \infty$ implies that z and u do not share an ancestor in N. Hence, $\tilde{D}(x, z) = \tilde{D}(y, z) > \tilde{D}(x, y)$ must hold. By symmetry, we also have that $\tilde{D}(x, u) = \tilde{D}(y, u) > \tilde{D}(x, y)$ holds.

Conversely, suppose that $\tilde{D}$ satisfies Properties (U1), (U2) and (U3). We begin by showing that $\tilde{D}$ satisfies Properties (A1) to (A4). Since $\tilde{D}$ satisfies Property (U1), $G_{\tilde{D}}$ is connected and chordal. Moreover, by Observation 4.4, $G_{\tilde{D}}$ is gem-free. Hence, $G_{\tilde{D}}$ is Ptolemaic, so Property (A1) holds.

We now show that Property (A2) is a consequence of Property (U2). Let $x, y, z \in X$ be such that $\odot = \infty \notin \{\tilde{D}(x, y), \tilde{D}(x, z), \tilde{D}(y, z)\}$. Up to permutation of the elements in $\{x, y, z\}$, we may assume that $\tilde{D}(x, y) = \max\{\tilde{D}(x, y), \tilde{D}(x, z), \tilde{D}(y, z)\}$. By (U2), $\tilde{D}(x, y) \leq \max\{\tilde{D}(x, z), \tilde{D}(y, z)\}$, so by choice of the pair x, y, it follows that $\tilde{D}(x, y) = \max\{\tilde{D}(x, z), \tilde{D}(y, z)\}$ follows. Hence, we have $|\{\tilde{D}(x, y), \tilde{D}(x, z), \tilde{D}(y, z)\}| < 3$, so (A2) holds.

Next, we show that Property (A3) holds. Let $x, y, z, u \in X$ be such that $\tilde{D}(x, y) = \tilde{D}(y, z) = \tilde{D}(z, u) \neq \tilde{D}(z, x) = \tilde{D}(x, u) = \tilde{D}(u, y)$ and $\infty \notin \{\tilde{D}(x, y), \tilde{D}(x, z)\}$. Using Property (U2) on the sets $\{x, y, z\}$ and $\{x, y, u\}$, we must have $\tilde{D}(x, y) = \tilde{D}(y, z) > D(x, z)$ and $\tilde{D}(x, u) = \tilde{D}(u, y) > \tilde{D}(x, y)$, which is impossible since $\tilde{D}(x, z) = \tilde{D}(x, u)$. Hence, Property (A3) holds.

Finally, we show that $\tilde{D}$ satisfies Property (A4). Let $x, y, z, u \in X$ be pairwise distinct such that $d(z, u) = \odot$ while d maps all other pairs of elements of $\{x, y, z, u\}$ to an element of $M = \mathbb{R}_{>0}$. By

(U3), we have $\tilde{D}(x,y) < \min\{\tilde{D}(x,z), \tilde{D}(x,u), \tilde{D}(y,z), \tilde{D}(y,u)\}$. Moreover, (U2) applied to the set $\{x,y,z\}$ gives $\tilde{D}(y,z) \leq \max\{\tilde{D}(x,y), \tilde{D}(x,z)\} = \tilde{D}(x,z)$ and $\tilde{D}(x,z) \leq \max\{\tilde{D}(x,y), \tilde{D}(y,z)\} = \tilde{D}(y,z)$, so $\tilde{D}(x,y) < \tilde{D}(x,z) = \tilde{D}(y,z)$ follows. Applying (U2) to the set $\{x,y,u\}$ implies $\tilde{D}(x,y) < \tilde{D}(x,u) = \tilde{D}(y,u)$ in a similar fashion.

Since $\tilde{D}$ satisfies Properties (A1)-(A4), Theorem 4.1 implies that there exists a labelled arboreal network (N,t) that explains $\tilde{D}$. Without loss of generality, we may assume that (N,t) is such that no arc (u,v) of N satisfies $t(u) = t(v)$ as otherwise we could contract that arc and the resulting arboreal network would also explain $\tilde{D}$. We next construct a weighting ω of N such that (N,ω) represents $\tilde{D}$. To this end, we first define a map $\delta : V(N) \to \mathbb{R}_{\geq 0}$ as follows. If v is a leaf of N, we put $\delta(v) = 0$. If v has outdegree at least 2, we put $\delta(v) = \frac{1}{2}t(v)$. To be able to extend the definition of δ to $V(N)$, we claim that for all vertices u and v of N distinct such that both u and v have outdegree at least 2 and u is an ancestor of v in N, we have $\delta(u) > \delta(v)$.

Let u and v be two such vertices of N. First, note that if $u = v_1, \ldots, v_k = v$, $k \geq 2$, is the subsequence of vertices of outdegree at least 2 on the path $P_N(u,v)$ from u to v, then it suffices to show that $\delta(v_i) > \delta(v_{i+1})$ holds for all $1 \leq i \leq k-1$. By definition of the vertices $v_1, \ldots, v_k$, there is no vertex of outdegree 2 or more on the path from v_i to v_{i+1}. Hence to prove the claim, we may assume without loss of generality that u and v are such that other than possibly u or v, no other vertex on $P_N(u,v)$ has outdegree 2 or more in N.

Now, suppose $x, y \in C_N(v)$ are such that $v = \mathrm{lca}_N(x,y)$, and let $z \in C_N(u)$ be such that $z \notin C_N(v)$. Note that since both u and v have outdegree at least 2 in N, and N is arboreal, the leaves x, y and z always exist. In particular, $u = \mathrm{lca}_N(x,z) = \mathrm{lca}_N(y,z)$. Since (N,t) explains $\tilde{D}$, it follows that $\tilde{D}(x,y) = t(v)$ and $\tilde{D}(x,z) = \tilde{D}(y,z) = t(u)$. By Property (U2), $t(u) \geq t(v)$ holds. We now show that this inequality is strict which immediately implies our claim by the definition of the map δ. To do this we distinguish between two cases: (a) (u,v) is an arc of N, and (b) there exists a vertex h of indegree 2 or more on the path from u to v.

