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Isomorphism of Trees and Isometry of Ultrametric Spaces

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Cover Page Footnote

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Abstract

We study the conditions under which the isometry of spaces with metrics generated by weights given on the edges of finite trees is equivalent to the isomorphism of these trees. Similar questions are studied for ultrametric spaces generated by labelings given on the vertices of trees. The obtained results generalized some facts previously known for phylogenetic trees and for Gurvich—Vyalyi monotone trees.

Keywords and phrases. Monotone tree, equidistant tree, phylogenetic tree, planted tree, finite ultrametric space, isometry of ultrametric spaces, isomorphism of trees, star.

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1 Introduction

In 2001 Gelfand caught the attention of the experts in the theory of lattices with the following problem: using graph theory describe up to isometry all finite ultrametric spaces [18]. An appropriate representation of ultrametric spaces by monotone rooted trees was proposed by V. Gurvich and M. Vyalyi in [15]. A simple geometric description of Gurvich—Vyalyi representing trees was found in [21]. This description allows us to use effectively the Gurvich—Vyalyi representation in various problems associated with finite ultrametric spaces. In particular, this leads to a graph-theoretic interpretation of the Gomory-Hu Inequality [13]. A characterization of finite ultrametric spaces which are as rigid as possible also was obtained [14] on the basis of the Gurvich—Vyalyi representation. Some other extremal properties of finite ultrametric spaces and related properties of monotone rooted trees have been found in [12]. The interconnections between the Gurvich—Vyalyi representation and the space of balls endowed with the Hausdorff metric are discussed in [7] (see also [10, 20, 22–24]).

It is well-known that the sets of leaves of phylogenetic equidistant trees with shortest-path metric are ultrametric. The finite equidistant trees can be considered as finite subtrees of the so-called R-trees (see [1] for some interesting results related to R-trees and ultrametrics). The categorical equivalence of trees and ultrametric spaces was investigated in [17] and [19].

It is interesting to note that, in fact, both the monotone trees and equidistant trees were used in the phylogenetic for the description of related ultrametric spaces long before the publication of paper [15] (see, for example, [25]). The monotone trees and the equidistant trees are dual in a certain sense, but it seems that the description of this duality can be found in Section 7.1 of book [25] only.

In the present paper we discuss the interrelations between weighted trees with shortest-path metrics and labeled trees with corresponding ultrametrics. In particular, the duality of equidistant trees and monotone trees is studied in details for trees which are more general than the classical phylogenetic trees.

The paper is organized as follows.

Section 2 contains some standard definitions from the theory of metric spaces and the theory of graphs. A short list of known properties of Gurvich—Vyalyi representing trees is also given there.

Section 3 deals with the weights and labelings on unrooted trees. In Theorem 3.1 we prove that, for all weights, the isomorphisms of weighted trees coincide with isometries of metric spaces endowed with the corresponding shortest-path metrics and, in Proposition 3.1, we show that this property characterizes the trees among all connected weighted graphs. Proposition 3.2 describes conditions under which the labelings on the vertex sets of trees generate ultrametrics. In Theorem 3.5 it is shown that under the same conditions every connected labeled graph G contains a spanning tree T such that labeling, induced on T, generates the same ultrametric as an original labeling on G. Theorem 3.7, one of the main results of the section, shows that, in the contrast with the weighted trees, the isomorphisms of labeled trees coincide with isometries of generated ultrametric spaces only for trees with one vertex.

In Section 4, after defining the concepts of equidistant weight and monotone labeling for the case of an arbitrary rooted tree, we find explicit formulas describing the transition between these weights and labelings in Proposition 4.1. Good functorial properties of such transition are described by Proposition 4.2.

Theorem 4.3, Theorem 4.4 and Theorem 4.5 are generalizations of the well-known fact about representation of finite ultrametric spaces by phylogenetic trees and by Gurvich—Vyalyi monotone trees.

Proposition 4.5 describes the necessary and sufficient conditions under which isomorphism of equidistant trees (monotone trees) is equivalent to isometricity of corresponding ultrametric spaces.

Section 5 of the paper contains some characteristic properties of ultrametric spaces of leaves of equidistant rooted trees with pendant roots. In particular, Proposition 5.4 describes a new characteristic property of stars in the language of equidistant weights.

Table of notation and symbols

$B(c,r)$	— a ball with radius r and center c, 7.
$\mathbf{B}_X$	— the set of all balls (the ballean) of ultrametric space X, 7.
d_H	— the Hausdorff distance between subsets of metric space, 18.
d_l	— the pseudoultrametric on vertices of tree, 13.
d_w	— the shortest-path metric on vertices of connected, weighted graph, 10.
$\operatorname{diam}(A)$	— the diameter of set A, 3.
$\operatorname{dist}(x,A)$	— the distance from point x to set A, 32.
$\delta(v)$	— the degree of vertex v of graph, 4.
$\delta^+(v)$	— the out-degree of vertex v of rooted tree, 4.
$E(G)$	— the set of all edges of graph G, 4.
$G[X_1,\ldots,X_k]$	— a complete k-partite graph, 5.
$G_{D,X}$	— the diametrical graph of ultrametric space X, 5.
$H \subseteq G$	— H is a subgraph of G, 4.
$H \simeq G$	— the graphs H and G are isomorphic, 6.
$L(T)$	— the set of all leaves of tree T, 4.
$\hat{l} * w$	— the monotone labeling generated by equidistant weight w, 23.
ρ_l	— the pseudoultrametric on vertices of connected, labeled graph, 15.
$T(r)$	— a rooted tree with root r, 4.
$T(r,l)$	— a labeled, rooted tree with root r and labeling l, 4.
$T(r,w)$	— a weighted, rooted tree with root r and weight w, 4.