If case (a) holds, we have $t(u) \neq t(v)$ by assumption on (N,t), so $t(u) > t(v)$. Hence, $\delta(u) > \delta(v)$ holds as claimed. If case (b) holds, let r be a root of N such that h is a descendant of r and u is not, and let $z' \in X$ be a descendant of r that is not also a descendant of h. Note that x, y, z, z' are pairwise distinct. Since (N,t) explains $\tilde{D}$, we have $\tilde{D}(z,z') = \infty$, while $\tilde{D}$ maps all other elements in $\binom{\{x,y,z,z'\}}{2}$ to an element in $\mathbb{R}_{>0}$. By Property (U3), it follows that $t(u) = \tilde{D}(x,z) = \tilde{D}(y,z) > \tilde{D}(x,y) = t(v)$, so $\delta(u) > \delta(v)$ also holds in this case. This completes the proof of the claim.

The claim being true, it is therefore always possible to extend the definition of δ to $V(N)$ in such a way that $\delta(u) > \delta(v)$ holds for all arcs (u,v) of N. Putting $\omega(a) = \delta(u) - \delta(v)$ for all arcs $a = (u,v)$ of N, it follows that $\omega(a) > 0$. Thus, (N,ω) is a weighted arboreal network.

We now show that (N,ω) is an ultrametric arboreal network. Let v be a non-leaf vertex of N and let $x \in X$ such that x is a descendant of v in N. Let $v_1 = v, v_2, \ldots, v_k = x$, $k \geq 2$, be a path from v to x in N. By definition, we have $l_{(N,\omega)}(v,x) = \sum_{i=1}^{k-1} \omega((v_i, v_{i+1}))$. Since $\omega((v_i, v_{i+1})) = \delta(v_i) - \delta(v_{i+1})$, and $\delta(x) = 0$, it follows that $l_{(N,\omega)}(v,x) = \delta(v)$. In particular, $l_{(N,\omega)}(v,x)$ does not depend on the choice of x in $C_N(v)$, so (N,ω) is an ultrametric arboreal network.

To complete the proof, it remains to show that (N,ω) represents $\tilde{D}$. Since $\tilde{D}$ is a partial distance and (N,t) explains $\tilde{D}$, we have $\tilde{D}(x,y) = \infty$ if and only if x and y do not share an ancestor in N. Now, let $x, y \in X$ distinct be such that $\tilde{D}(x,y) \neq \infty$, and let $v = \mathrm{lca}_N(x,y)$. By definition, and since (N,ω) is ultrametric, we have $D_{(N,\omega)}(x,y) = l_{(N,\omega)}(v,x) + l_{(N,\omega)}(v,y) = 2l_{(N,\omega)}(v,x)$. As observed in the

previous paragraph, $l_{(N,\omega)}(v,x) = \delta(v)$, and $\delta(v) = \frac{1}{2}t(v)$ by definition of δ. Since $t(v) = \tilde{D}(x,y)$ as (N,t) explains $\tilde{D}$ and $v = \mathrm{lca}_N(x,y)$, it follows that $D_{(N,\omega)}(x,y) = \tilde{D}(x,y)$. This concludes the proof of the theorem. □

A first immediate consequence of Theorem 4.3 is the following, computational complexity result:

Corollary 4.5. *For $\tilde{D}$ a partial distance on X, we can decide in time $O(|X|^4)$ whether or not $\tilde{D}$ is an arboreal ultrametric.*

The following corollary characterizes when the restriction of an arboreal ultrametric on X to a subset of X is also an arboreal ultrametric.

Corollary 4.6. *Let $\tilde{D}$ be an arboreal ultrametric on X, and let Y be a nonempty subset of X. The restriction $\tilde{D}_Y$ of $\tilde{D}$ to $Y \times Y$ is an arboreal ultrametric if and only if $G_{\tilde{D}_Y}$ is connected.*

Proof: Since $\tilde{D}$ is an arboreal ultrametric, $\tilde{D}$ satisfies Properties (U1), (U2) and (U3) of Theorem 4.3.

Since $\tilde{D}$ satisfies (U1), $G_{\tilde{D}}$ is connected and chordal. Moreover, $G_{\tilde{D}_Y}$ is precisely the subgraph of $G_{\tilde{D}}$ induced by the elements of Y. In particular, $G_{\tilde{D}_Y}$ is chordal. Moreover, it is straightforward to verify that if $\tilde{D}$ satisfies (U2) (*resp.* (U3)), then $\tilde{D}_Y$ also satisfies (U2) (*resp.* (U3)). In summary, $\tilde{D}_Y$ satisfies (U2) and (U3), and $G_{\tilde{D}_Y}$ is chordal. By Theorem 4.3, $\tilde{D}$ is an arboreal ultrametric if and only if $G_{\tilde{D}_Y}$ is connected. □

We conclude this section with a uniqueness result. For the purpose of this result, we will relax the definition of a network, by allowing leaves to have degree more than one. Note that if a network N contains such leaves, it can be transformed into a network in the sense given above by applying the following three steps for all leaves x of indegree 2 or more. First, introduce a new vertex v. Then, replace all arcs (u,x) with the arc (u,v). Finally, add the arc (v,x). Note that the network N^+ obtained this way is unique. However, if (N,ω) is edge weighted, then there are infinitely many ways to assign weights ω' to the arcs of N^+ in such a way that (N^+,ω') is a weighted network satisfying $\tilde{D}_{(N^+,\omega')} = \tilde{D}_{(N,\omega)}$.