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$T'(r', w')$	— the weighted rooted tree obtained from a weighted rooted tree $T(r, w)$ by gluing together all pairs of edges with common one-degree vertex, 27.
$T(l)$	— a labeled tree with labeling l, 4.
$T(w)$	— a weighted tree with weight w, 4.
T_v	— the subtree of rooted tree T lying below the vertex v of T, 7.
$T_X = T_X(r, l)$	— the representing tree of ultrametric space X, 5.
$V(G)$	— the set of all vertices of graph G, 4.
$V_0^+(T)$	— the set of vertices of rooted tree T with out-degree equals zero, 21.
$V_1^+(T)$	— the set of vertices of rooted tree T with out-degree equals one, 26.
$V_2^{++}(T)$	— the set of vertices of rooted tree T which have the out-degree greater than or equal two, 27.
$\hat{w} * l$	— the equidistant weight generated by monotone labeling l, 23.
$\|X\|$	— the cardinal number of X, 4.
(X, d)	— a metric space with metric d, 3.
$(X, d) \simeq (Y, \rho)$	— the metric spaces (X, d) and (Y, ρ) are isometric, 3.

2 Initial definitions and facts

Let us recall some concepts from the theory of metric spaces and graph theory.

A *metric* on a set X is a function $d\colon X \times X \to \mathbb{R}^+$, $\mathbb{R}^+ = [0, \infty)$, such that for all x, y, $z \in X$

(i) $d(x, y) = d(y, x)$,

(ii) $(d(x, y) = 0) \Leftrightarrow (x = y)$,

(iii) $d(x, y) \leq d(x, z) + d(z, y)$.

The quantity

$$\operatorname{diam} X = \sup\{d(x, y)\colon x, y \in X\}$$

is the *diameter* of (X, d).

A metric space (X, d) is *ultrametric* if the *strong triangle inequality*

$$d(x, y) \leq \max\{d(x, z), d(z, y)\}.$$

holds for all x, y, $z \in X$. In this case d is called *an ultrametric* on X and (X, d) is an *ultrametric space.*

Definition 2.1. *Metric spaces (X, d) and (Y, ρ) are* isometric *if there is a bijective mapping $\Phi\colon X \to Y$ such that*

$$d(x, y) = \rho(\Phi(x), \Phi(y))$$

holds for all x, $y \in X$. In this case we write $(X, d) \simeq (Y, \rho)$ and say that Φ is an isometry *of (X, d) and (Y, ρ).*

A *graph* is a pair (V, E) consisting of a nonempty set V and a (possibly empty) set E whose elements are unordered pairs of different points from V. For a graph $G = (V, E)$, the sets $V = V(G)$ and $E = E(G)$ are called *the set of vertices (or nodes)* and *the set of edges*, respectively. We say that G is *nonempty* if $E(G) \neq \varnothing$. If $\{x, y\} \in E(G)$, then the vertices x and y are *adjacent*. Recall that a *path* is a nonempty graph P whose vertices can be numbered so that

$$V(P) = \{x_0, x_1, ..., x_k\},\ k \geqslant 1, \quad \text{and} \quad E(P) = \{\{x_0, x_1\}, ..., \{x_{k-1}, x_k\}\}.$$

In this case we say that P is a path joining x_0 and x_k.

A graph G is *finite* if $V(G)$ is a finite set, $|V(G)| < \infty$. In this paper we consider finite graphs only. A finite graph C is a *cycle* if $|V(C)| \geq 3$ and there exists an enumeration v_1, v_2, ..., v_n of its vertices such that

$$(\{v_i, v_j\} \in E(C)) \Leftrightarrow (|i - j| = 1 \quad \text{or} \quad |i - j| = n - 1).$$

A graph H is a *subgraph* of a graph G if

$$V(H) \subseteq V(G) \quad \text{and} \quad E(H) \subseteq E(G).$$

We write $H \subseteq G$ if H is a subgraph of G.

A graph G is *connected* if for every two distinct u, $v \in V(G)$ there is a path $P \subseteq G$ joining u and v. A connected graph without cycles is called a *tree*. A vertex v of a tree T is a *leaf* if the *degree* of v is less than two,

$$\delta(v) = |\{u \in V(T) \colon \{u, v\} \in E(T)\}| < 2.$$

If a vertex v is not a leaf of T, then we say that v is an *internal node* of T.

A tree T may have a distinguished vertex r called the *root*; in this case T is called a *rooted tree* and we write $T = T(r)$.

Let $T = T(r)$ be a rooted tree, let $v \in V(T)$ and let $L(T)$ be the set of all leaves of T. As in [7, 9–14], we will denote by $\delta^+(v)$ the *out-degree* of v,

$$\delta^+(v) = \begin{cases} \delta(v) & \text{if } v = r, \\ \delta(v) - 1 & \text{if } v \neq r. \end{cases}$$

Then $r \in L(T)$ if and only if $\delta^+(r) \leqslant 1$. Moreover, for a vertex v different from the root r, the equality $\delta^+(v) = 0$ holds if and only if $v \in L(T)$.

Definition 2.2. *A* labeled tree $T = T(l)$ *is a tree* T *with a* labeling $l \colon V(T) \to \mathbb{R}^+$. *A* weighted tree $T = T(w)$ *is a nonempty tree* T *with a* weight $w \colon E(T) \to \mathbb{R}^+$. *A labeled (weighted) rooted tree* $T(r, l)$ *(*$T(r, w)$*) is a rooted tree endowed with given labeling* l *(weight* w*).*

Thus, in what follows, we assume that the labels on the tree vertices are some nonnegative numbers.

We also use the notion of complete multipartite graph.

Definition 2.3. *A finite, nonempty graph G is called* complete k-partite *if its vertices can be divided into disjoint nonempty sets $X_1, \ldots, X_k$ so that $k \geqslant 2$ and there are no edges joining the vertices of the same set X_i and any two vertices from different X_i, X_j, $1 \leqslant i, j \leqslant k$ are adjacent. In this case we write $G = G[X_1, \ldots, X_k]$.*

We shall say that G is a *complete multipartite graph* if there exists k such that G is complete k-partite.

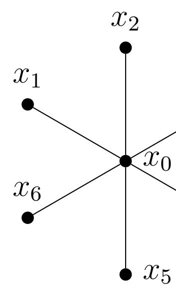

Figure 1: A star $G[X_1, X_2]$, $X_1 = \{x_0\}$, $X_2 = \{x_1, x_2, x_3, x_4, x_5, x_6\}$.

In particular, a *star* is a complete bipartite graph $G[X_1, X_2]$ with $|X_1| = 1$ or $|X_2| = 1$ [2, p. 4].

Definition 2.4 ([6])**.** *Let (X, d) be a finite ultrametric space with $|X| \geqslant 2$. Define a graph $G_{D,X}$ as $V(G_{D,X}) = X$ and*

$$(\{u, v\} \in E(G_{D,X})) \Leftrightarrow (d(u, v) = \operatorname{diam} X)$$

for all u, $v \in V(G_{D,X})$. We call $G_{D,X}$ the diametrical graph *of X.*

Theorem 2.1 ([6])**.** *Let (X, d) be a finite ultrametric space, $|X| \geqslant 2$. Then $G_{D,X}$ is complete multipartite.*

For every nonempty, finite ultrametric space (X, d) we can associate a labeled rooted tree $T_X = T_X(r, l)$ with $r = X$ and $l \colon V(T_X) \to \mathbb{R}^+$ by the following rule (see [21]).

If X is a one-point set, then T_X is the rooted tree consisting of the node X with the label $\operatorname{diam} X = 0$. Note that for the rooted trees consisting only of one node, we consider that this node is the root as well as a leaf.

Let $|X| \geqslant 2$. According to Theorem 2.1 we have $G_{D,X} = G_{D,X}[X_1, ..., X_k]$ and $k \geqslant 2$. In this case the root of the tree T_X is labeled by $\operatorname{diam} X$ and T_X has the nodes $X_1, ..., X_k$ of the first level with the labels

$$l(X_i) = \operatorname{diam} X_i, \tag{2.1}$$

$i = 1, ..., k$. The nodes of the first level with the label 0 are leaves, and those indicated by strictly positive labels are internal nodes of the tree T_X. If the first level has no internal nodes, then the tree T_X is constructed. Otherwise, by repeating the above-described procedure with $X_1, ..., X_k$ instead of X, we obtain the nodes of the second level, etc. Since X is finite, all vertices on some level will be leaves, and the construction of T_X is completed.

The above-constructed labeled rooted tree T_X is called the *representing tree* of the ultrametric space (X, d).

Example 2.1. *Let $X = \{x_1, x_2, x_3, x_4, x_5\}$ be a five-point set and let $d\colon X \times X \to \mathbb{R}^+$ be an ultrametric such that, for all distinct x, $y \in X$, we have*

$$d(x,y) = \begin{cases} 1 & \text{if } x, y \in \{x_1, x_2\}, \\ 2 & \text{if } x, y \in \{x_3, x_4, x_5\}, \\ 3 & \text{if } x \in \{x_1, x_2\} \text{ and } y \in \{x_3, x_4, x_5\}. \end{cases}$$

Then the representing tree of (X, d) is depicted by Figure 2.

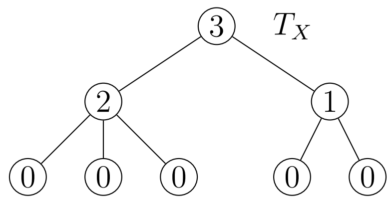

Figure 2: The circles labeled by 0 are the one-point subsets of X and $l^{-1}(1) = \big\{\{x_1, x_2\}\big\}$, $l^{-1}(2) = \big\{\{x_3, x_4, x_5\}\big\}$, $l^{-1}(3) = \big\{X\big\}$.

In the next sections we will need several concepts of isomorphism of graphs and, in particular, isomorphism of of trees.

Definition 2.5. *Let G and H be graphs. A bijection $f\colon V(G) \to V(H)$ is an* isomorphism *of G and H if*

$$(\{u, v\} \in E(G)) \Leftrightarrow (\{f(u), f(v)\} \in E(H))$$

is valid for all u, $v \in V(G)$. The graphs G and H are isomorphic *if there exists an isomorphism $f\colon V(G) \to V(H)$. In this case we write $G \simeq H$.*

For labeled rooted trees, the above definition must be modified as follows.

Definition 2.6. *Let $T_1 = T_1(r_1, l_1)$ and $T_2 = T_2(r_2, l_2)$ be labeled rooted trees. An isomorphism $f\colon V(T_1) \to V(T_2)$ of the free (unrooted, without labelings) trees T_1 and T_2 is an isomorphism of $T_1(r_1, l_1)$ and $T_2(r_2, l_2)$ if $f(r_1) = f(r_2)$ and the equality $l_2(f(v)) = l_1(v)$ holds for every $v \in V(T_1)$. The labeled rooted trees $T_1(r_1, l_1)$ and $T_2(r_2, l_2)$ are isomorphic if there is an isomorphism of these trees.*

Analogously, we can define the isomorphisms of weighted rooted trees, of weighted unrooted trees, of labeled unrooted trees, and of rooted trees without labelings or weights. Thus, if T_1 and T_2 are trees endowed with additional structure, then, by definition, T_1 and T_2 are isomorphic if there exists an isomorphism of (free) trees T_1 and T_2 and this isomorphism preserves the given structure. In this case we will write $T_1 \simeq T_2$. In particular, the formula $T_1(r_1, l_1) \simeq T_2(r_2, l_2)$ means that $T_1 = T_1(r_1, l_1)$ and $T_2 = T_2(r_2, l_2)$ are isomorphic as labeled rooted trees; $T_1(w_1) \simeq T_2(w_2)$ is abbreviation for the statement: $T_1 = T_1(w_1)$ and $T_2 = T_2(w_2)$ are isomorphic as weighted trees, and so on.