To state our uniqueness result, we shall use the following fact which follows by (Huber et al., 2024, Theorem 7.6). Suppose that d is a symbolic map, then there exists a unique (up to isomorphism) labelled arboreal network (N,t) such that (N,t) explains d, N does not contain vertices of outdegree 1, and $t(u) \neq t(v)$ for all arcs (u,v) of N with $u,v \in V(N)^-$.

Theorem 4.7. *Let $\tilde{D} : X \times X \to \mathbb{R}_{>0} \cup \{\infty\}$ be a partial distance on X. If $\tilde{D}$ satisfies properties (U1) to (U3), then, up to isomorphism, there exists a unique ultrametric arboreal network (N,ω) representing $\tilde{D}$ such that N does not contain vertices of outdegree* 1.

Proof: Since $\tilde{D}$ satisfies properties (U1) to (U3), Theorem 4.3 implies that there exists an ultrametric arboreal network representing $\tilde{D}$. Let (N,ω) be such a network, and suppose that N contains at least one vertex with outdegree 1. Let u be one such vertex, v denote the unique child of u, and let $p_1,\ldots,p_k$, $k \geq 2$, be the parents of u (note that $k \geq 2$ since u has outdegree 1 and N is a network, and therefore u is not a root and it does not have indegree 1). Consider the weighted network (N',ω') where N' is obtained by contracting the arc (u,v), and where $\omega'(a)$ is defined, for all arcs a of N' as $\omega'(a) = \omega(a) + \omega((u,v))$ if $a = (p_i,u)$ for some $i \in \{1,\ldots,k\}$, and $\omega'(a) = \omega(a)$. It is straightforward to check that (N',ω') remains an ultrametric arboreal network explaining $\tilde{D}$. By repeatedly applying this operation to vertices with outdegree 1, we can therefore assume without loss of generality that (N,ω) does not contain vertices of outdegree 1.

Now, let $t_\omega : V(N)^- \to \mathbb{R}_{>0}$ be the map defined, for all vertices v of N of outdegree 2 or more (that is, for all non-leaf vertices of N), by $t_\omega(v) = 2l_{(N,\omega)}(v, x)$, where $x \in C_N(v)$. Recall that since N is ultrametric, $l_{(N,\omega)}(v, x)$ does not depend on the choice of x in $C_N(v)$, so $t_\omega(v)$ is uniquely determined.

Clearly, (N, t_ω) explains the symbolic map $\tilde{D}$. Indeed, since (N, ω) represents $\tilde{D}$ as a partial distance, $\tilde{D}(x, y) = \infty$ for some $x, y \in X$ if and only if x and y do not share an ancestor in N. Otherwise, if x and y do share an ancestor in N, then for $v = \mathrm{lca}_N(x, y)$, we have $\tilde{D}(x, y) = l_{(N,\omega)}(v, x) + l_{(N,\omega)}(v, y)$, and since (N, ω) is ultrametric, $l_{(N,\omega)}(v, x) = l_{(N,\omega)}(v, y)$ and hence $\tilde{D}(x, y) = 2l_{(N,\omega)}(v, x) = t_\omega(v)$.

Now, by the fact mentioned before the statement of the theorem, there exists a unique (up to isomorphism) labelled arboreal network (N_0, t_0) such that (N_0, t_0) explains $\tilde{D}$, N_0 does not contain vertices of outdegree 1, and $t_0(u) \neq t_0(v)$ for all arcs (u, v) of N_0 with $u, v \in V(N)^-$. But as has already been established, (N, t_ω) satisfies (i) and (ii). Moreover, (N, t_ω) also satisfies (iii). Indeed, if (u, v) is an arc of N such that $u, v \in V(N)^-$, then $t_\omega(u) = t_\omega(v) + \omega((u, v))$ and, since $\omega((u, v)) > 0$, $t_\omega(u) \neq t_\omega(v)$ follows. Hence N and N_0 must be isomorphic.

In light of this last observation, it follows that if (N', ω') is an ultrametric arboreal network representing $\tilde{D}$ that does not contain any vertices of outdegree 1, then N' is isomorphic to N. It remains to show that the weighting ω is uniquely determined by N and $\tilde{D}$. So, let (u, v) be an arc of N. Suppose first that v is a leaf of N. Since u has outdegree 2 or more, there exists a leaf $x \in C_N(u)$ distinct from v. Since (N, ω) represents $\tilde{D}$, we have $\tilde{D}(x, v) = l_{(N,\omega)}(u, x) + l_{(N,\omega)}(u, v)$. Moreover, (N, ω) is ultrametric, so we have $l_{(N,\omega)}(u, x) = l_{(N,\omega)}(u, v)$. Since $l_{(N,\omega)}(u, v) = \omega((u, v))$, it follows that $\omega((u, v)) = \frac{1}{2}\tilde{D}(x, v)$.

Suppose now that v is not a leaf of N. Let $x, y \in C_N(v)$ distinct such that $v = \mathrm{lca}_N(x, y)$, and let $z \in C_N(u) \setminus C_N(v)$. Note that the existence of x, y and z is guaranteed by the fact that both u and v have outdegree 2 or more in N. Since (N, ω) represents $\tilde{D}$, we have $\tilde{D}(x, y) = l_{(N,\omega)}(v, x) + l_{(N,\omega)}(v, y)$ and $\tilde{D}(x, z) = l_{(N,\omega)}(u, x) + l_{(N,\omega)}(u, z)$. Moreover, (N, ω) is ultrametric, so we have $l_{(N,\omega)}(v, x) = l_{(N,\omega)}(v, y)$ and $l_{(N,\omega)}(u, x) = l_{(N,\omega)}(u, z)$. Finally, we have $l_{(N,\omega)}(u, x) = l_{(N,\omega)}(v, x) + \omega((u, v))$. In combination, these equalities imply $\omega((u, v)) = \frac{1}{2}(\tilde{D}(x, z) - \tilde{D}(x, y))$. This concludes the proof that ω is uniquely determined by N and $\tilde{D}$, and thus the proof of the theorem. □

5 Future directions

In this paper we have introduced the concept of arboreal ultrametrics and considered how to produce them from unrooted trees and how to characterize them. There remain several interesting open directions for research on arboreal ultrametrics and related structures.