Theorem 2.2 ([14]). *Let (X, d) and (Y, ρ) be nonempty, finite ultrametric spaces with the representing trees T_X and T_Y. Then*

$$((X, d) \simeq (Y, \rho)) \Leftrightarrow (T_X \simeq T_Y)$$

is valid.

If $T = T(r)$ is a rooted tree and $u, v \in V(T)$ are distinct, then we say that v is a *successor* of u whenever $u \in V(P)$, where P is the path joining v and r. A successor v of u is a *direct successor* of u if $\{u, v\} \in E(T)$.

The following theorem is a simple modification of Theorem 2.7 [11].

Theorem 2.3. *Let $T = T(r, l)$ be a finite labeled rooted tree. Then the following two conditions are equivalent:*

(i) *For every $u \in V(T)$ we have $\delta^+(u) \neq 1$ and*

$$(\delta^+(u) = 0) \Leftrightarrow (l(u) = 0)$$

and, in addition, the inequality $l(v) < l(u)$ holds whenever v is a direct successor of u.

(ii) *There is a finite, nonempty ultrametric space (X, d) such that*

$$T_X \simeq T(r, l).$$

Recall that a *phylogenetic tree* is a finite unrooted tree T, whose inner nodes have degree at least three, together with a labeling defined on the set of leaves of T (see, for example, [26]). Using Theorem 2.1 and above described procedure of construction of representing trees we can simply prove the following result.

Proposition 2.1. *The following statements are equivalent for every finite tree T.*

(i) *There is a phylogenetic tree T_1 such that T and T_1 are isomorphic as free (unrooted, without labelings) trees.*

(ii) *There is a finite ultrametric space (X, d) such that the diametrical graph $G_{D,X}$ is complete k-partite with $k \geqslant 3$ and T_X and T are isomorphic as free (unrooted, without labelings) trees.*

Let (X, d) be an ultrametric space. Recall that a *ball* with a radius $r \geqslant 0$ and a center $c \in X$ is the set

$$B_r(c) = \{x \in X : d(x, c) \leqslant r\}.$$

The *ballean* $\mathbf{B}_X$ of the ultrametric space (X, d) is the set of all balls of (X, d). Every one-point subset of X belongs to $\mathbf{B}_X$, it is called a *singular* ball.

Let $T = T(r)$ be a rooted tree. For every vertex v of T we denote by T_v the subtree of T such that v is the root of T_v,

$$V(T_v) = \{u \in V(T) : u = v \text{ or } u \text{ is a successor of } v\}, \tag{2.2}$$

and satisfying

$$(\{v_1, v_2\} \in E(T_v)) \Leftrightarrow (\{v_1, v_2\} \in E(T(r))) \tag{2.3}$$

for all v_1, $v_2 \in V(T_v)$. In this situation Charles Semple and Mike Steel say that T_v is a rooted subtree of $T(r)$ lying below v [25, p. 9]. See Figure 3 for an example of such a rooted subtree.

In what follows we write $L = L(T_v)$ to denote the set of all leaves of T_v.

If $T = T_X$ is the representing tree of a finite ultrametric space (X, d) and $v = \{x_1, x_2, \dots, x_n\}$ is a vertex of T_X, $x_i \in X$, $i = 1, \dots, n$, then we have

$$L(T_v) = \{\{x_1\}, \dots, \{x_n\}\}.$$

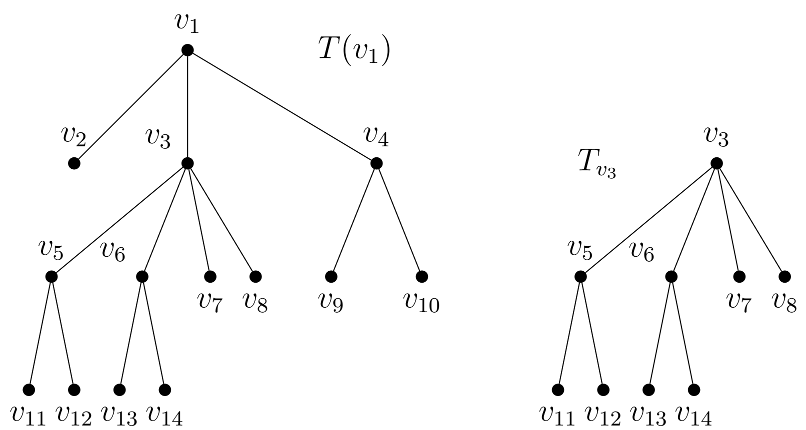

Figure 3: The rooted tree T_{v_3} is a rooted subtree of the rooted tree $T(v_1)$ lying below v_3. Here $L(T_{v_3}) = \{v_7, v_8, v_{11}, v_{12}, v_{13}, v_{14}\}$.

For T_X consisting of one node only, $V(T_X) = X$, we consider that X is the root of T_X as well as a leaf of T_X. Thus, if $X = \{x\}$, then we have $L(T_X) = \{\{x\}\}$.

The following proposition claims that the ballean of every finite ultrametric space (X, d) coincides with the vertex set of T_X.

Proposition 2.2. *Let (X, d) be a finite, nonempty ultrametric space with representing tree T_X. Then the following statements hold:*

(*i*) *For every node $v \in V(T_X)$ there is the unique $B \in \mathbf{B}_X$, $B = \{x_1, \dots, x_n\}$, such that $L(T_v) = \{\{x_1\}, \dots, \{x_n\}\}$. This ball B is singular if and only if $v \in L(T_X)$.*

(*ii*) *For every $B \in \mathbf{B}_X$, $B = \{x_1, \dots, x_n\}$, there is the unique $v \in V(T_X)$ such that $L(T_v) = \{\{x_1\}, \dots, \{x_n\}\}$. This vertex v is a leaf of T if and only if B is singular.*

This proposition is a simple modification of the corresponding result from [22] (see also Theorem 2.5 in [7]).

The proofs of Theorem 2.2, Theorem 2.3 and Proposition 2.2 are based on the next basic theorem.