First, as stated in Corollary 4.5, we can recognize whether or not a partial distance on a set of size n is an arboreal ultrametric in $O(n^4)$ time. It would be interesting to know if it is possible to obtain a better bound. Note that extending Bandelt's approach in Bandelt (1990) to recognizing whether or not a distance is an ultrametric on a set of size n in $O(n^2 log(n))$ time in the obvious way does appear to give a faster algorithm since checking Property (U3) in Theorem 4.3 is problematic. Thus some other approach is probably required if it is indeed possible to find an improvement (e.g. by considering approaches such as those in Culberson and Rudnicki (1989) which can recognize an ultrametric in $O(n^2)$ time).

More generally since distances can be defined in various way and for many different types of data (Felsenstein, 2004, Chapter 11), it would be interesting to develop an algorithm that not only recognizes arboreal ultrametrics but also constructs them from distances arising from real data. The unweighted pair group method with arithmetic mean (UPGMA) Sokal and Michener (1958) is a popular algorithm that

takes as input a distance matrix and outputs an ultrametric tree. It also has the property that if the input is an ultrametric then is produces the unique ultrametric tree that realizes this ultrametric. It could be worthwhile exploring if some algorithm could be developed for producing ultrametric arboreal networks from partial distances that generalizes UPGMA.

In another but related direction, there are several results concerning the approximation of distances by ultrametrics (see e.g. (Chepoi and Fichet, 2000, Section 3) for a review). It could be worth exploring which of these results might extend to approximations of partial distances by arboreal ultrametrics. For example, it is well-known (see e.g. Chepoi and Fichet (2000)) that any distance has an ultrametric subdominant (or lower maximum approximation); is there such a result for partial distances? Note that computing subdominants is closely related to the concept of the Farris tranform (see e.g. Dress et al. (2007) for a review), which could also be interesting to investigate in the context of arboreal ultrametrics

Finally, as we have seen above, our characterization for arboreal ultrametrics is closely related to the theory of symbolic ultrametrics. In particular, for arboreal ultrametrics we are considering the situation where the symbols are real numbers. It would be interesting to study what might happen if we replace real numbers with other algebraic structures such as groups. Note that this problem has already been considered in the context of symbolic ultrametrics (see e.g. (Semple and Steel, 2003, Section 7.6) for an overview). More generally, it was recently shown that the class of distance-hereditary graphs is precisely the class of undirected graphs that can be explained by arboreal networks Scholz (2025). Thus, it could be interesting to investigate if our results lead to new directions of study in the theory of distance-hereditary graphs.

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Appendix: Proof of Proposition 3.1

Proof: Throughout the proof, we will use the notation given in Algorithm 1. Put $n = |X|$. Let $x_1, \ldots, x_n$ be the wcps computed at Line 1. Let (N_2, ω_2) be the weighted network built at Lines 2 and 3, and for $i \in \{3, \ldots, n\}$, let (N_i, ω_i) be the weighted network obtained after the $(i-2)^{\text{th}}$ instance of the loop initiated at Line 4. Note that for $i \in \{2, \ldots, n\}$, (N_i, ω_i) is a weighted network on $\{x_1, \ldots, x_i\}$. Moreover, since the algorithm terminates immediately after the last instance of the loop, the weighted network (N, ω) returned by Algorithm 1 satisfies $(N, \omega) = (N_n, \omega_n)$. Therefore, it suffices to show that for all $i \in \{2, \ldots, n\}$, (N_i, ω_i) is an ultrametric uprooting of (T_i, λ_i). We shall do this by using induction on i.

As base case, consider the case $i = 2$. Then T_2 has two vertices x_1 and x_2, and one edge $\{x_1, x_2\}$. By construction, N_2 is the rooted tree with vertex set $\{r_2, x, y\}$ and arc set $\{(r_2, x_1), (r_2, x_2)\}$ (Line 2), and we have $\omega((r_2, x_1)) = \omega((r_2, x_2)) = \frac{1}{2}\lambda_2(\{x_1, x_2\})$ (Line 3). From there, one can easily verify that, N_2 is an uprooting of T_2, and since, $\omega((r_0, x_1)) + \omega((r_0, x_2)) = \lambda_2(\{x_1, x_2\})$, it follows that (N_2, ω_2) is a weight-preserving uprooting of (T_2, λ_2). Moreover, $\omega((r_2, x_1)) = \omega((r_2, x_2))$, so (N_2, ω_2) is an ultrametric arboreal network.

Now, let $i > 2$, and suppose that (N_{i-1}, ω_{i-1}) is an ultrametric uprooting of (T_{i-1}, λ_{i-1}). To ease notation, we now put $(N, \omega) = (N_{i-1}, \omega_{i-1})$, and $(N^+, \omega^+) = (N_i, \omega_i)$ (that is, the network obtained after completion of the $(i-2)^{\text{th}}$ instance of the loop). We now show that (N^+, ω^+) is an ultrametric uprooting of (T_i, λ_i), which will complete the proof of the proposition since it implies that the network that is returned in Line 26 has the desired properties.

Let v_i, x_i and x be the elements picked on Line 6, and let p_x be as defined at Line 7. Note that the operations inside of the loop starting on Line 4 are divided into two independent parts. The first part from Line 8 to 19 is concerned with adding a vertex v to the network N, and depends on the relative values of $\omega((p_x, x))$ and $\lambda_i(\{v_i, x\})$. The second part, from Line 20 to Line 25, is concerned with adding the leaf x_i to the network N, and depends on the relative values of $\lambda_i(\{v_i, x_i\})$ and $l_{(N,\omega)}(v, z)$ for some $z \in C_N(v)$. Note that by our induction hypothesis, (N, ω) is ultrametric, so $l_{(N,\omega)}(v, z)$ is independent from the choice of z in $C_N(v)$. In the following, we always understand z as some element in $C_N(v)$, without mentioning this explicitly.

Next, note that the first part has three subcases, respectively $\omega((p_x, x)) > \lambda_i(\{v_i, x\})$ (Line 8), $\omega((p_x, x)) < \lambda_i(\{v_i, x\})$ (Line 11) and $\omega((p_x, x)) = \lambda_i(\{v_i, x\})$ (Line 18), and the second part has two subcases, namely, $\lambda_i(\{v_i, x_i\}) = l_{(N,\omega)}(v, z)$ (Line 20) and $\lambda_i(\{v_i, x_i\}) \neq l_{(N,\omega)}(v, z)$ (Line 23). Therefore, we will complete the proof that (N^+, ω^+) is an ultrametric uprooting of (T_i, λ_i) by considering each of the six resulting combinations.

(1): $\omega((p_x, x)) > \lambda_i(\{v_i, x\})$ and $\lambda_i(\{v_i, x_i\}) = l_{(N,\omega)}(v, z)$ (Lines 8 and 20). In this case N^+ is obtained from N by first subdividing (p_x, x) with the introduction of a new vertex v (Line 9), and adding the arc (v, x_i) (Line 21). By our induction hypothesis, N is an uprooting of T_{i-1}, so $\overline{N}$ and T_{i-1} are isomorphic. Moreover, by construction, $\overline{N^+}$ is obtained from $\overline{N}$ by subdividing the edge incident to x with the introduction of vertex v, and adding the edge $\{v, x_i\}$. Since x and x_i are part of a cherry in T_i, there are two possibilities. Either $v_i = u$ where u is the vertex adjacent to x in T_{i-1}, or v_i has degree 3 and is adjacent to u, x and x_i. The first possibility cannot hold since $\lambda_{i-1}(\{u, x\}) = \lambda_i(\{v_i, x\})$ and $\omega((p_x, x)) \leq \lambda_{i-1}(\{u, x\})$ must hold, which contradicts our assumption that $\omega((p_x, x)) > \lambda_i(\{v_i, x\})$. Therefore the second possibility holds, and so v_i has degree 3 and is adjacent to u, x and x_i. In other

words, T_i can be obtained from T_{i-1} by subdividing the edge (u, x) with the introduction of vertex v_i, and adding the edge $\{v_i, x\}$. Since T_{i-1} and $\overline{N}$ are isomorphic, it follows that T_i and $\overline{N^+}$ are isomorphic. Hence, N^+ is an uprooting of T_i.

We now show that (N^+, ω^+) is an uprooting of (T_i, λ_i). Let $\{w, w'\}$ be an edge of T_i. Suppose first that neither $w = v_i$ nor $w' = v_i$ holds. In this case, w and w' are vertices of N, and by our induction hypothesis, we have $\lambda_{i-1}(\{w, w'\}) = \overline{\omega}(\{w, w'\})$. Moreover, since w and w' are both distinct from v_i, we have $\lambda_{i-1}(\{w, w'\}) = \lambda_i(\{w, w'\})$ and $\overline{\omega^+}(\{w, w'\}) = \overline{\omega}(\{w, w'\})$. Hence, $\overline{\omega^+}(\{w, w'\}) = \lambda_i(\{w, w'\})$ follows. Suppose now that $w = v_i$. Then, w' is one of x, x_i or u. Since $\omega^+(\{v, x\}) = \lambda_i(\{v_i, x\})$ (Line 10), $\overline{\omega^+}(\{v_i, x\}) = \lambda_i(\{v_i, x\})$ follows. Similarly, $\omega^+(\{v, x_i\}) = \lambda_i(\{v_i, x_i\})$ (Line 22), so $\overline{\omega^+}(\{v_i, x_i\}) = \lambda_i(\{v_i, x_i\})$ follows. Finally, we have $\lambda_i(\{v_i, u\}) = \lambda_{i-1}(\{u, x\}) - \lambda_i(\{u, x\})$. If p_x is not a root of N of degree 2, then $\overline{\omega^+}(\{v_i, u\}) = \omega^+((p_x, v)) = \omega((p_x, x)) - \lambda_i(\{v_i, x\})$. By our induction hypothesis, $\omega((p_x, x)) = \overline{\omega}\{u, x\} = \lambda_{i-1}(\{u, x\})$, and so $\overline{\omega^+}((v_i, u)) = \lambda_i(\{v_i, u\})$. This concludes the proof that (N^+, ω^+) is an uprooting of (T_i, λ_i).