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Theorem 2.4 ([10]). *Let (X, d) be a finite ultrametric space and let x_1 and x_2 be two distinct points of X. If P is the path joining the distinct leaves $\{x_1\}$ and $\{x_2\}$ in T_X, then we have*

$$d(x_1, x_2) = \max_{v \in V(P)} l(v),$$

where the labeling $l\colon V(T_X) \to \mathbb{R}^+$ is defined as in (2.1).

The next section of the paper contains several results which can be considered as extensions of Theorem 2.4 to the case of unrooted, labeled trees.

Comments on the concept of graph isomorphism

All above introduced notions of isomorphism can be considered as some specifications of the following general definition. (See Definition 1 in [16].)

Let $G = (V, E, L_V, L_E, l)$ be a graph with $V(G) = V$, $E(G) = E$ and such that L_V and L_E are some sets of vertex labels and edge labels, respectively, and let $f\colon (V \cup E) \to L_V \cup L_E$ be a mapping for which $f(V) \subseteq L_V$ and $f(E) \subseteq L_E$ hold.

Definition 2.7. *The graphs*

$$G_1 = (V_1, E_1, L_{V_1}, L_{E_1}, l_1) \quad \textit{and} \quad G_2 = (V_2, E_2, L_{V_2}, L_{E_2}, l_2)$$

are isomorphic if there is a bijection $f\colon V_1 \to V_2$ such that:

(i) $l_1(v) = l_2(f(v))$ *for every* $v \in V_1$.

(ii) $(\{u, v\} \in E_1) \Leftrightarrow (\{f(u), f(v)\} \in E_2)$ *for all* u, $v \in V_1$.

(iii) $l_1(\{u, v\}) = l_2(\{f(u), f(v)\})$ *for every* $\{u, v\} \in E_1$.

Two definitions of graph isomorphism are equivalent if any two graphs are isomorphic w.r.t the first definition if and only if these graphs are isomorphic w.r.t. the second one. For the case when

$$G_1 = (V_1, E_1, L_{V_1}, L_{E_1}, l_1) \quad \text{and} \quad G_2 = (V_2, E_2, L_{V_2}, L_{E_2}, l_2)$$

are trees, Definition 2.7 is equivalent to:

- Definition 2.5 if $L_{V_1} \cup L_{E_1} = L_{V_2} \cup L_{E_2} = \{0\}$.
- The definition of isomorphic rooted trees if $L_{V_1} \cup L_{E_1} = L_{V_2} \cup L_{E_2} = \{0, 1\}$ and there are the unique $v_1^* \in V_1$ and $v_2^* \in V_2$ such that $l_i(v_i^*) = 1$ and $l_i(e) = l_i(v) = 0$ whenever $e \in E_i$ and $v \in V_i \setminus \{v_i^*\}$, $i = 1$, 2.
- The definition of isomorphic labeled trees if $L_{V_1} = L_{V_2} = \mathbb{R}^+$ and $L_{E_1} = L_{E_2} = \{0\}$.

Similarly, we can find specifications of Definition 2.7 which are equivalent to definitions of isomorphisms of phylogenetic trees, weighted trees, weighted rooted trees, and weighted labeled trees, but we prefer to use several independent definitions of isomorphism to simplify the statements of future results.

The concept of equivalent isomorphisms (= equivalent definitions of isomorphism) can be more satisfactory described on the basis of category theory, but this is not the subject of the paper.

3 Weights and labelings on unrooted trees

Let $G(w)$ be a finite weighted graph. The weight $w\colon E(G) \to \mathbb{R}^+$ is *strictly positive* if $w(e) > 0$ holds for every $e \in E(G)$.

If $w\colon E(G) \to \mathbb{R}^+$ is strictly positive, then the weighted *shortest-path metric* is the mapping $d_w\colon V(G) \times V(G) \to \mathbb{R}^+$ defined as

$$d_w(u,v) = \begin{cases} 0, & \text{if } u = v \\ \min_{P \in \mathcal{P}_{u,v}} \sum_{e \in P} w(e), & \text{if } u \neq v, \end{cases} \tag{3.1}$$

where $\mathcal{P}_{u,v}$ is the set of all paths joining u and v in G. (If G is a tree, then, for any pair of distinct u, $v \in V(G)$, the set $\mathcal{P}_{u,v}$ contains the unique path.) For the case when $w(e) = 1$ holds for every $e \in E(G)$, the metric d_w is called the *graph metric* on G.

It is easy to prove that the connected graphs G_1 and G_2 are isomorphic as free, unweighted graphs if and only if the metric spaces $(V(G_1), d_1)$ and $(V(G_2), d_2)$ are isometric, where d_i is the graph metric on G_i, $i = 1, 2$. The following theorem is a partial generalization of this fact.

Theorem 3.1. *Let $T_1 = T_1(w_1)$ and $T_2 = T_2(w_2)$ be finite weighted trees with strictly positive weights. Then a mapping $f\colon V(T_1) \to V(T_2)$ is an isometry of the metric spaces $(V(T_1), d_{w_1})$ and $(V(T_2), d_{w_2})$ if and only if it is an isomorphism of the weighted trees $T_1(w_1)$ and $T_2(w_2)$.*

Proof. Let u, $v \in V(T_1)$. If f is an isomorphism of $T_1(w_1)$ and $T_2(w_2)$, then, using the definition of isomorphism of weighted trees, (3.1) and the uniqueness of the path $P_{u,v}$ joining u and v in T_1, we obtain the equality

$$d_{w_1}(u,v) = d_{w_2}(f(u), f(v)).$$

Hence, f is an isometry of the metric spaces $(V(T_1), d_{w_1})$ and $(V(T_2), d_{w_2})$.