It remains to show that (N^+, ω^+) is an ultrametric network. Let w be a root of N^+, and let $z \in C_{N^+}(w)$. Note that $w \neq v$ holds, since v is not a root of N^+. In particular, w is also a root of N. If z is distinct from x and x_i, then z is not a descendant of v. In particular, all arcs on the path from w to z in N^+ are arcs of N, and for all such arcs a, $\omega(a) = \omega^+(a)$ holds. Therefore, $l_{(N^+,\omega^+)}(w, z) = l_{(N,\omega)}(w, z)$. If $z = x$ then the fact that $w \neq v$, together with the fact that $\omega^+((p_x, v)) + \omega^+((v, x)) = \omega((p_x, x))$ (Line 10), also implies that $l_{(N^+,\omega^+)}(w, z) = l_{(N,\omega)}(w, z)$. Using the induction hypothesis that (N, ω) is ultrametric, it follows that for all $z, z' \in C_N(w)$ distinct from x_i, $l_{(N^+,\omega^+)}(w, z) = l_{(N^+,\omega^+)}(w, z')$. Finally, consider the case where $z = x_i$. Then, we have $l_{(N^+,\omega^+)}(w, x_i) = l_{(N^+,\omega^+)}(w, v) + \omega^+((v, x_i))$. Since $\omega^+((v, x_i)) = \omega((v, x))$ (Lines 10 and 22), it follows that $l_{(N^+,\omega^+)}(w, x_i) = l_{(N^+,\omega^+)}(w, x)$. Since, as shown above, $l_{(N^+,\omega^+)}(w, x) = l_{(N^+,\omega^+)}(w, z)$ holds for all $z \in C_{N^+}(w)$ distinct from x_i, we have $l_{(N^+,\omega^+)}(w, x_i) = l_{(N^+,\omega^+)}(w, z)$ for all $z \in C_{N^+}(w)$. This concludes the proof that (N^+, ω^+) is an ultrametric network, and therefore, the proof that (N^+, ω^+) is an ultrametric uprooting of (T_i, λ_i) and the proof for Case **(1)**.

(2): $\omega((p_x, x)) > \lambda_i(\{v_i, x\})$ and $\lambda_i(\{v_i, x_i\}) \neq l_{(N,\omega)}(v, z)$ (Lines 8 and 23). In this case N^+ is obtained from N by first subdividing (p_x, x) with the introduction of a new vertex v (Line 9), and adding a new vertex r and the arcs (r, x_i) and (r, v) (Line 24). By construction, $\overline{N^+}$ is obtained from $\overline{N}$ by subdividing the edge incident to x with the introduction of vertex v, and adding the edge $\{v, x_i\}$. From there, arguments similar as in case (1) imply that N^+ is an uprooting of T_i.

To prove that (N^+, ω^+) is an uprooting of (T_i, λ_i), we first show that $\omega((r, v)) > 0$. By Line 25, we have $\omega((r, v)) = \frac{1}{2}(\lambda_i(\{v_i, x_i\}) - l_{(N,\omega)}(v, z))$ for some $z \in C_N(v)$. Note that since by assumption, $\lambda_i(\{v_i, x_i\}) \neq l_{(N,\omega)}(v, z)$, we have $\omega((r, v)) \neq 0$. Therefore, it suffices to show that $\omega((r, v)) \geq 0$ holds. We next remark that the only possible choice for z is x. So,we have $\omega((r, v)) = \frac{1}{2}(\lambda_i(\{v_i, x_i\}) - l_{(N,\omega)}(v, x)) = \frac{1}{2}(\lambda_i(\{v_i, x_i\}) - \omega((v, x))) = \frac{1}{2}(\lambda_i(\{v_i, x_i\}) - \lambda_i(\{v_i, x\}))$, where the latter equality comes from Line 10. Since $\{v_i, x_i\}$ is the long end of the cherry, $\lambda_i(\{v_i, x_i\}) \geq \lambda_i(\{v_i, x\})$ follows, from which we obtain $\omega((r, v)) \geq 0$. Hence, $\omega((r, v)) > 0$ holds as desired.

Now, let $\{w, w'\}$ be an edge of T_i. If neither $w = v_i$ nor $w' = v_i$ holds, then by the arguments of case (1), we have $\overline{\omega^+}(\{w, w'\}) = \lambda_i(\{w, w'\})$. The same arguments imply that $\overline{\omega^+}(\{v_i, x\}) = \lambda_i(\{v_i, x\})$ and $\overline{\omega^+}((v_i, u)) = \lambda_i(\{v_i, u\})$ hold, as $\omega((p_x, v))$ and $\omega((v, x))$ are defined the same way as in case (1) (Line 10). Finally we have $\overline{\omega^+}(\{v_i, x_i\}) = \omega((r, v)) + \omega((r, x_i)) = \lambda_i(\{v_i, x_i\})$ (Line 25). This concludes the proof that (N^+, ω^+) is an uprooting of (T_i, λ_i).

It remains to show that (N^+, ω^+) is ultrametric. Let w be a root of N^+. If $w = r$, then $C_{N^+}(w)$ con-

tains exactly 2 elements, x and x_i. We have $l_{(N^+,\omega^+)}(r,x) = \omega((r,v)) + \omega((v,x)) = \frac{1}{2}(\lambda_i(\{v_i,x_i\}) - l_{(N,\omega)}(v,z)) + \lambda_i(\{v_i,x\})$ for some $z \in C_N(v)$ (Lines 10 and 25), and $l_{(N^+,\omega^+)}(r,x_i) = \omega((r,x_i)) = \frac{1}{2}(\lambda_i(\{v_i,x_i\}) + l_{(N,\omega)}(v,z))$ for some $z \in C_N(v)$ (Line 25). Hence, $l_{(N^+,\omega^+)}(r,x) = l_{(N^+,\omega^+)}(r,x_i)$ holds. Suppose now that w is distinct from r, and let $z \in C_{N^+}(w)$. Note that z is distinct from x_i since $w \neq r$. Now, let a be an arc from w to z. If a is an arc of N, then $\omega(a) = \omega^+(a)$ holds. Otherwise, a is one of the arcs (p_x,v) or (v,x). Next, we remark that since v has indegree 2 and outdegree 1, and w is distinct from r, the presence of one of these arcs on the path from w to z implies that the other is also present. Moreover, in that case, the arc (p_x,x) is present on the path from w to z in N. Since $\omega((p_x,v)) + \omega((v,x)) = \omega((p_x,x))$ (Line 10), $l_{(N^+,\omega^+)}(w,z) = l_{(N,\omega)}(w,z)$ always holds. Together with the induction hypothesis that (N,ω) is ultrametric, it follows that for all $z,z' \in C_N(w)$, $l_{(N^+,\omega^+)}(w,z) = l_{(N^+,\omega^+)}(w,z')$. This concludes the proof that (N^+,ω^+) is an ultrametric network, and so (N^+,ω^+) is an ultrametric uprooting of (T_i,λ_i) which completes Case **(2)**.

(3): $\omega((p_x,x)) < \lambda_i(\{v_i,x\})$ and $\lambda_i(\{v_i,x_i\}) = l_{(N,\omega)}(v,z)$ (Lines 11 and 20). We claim that this case is impossible. Indeed, by definition, we have $l_{(N,\omega)}(v,z) = l_{(N,\omega)}(p_x,z) - \omega((p_x,v))$. Moreover, $\omega((p_x,v)) = \lambda_i(\{v_i,x\}) - \omega((p_x,x)) > 0$, where the equality comes from Line 17 and the inequality from our assumption $\omega((p_x,x)) < \lambda_i(\{v_i,x\})$. Hence, we have $l_{(N,\omega)}(v,z) < l_{(N,\omega)}(p_x,z)$. Since (N,ω) is ultrametric by our induction hypothesis, we have $l_{(N,\omega)}(p_x,z) = l_{(N,\omega)}(p_x,x)$, and since x is a child of p_x, $l_{(N,\omega)}(p_x,x) = \omega((p_x,x))$. By assumption, $\omega((p_x,x)) < \lambda_i(\{v_i,x\})$. Putting these inequalities together, $l_{(N,\omega)}(v,z) < \lambda_i(\{v_i,x\})$ follows. Finally, since $\lambda_i(\{v_i,x_i\}) = l_{(N,\omega)}(v,z)$ by assumption, we obtain $\lambda_i(\{v_i,x_i\}) < \lambda_i(\{v_i,x\})$, which is impossible by our choice of x_i as the long end of a cherry in (T_i,λ_i).

(4): $\omega((p_x,x)) < \lambda_i(\{v_i,x\})$ and $\lambda_i(\{v_i,x_i\}) \neq l_{(N,\omega)}(v,z)$ (Lines 11 and 23). We first show that in this case, p_x is a root of N of outdegree 2. So, suppose for contradiction that this is not the case. Then p_x is a vertex of T_{i-1}, and therefore, also a vertex of T_i. In particular, we have $\lambda_{i-1}(\{p_x,x\}) \geq \lambda_i(\{v,x\})$. Since $\lambda_{i-1}(\{p_x,x\}) = \omega((p_x,x))$, this contradicts our assumption that $\omega((p_x,x)) < \lambda_i(\{v_i,x\})$.

We now show that N^+ is an uprooting of T_i. Let u be the child of p_x distinct from x. Since p_x is a root of N of degree 2 with children u and x, and T_i and $\overline{N}$ are isomorphic, we have that u is the vertex adjacent to x in T_i. We now consider two subcases, $u = v_i$ and $u \neq v_i$. First, if $u = v_i$, we have $\lambda_{i-1}(\{u,x\}) = \lambda_i(\{v_i,x\})$, and since $\lambda_{i-1}(\{u,x\}) = \overline{\omega}(\{u,x\}) = \omega((p_x,u)) + \omega((p_x,x))$, $\lambda_i(\{v_i,x\}) = \omega((p_x,u)) + \omega((p_x,x))$. Hence, we build N^+ from N by putting $u = v$ (Line 14), adding a new vertex r, and adding the arcs (r,v) and (r,x_i) (Line 24). In particular, $\overline{N^+}$ is obtained from $\overline{N}$ by adding the edge $\{u,x_i\}$. Since $\overline{N}$ and T_{i-1} are isomorphic, and T_i is obtained from T_{i-1} by adding the arc $\{u,x_i\}$, it follows that $\overline{N^+}$ and T_i are isomorphic. Second, if $u \neq v_i$, we have $\lambda_{i-1}(\{u,x\}) > \lambda_i(\{v_i,x\})$, and since $\lambda_{i-1}(\{u,x\}) = \overline{\omega}(\{u,x\}) = \omega((p_x,u)) + \omega((p_x,x))$, $\lambda_i(\{v_i,x\}) < \omega((p_x,u)) + \omega((p_x,x))$. Hence, we build N^+ from N by subdividing the arc (p_x,u) with the introduction of vertex v (Line 16), adding a new vertex r, and adding the arcs (r,v) and (r,x_i) (Line 24). In particular, $\overline{N^+}$ is obtained from $\overline{N}$ by subdividing the edge $\{u,x\}$ with the introduction of vertex v, and adding the edge $\{v,x_i\}$. Since $\overline{N}$ and T_{i-1} are isomorphic, and T_i is obtained from T_{i-1} by subdividin the arc $\{u,x\}$ with the introduction of vertex v_i, and adding the edge $\{v_i,x_i\}$, it follows that $\overline{N^+}$ and T_i are isomorphic. In summary, in both cases, we can conclude that N^+ is an uprooting of T_i.