Conversely, let f be an isometry of $(V(T_1), d_{w_1})$ and $(V(T_2), d_{w_2})$. Then it is easy to see that f is an isomorphism of weighted trees $T_1(w_1)$ and $T_2(w_2)$ if and only if f is an isomorphism of free (unweighted) trees T_1 and T_2. To prove that f is an isomorphism of T_1 and T_2 it suffices to show that the implication

$$(\{u_1, v_1\} \in E(T_1)) \Rightarrow (\{f(u_1), f(v_1)\} \in E(T_2)) \tag{3.2}$$

is valid for all u_1, $v_1 \in V(T_1)$. Indeed, (3.2) implies

$$E(T_2) \supseteq \{\{f(u_1), f(v_1)\} \colon \{u_1, v_1\} \in E(T_1)\}.$$

Since f is bijective, we have $|V(T_1)| = |V(T_2)|$. Moreover, since T_1 and T_2 are trees, the equalities $|V(T_1)| = |E(T_1)| + 1$ and $|V(T_2)| = |E(T_2)| + 1$ (see, for example, [5, Corollary 1.53]) hold. Consequently, we have

$$|E(T_1)| = |E(T_2)|. \tag{3.3}$$

Now from (3.2) and (3.3) it follows that

$$(\{u_1, v_1\} \in E(T_1)) \Leftrightarrow (\{f(u_1), f(v_1)\} \in E(T_2)).$$

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Let us prove (3.2). Suppose contrary that $\{f(u_1), f(v_1)\} \notin E(T_2)$. Then there exists a path $P^2 = (v_1^*, v_2^*, \ldots, v_n^*)$ such that $P^2 \subseteq T_2$, $n \geqslant 3$, and $v_1^* = f(u_1)$, $v_n^* = f(v_1)$. By (3.1), we have

$$d_{w_2}(v_1^*, v_n^*) = \sum_{i=1}^{n-1} w_2(\{v_i^*, v_{i+1}^*\}) = \sum_{i=1}^{n-1} d_{w_2}(v_i^*, v_{i+1}^*). \tag{3.4}$$

Since f is an isometry of $(V(T_1), d_{w_1})$ and $(V(T_2), d_{w_2})$, from (3.4) it follows that

$$\begin{aligned} d_{w_1}(u_1, v_1) = d_{w_1}(u_1, f^{-1}(v_2^*)) + d_{w_1}(f^{-1}(v_{n-1}^*), v_1) \\ + \sum_{i=2}^{n-2} d_{w_1}(f^{-1}(v_i^*), f^{-1}(v_{i+1}^*)). \end{aligned} \tag{3.5}$$

(For $i = 2, \ldots, n-2$ we identify the one-point set $f^{-1}(v_i^*)$ with the unique point of this set.)

Since T_1 is a tree, there are

a path $P_1^1 \subseteq T_1$ joining $f^{-1}(v_1^*) = u_1$ and $f^{-1}(v_2^*)$,

a path $P_2^1 \subseteq T_1$ joining $f^{-1}(v_2^*)$ and $f^{-1}(v_3^*)$,

$\ldots$,

and a path $P_{n-1}^1 \subseteq T_1$ joining $f^{-1}(v_{n-1}^*)$ and $f^{-1}(v_n^*) = v_1$.

Using (3.1) again we can write (3.5) as

$$w_1(\{u_1, v_1\}) = \sum_{i=1}^{n-1} \sum_{e \in E(P_i^1)} w(e). \tag{3.6}$$

Let us consider a graph G such that

$$V(G) = \bigcup_{i=1}^{n-1} V(P_i^1) \quad \text{and} \quad E(G) = \bigcup_{i=1}^{n-1} E(P_i^1).$$

It is clear that G is connected, $G \subseteq T_1$, and u_1, $v_1 \in V(G)$. Since T_1 is a tree, G is a subtree of T_1. Consequently, there is a unique path $P_{u,v}$ joining u_1 and v_1 in G. From $G \subseteq T_1$ it follows that $P_{u,v}$ is a path joining u_1 and v_1 in T_1. But the unique path joining u_1 and v_1 in T_1 is $(\{u_1, v_1\}$. Thus, $\{u_1, v_1\} \in E(G)$. Since $w_1(e) > 0$ holds for every $e \in E(T_1)$, equality (3.6) implies $E(G) = \{\{u_1, v_1\}\}$. The last equality contradicts the definition of the path P^2.

The validity of (3.2) follows. □

Corollary 3.2. *Let (X, d) be a finite metric space. Suppose that $T_1 = T_1(w_1)$ and $T_2 = T_2(w_2)$ are weighted trees with strictly positive weights such that*

$$X = V(T_1) = V(T_2).$$

Then the equalities $d = d_{w_1} = d_{w_2}$ imply $T_1(w_1) = T_2(w_2)$.

Proof. It follows from Theorem 3.1 with identical $f\colon X \to X$, $f(x) = x$ for every $x \in X$. □

Corollary 3.3. *Let $T_1 = T_1(w_1)$ and $T_2 = T_2(w_2)$ be finite weighted trees with strictly positive weights. Then the equivalence*

$$(T_1(w_1) \simeq T_2(w_2)) \Leftrightarrow ((V(T_1), d_{w_1}) \simeq (V(T_2), d_{w_2})) \tag{3.7}$$

is valid.

The concept of isomorphism of weighted trees can be naturally extended to the concept of isomorphism of weighted graphs. Let $G_1 = G_1(w_1)$ and $G_2 = G_2(w_2)$ be connected, nonempty graphs with the weights $w_1\colon E(G_1) \to \mathbb{R}^+$ and $w_2\colon E(G_2) \to \mathbb{R}^+$. We write $G_1(w_1) \simeq G_2(w_2)$ and say that $G_1(w_1)$ and $G_2(w_2)$ are isomorphic if there is a bijection $f\colon V(G_1) \to V(G_2)$ such that

$$(\{u, v\} \in E(G_1)) \Leftrightarrow (\{f(u), f(v)\} \in E(G_2))$$

for all u, $v \in V(G_1)$ and, moreover,

$$w_1(\{u, v\}) = w_2(\{f(u), f(v)\})$$

holds whenever $\{u, v\} \in E(G_1)$.

The following result shows that the validity of (3.7) is a characteristic property of trees.

Proposition 3.1. *Let G_1 and G_2 be finite, connected, nonempty graphs. Then the following statements are equivalent:*

(*i*) *G_1 and G_2 are trees.*

(*ii*) *The equivalence*

$$(G_1(w_1) \simeq G_2(w_2)) \Leftrightarrow ((V(G_1), d_{w_1}) \simeq (V(G_2), d_{w_2}))$$

is valid for all strictly positive $w_1\colon E(G_1) \to \mathbb{R}^+$ and $w_2\colon E(G_2) \to \mathbb{R}^+$.

Proof. $(i) \Rightarrow (ii)$. This implication is valid by Corollary 3.3.

$(ii) \Rightarrow (i)$. As in the proof of Theorem 3.1, it is easy to see that the implication

$$(G_1(w_1) \simeq G_2(w_2)) \Rightarrow ((V(G_1), d_{w_1}) \simeq (V(G_2), d_{w_2}))$$

is valid. But, in general, the converse implication is false.

Indeed, suppose that G is a finite, connected, nonempty graph which contains a cycle C, $C \subseteq G$. Let e_0 be a fixed edge of C. Write $G_i = G$ for $i = 1, 2$. We can define two weights $w_1\colon E(G_1) \to \mathbb{R}^+$ and $w_2\colon E(G_2) \to \mathbb{R}^+$ such that

$$w_1(e_0) = 1 + |E(G)|, \quad w_2(e_0) = 2 + |E(G)| \tag{3.8}$$

and $w_1(e) = w_2(e) = 1$ whenever $e \in E(G)$ but $e \neq e_0$. Since

$$w_1(E(G_1)) = \{1, 1 + |E(G)|\} \neq \{1, 2 + |E(G)|\} = w_2(E(G_2))$$

holds, the weighted graphs $G_1(w_1)$ and $G_2(w_2)$ cannot be isomorphic. Now using (3.1) and (3.8) we see that both the metric spaces $(V(G_1), d_{w_1})$ and $(V(G_2), d_{w_2})$ are isometric to the metric space $(V(G \setminus e_0), d)$, where $G \setminus e_0$ denotes the connected graph obtained from G by deleting e_0 and d is the graph metric on $V(G \setminus e_0)$. □

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Remark 3.1. *The characterization of trees obtained in Proposition 3.1 is similar to the characterizations of trees which were given in Corollary 3.6 of [8] and Corollary 5 of [9].*

Remark 3.2. *It was noted by referee of the present paper that Theorem 3.1, Proposition 3.1 and Theorem 4.3 from the next section are closely connected with Buneman's four-point condition [3].*

Theorem 3.1 and Proposition 3.1 give rise the following problem:

Problem 3.1. *Let $G_1(w_1)$ and $G_2(w_2)$ be connected, weighted graphs with strictly positive weights. Find conditions under which every isometry $f\colon V(G_1) \to V(G_2)$ of the metric spaces $(V(G_1), d_{w_1})$ and $(V(G_2), d_{w_2})$ is an isomorphism of $G_1(w_1)$ and $G_2(w_2)$.*

In the rest of the section we consider the labeled, unrooted trees and related ultrametric spaces and find some modifications of Theorem 2.4, Theorem 3.1, Proposition 3.1 and Problem 3.1 in this case.

Let $T = T(l)$ be a labeled tree with labeling $l\colon V(T) \to \mathbb{R}^+$ and let $d_l\colon V(T)\times V(T) \to \mathbb{R}^+$ be a mapping defined as

$$d_l(u, v) = \begin{cases} 0, & \text{if } u = v \\ \max\limits_{v^* \in V(P)} l(v^*), & \text{if } u \neq v, \end{cases} \tag{3.9}$$

where P is the unique path joining u and v in T.

In the next proposition we consider arbitrary (infinite, finite or empty) trees (cf. Theorem 2.4).

Proposition 3.2. *The following statements are equivalent for every labeled tree $T = T(l)$.*

(i) The function d_l is an ultrametric on $V(T)$.

(ii) The function d_l is a metric on $V(T)$.

(iii) The inequality

$$\max\{l(u_1), l(v_1)\} > 0 \tag{3.10}$$

holds for every $\{u_1, v_1\} \in E(T)$.

Proof. $(i) \Rightarrow (ii)$. It follows directly from the definitions of metrics and ultrametrics.

$(ii) \Rightarrow (iii)$. Let (ii) hold and let $\{u_1, v_1\} \in E(T)$. Then $u_1 \neq v_1$ holds because T has no loops. Since d_l is a metric, from $u_1 \neq v_1$ it follows that

$$d_l(u_1, v_1) > 0. \tag{3.11}$$

Since $P = (u_1, v_1)$ is the unique path joining u_1 and v_1 in T, by (3.9) we have

$$d_l(u_1, v_1) = \max_{v \in V(P)} l(v) = \max\{l(u_1), l(v_1)\}.$$

Now using (3.11) we obtain (3.10).

$(iii) \Rightarrow (i)$. Let (iii) hold. It is clear that d_l is symmetric and nonnegative. Statement (iii) and the definition of d_l imply that the inequality $d_l(u, v) > 0$ holds for all pairs of distinct u, $v \in V(T)$. Thus, to complete the proof of validity of (i), it suffices to show that the strong triangle inequality

$$d_l(v_1, v_2) \leqslant \max\{d_l(v_1, v_3), d_l(v_3, v_2)\} \tag{3.12}$$

holds for all v_1, v_2, $v_3 \in V(T)$.