We now show that (N^+,ω^+) is an uprooting of (T_i,λ_i). First, we show that $\omega((r,v)) > 0$, and in case $\lambda_i(\{v_i,x\}) \neq \omega((p_x,u)) + \omega((p_x,x))$, that $\omega((v,u)) > 0$. To see the latter, recall that in the last paragraph, we showed that $\lambda_i(\{v_i,x\}) \leq \omega((p_x,u)) + \omega((p_x,x))$ always holds. In particular, $\omega((v,u)) = \omega((p_x,u)) + \omega((p_x,x)) - \lambda_i(\{v_i,x\}) \geq 0$, and since $\lambda_i(\{v_i,x\}) \neq \omega((p_x,u)) + \omega((p_x,x))$, the inequality

is strict. We now show that $\omega((r,v)) > 0$. By Line 25, we have $\omega((r,v)) = \frac{1}{2}(\lambda_i(\{v_i,x_i\}) - l_{(N,\omega)}(v,z))$ for some $z \in C_N(v)$. By construction, and since $\omega((v,u)) > 0$, we have $l_{(N,\omega)}(v,z) \leq l_{(N,\omega)}(p_x,z)$. Moreover, (N,ω) is ultrametric by our induction hypothesis, so we have $l_{(N,\omega)}(p_x,z) = l_{(N,\omega)}(p_x,x)$. Since $l_{(N,\omega)}(p_x,x) = \omega((p_x,x))$, we have $l_{(N,\omega)}(v,z) \leq \omega((p_x,x))$. Moreover since by assumption, $\omega((p_x,x)) < \lambda_i(\{v_i,x\})$, we get $l_{(N,\omega)}(v,z) < \lambda_i(\{v_i,x\})$. Finally, since x_i is the long end of its cherry, we have $\lambda_i(\{v_i,x\}) \leq \lambda_i(\{v_i,x_i\})$, and so $l_{(N,\omega)}(v,z) < \lambda_i(\{v_i,x_i\})$ which proves, using the definition of $\omega((r,v))$ at Line 25, that $\omega((r,v)) > 0$.

Now, let $\{w,w'\}$ be an edge of T_i. If $\{w,w'\}$ is an edge of T_{i-1}, then by the arguments used in Case **(1)**, we have $\overline{\omega^+}(\{w,w'\}) = \lambda_i(\{w,w'\})$. Suppose now that $\{w,w'\}$ is not an edge of T_i. If $v_i = u$, the only such edge is $\{v_i,x_i\}$. If otherwise, $v_i \neq u$, then there are three such edges, namely, $\{v_i,x_i\}$, $\{u,v_i\}$ and $\{v_i,x\}$. For $\{v_i,x_i\}$, we have $\overline{\omega^+}(\{v_i,x_i\}) = \omega((r,v)) + \omega((r,x_i)) = \lambda_i(\{v_i,x_i\})$ (Line 25). For $\{u,v_i\}$, we have $\overline{\omega^+}(\{u,v_i\}) = \omega((v,u)) = \omega((p_x,u)) + \omega((p_x,x)) - \lambda_i(\{v_i,x\})$ (Line 17). Since (N,ω) is an uprooting of (T_{i-1},ω_{i-1}), and p_x is a root of N of degree 2, $\omega((p_x,u)) + \omega((p_x,x)) = \lambda_{i-1}(\{u,x\})$. Therefore, we have $\overline{\omega^+}(\{u,v_i\}) = \lambda_{i-1}(\{u,x\}) - \lambda_i(\{v_i,x\}) = \lambda_i(\{u,v_i\})$. Finally, for $\{v_i,x\}$, we have $\overline{\omega^+}(\{v_i,x\}) = \omega((p_x,x)) + \omega((p_x,v)) = \lambda_i(\{v_i,x\})$ (Line 17). This concludes the proof that (N^+,ω^+) is an uprooting of (T_i,λ_i).

It remains to show that (N^+,ω^+) is ultrametric. Let w be a root of N^+. Suppose first that $w = r$, and let $z,z' \in C_N(w)$. If z and z' are distinct from x_i, then z and z' are both descendants of v. In particular, we have $l_{(N^+,\omega^+)}(r,z) = \omega((r,v)) + l_{(N^+,\omega^+)}(v,z)$ and $l_{(N^+,\omega^+)}(r,z') = \omega((r,v)) + l_{(N^+,\omega^+)}(v,z')$. By our induction hypothesis, (N,ω) is ultrametric, so we have $l_{(N^+,\omega^+)}(v,z) = l_{(N^+,\omega^+)}(v,z')$, and $l_{(N^+,\omega^+)}(r,z) = l_{(N^+,\omega^+)}(r,z')$. Otherwise, if $z' = x_i$, then we have $l_{(N^+,\omega^+)}(r,x_i) = \omega^+((r,x_i)) = \frac{1}{2}(\lambda_i(\{v_i,x_i\}) + l_{(N,\omega)}(v,z))$ (Line 25), and $l_{(N^+,\omega^+)}(r,z) = \omega((r,v)) + l_{(N^+,\omega^+)}(v,z) = \frac{1}{2}(\lambda_i(\{v_i,x_i\}) - l_{(N,\omega)}(v,z)) + l_{(N^+,\omega^+)}(v,z)$. Hence $l_{(N^+,\omega^+)}(r,x_i) = l_{(N^+,\omega^+)}(r,z)$. Suppose now that w is distinct from r. Then, arguments similar to the ones used in Case **(2)** (replacing arcs (p_x,x) and (v,x) with (p_x,u) and (v,u), respectively, and remarking that $\omega^+((p_x,v)) + \omega^+((v,u)) = \omega((p_x,u))$ holds by Line 17) lead to the conclusion that $l_{(N^+,\omega^+)}(w,z) = l_{(N^+,\omega^+)}(w,z')$ holds for all $z,z' \in C_N(v)$. It follows that (N^+,ω^+) is ultrametric, which completes Case **(4)**.

(5): $\omega((p_x,x)) = \lambda_i(\{v_i,x\})$ and $\lambda_i(\{v_i,x_i\}) = l_{(N,\omega)}(v,z)$ (Lines 18 and 20). This is a special case of **(1)**, where v is chosen as p_x instead of resulting from a subdivision (Line 19).

(6): $\omega((p_x,x)) = \lambda_i(\{v_i,x\})$ and $\lambda_i(v_i,x_i) \neq l_{(N,\omega)}(v,z)$ (Lines 18 and 23). This is a special case of **(2)**, where v is chosen as p_x instead of resulting from a subdivision (Line 19). □