Let v_1, v_2, $v_3 \in V(T)$. It is easy to see (3.12) holds if we have $v_i = v_j$ for some different i, $j \in \{1, 2, 3\}$. Suppose that $v_1 \neq v_2 \neq v_3 \neq v_1$. Write $P_{i,j}$ for the path joining v_i and v_j in T. $1 \leqslant i < j \leqslant 3$. From (3.9) it follows that

$$\max\{d_l(v_1, v_3), d_l(v_3, v_2)\} = \max\{l(v) \colon v \in V(P_{1,3}) \cup V(P_{3,2})\}. \tag{3.13}$$

Let

$$T_{1,2,3} = T[V(P_{1,3}) \cup V(P_{3,2})]$$

be the subgraph of T induced by $V(P_{1,3}) \cup V(P_{3,2})$. Since v_1, $v_2 \in T_{1,2,3}$ and $T_{1,2,3}$ is connected, the uniqueness of path joining v_1 and v_2 implies $P_{1,2} \subseteq T_{1,2,3}$. Hence, $V(P_{1,2}) \subseteq V(T_{1,2,3})$ holds. Consequently

$$\max\{l(v) \colon v \in V(P_{1,2})\} \leqslant \max\{l(v) \colon v \in V(T_{1,2,3})\}. \tag{3.14}$$

The equality

$$d_l(v_1, v_2) = \max\{l(v) \colon v \in V(P_{1,2})\},$$

(3.13) and (3.14) imply (3.12). □

Remark 3.3. *If $T = T(l)$ is a labeled tree but there is $\{u_1, v_1\} \in E(T)$ such that $l(u_1) = l(v_1) = 0$, then the mapping $d_l \colon V(T) \times V(T) \to \mathbb{R}^+$ is an pseudoultrametric on $V(T)$, i.e., d_l is a symmetric, nonnegative mapping satisfying the strong triangle inequality.*

Corollary 3.4. *Let $T_1 = T_1(l_1)$ and $T_2 = T_2(l_2)$ be labeled trees such that*

$$\max\{l_i(u_i), l_i(v_i)\} > 0 \tag{3.15}$$

for every $\{u_i, v_i\} \in E(T_i)$, $i = 1, 2$. Then the implication

$$(T_1(l_1) \simeq T_2(l_2)) \Rightarrow (V(T_1, d_{l_1}) \simeq V(T_2, d_{l_2})) \tag{3.16}$$

is valid.

Proof. By Proposition 3.2, inequality (3.15) implies that d_{l_1} and d_{l_2} are ultrametrics. Hence, the right hand side in (3.15) is defined correctly. Now (3.16) follows directly from the definition of isomorphism of labeled rooted trees and formula (3.9). □

The following example shows that the converse implication

$$(V(T_1, d_{l_1}) \simeq V(T_2, d_{l_2})) \Rightarrow (T_1(l_1) \simeq T_2(l_2))$$

is false in general.

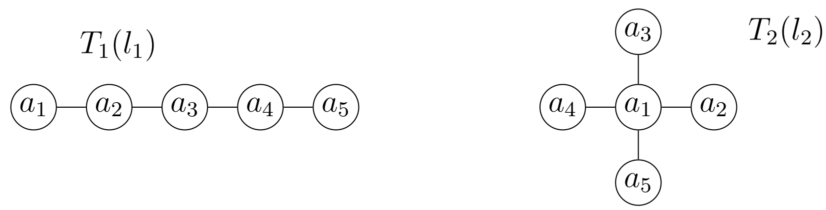

Figure 4: The labeled path $T_1(l_1)$ and the labeled star $T_2(l_2)$ generate some isometric ultrametric spaces.

Example 3.1. *Let $a_1, \ldots, a_5$ be a sequence of real numbers such that*

$$0 = a_1 < a_2 \leqslant \ldots \leqslant a_5.$$

Then the ultrametric spaces $V(T_1, d_{l_1})$ and $V(T_2, d_{l_2})$ are isometric for the labeled trees $T_1 = T_1(l_1)$ and $T_2 = T_2(l_2)$ depicted by Figure 4.

Now we expand the construction of mapping d_l, defined by formula (3.9) for labeled trees, to the case of arbitrary finite connected, labeled graph.

Let $G = G(l)$ be a connected, finite graph with a labeling $l\colon V(G) \to \mathbb{R}^+$ and let $\rho_l\colon V(G) \times V(G) \to \mathbb{R}^+$ be a mapping defined as

$$\rho_l(u,v) = \begin{cases} 0, & \text{if } u = v \\ \min\limits_{P \in \mathcal{P}_{u,v}} \max\limits_{v^* \in V(P)} l(v^*), & \text{if } u \neq v, \end{cases} \tag{3.17}$$

where $\mathcal{P}_{u,v}$ is the set of all paths joining u and v in G.

In the formulation of the next theorem we use the notion of *spanning tree*. Recall that a tree T is a *spanning tree* for a graph G if $T \subseteq G$ and $V(T) = V(G)$ hold. It is well-known that a graph G is connected if and only if G contains a spanning tree (see, for example, [2, Theorem 4.6]).

Theorem 3.5. *For every finite connected graph $G = G(l)$ with labeling $l\colon V(G) \to \mathbb{R}^+$ there is a labeled tree $T = T(l)$ such that T is a spanning tree for G and the equality $\rho_l = d_l$ holds.*

Proof. Let us denote by $\Delta(G)$ the number $|E(G)| + 1 - |V(G)|$,

$$\Delta(G) = |E(G)| + 1 - |V(G)|.$$

We give a proof by induction on $\Delta(G)$.

Since G is connected, we have $|V(G)| \geqslant |E(G)| + 1$. The equality $|V(G)| = |E(G)| + 1$ holds if and only if G is tree (see, for example, [5, Corollary 1.53]). Hence, for $\Delta(G) = 0$, the graph G is a tree and the theorem is valid. Suppose the theorem is valid if $\Delta(G) \leqslant N$ for some nonnegative integer N. Let $\Delta(G) = N + 1$ hold. Then G contains a cycle C. Let v_1 be a vertex of C such that

$$l(v_1) = \max\{l(v)\colon v \in V(C)\} \tag{3.18}$$

and let u_1 be a vertex of C for which the edge $e_1 = \{u_1, v_1\}$ belongs to $E(C)$. Write G^1 for the graph $G \setminus \{e_1\}$ obtained from G by deleting e_1. Then G^1 is connected and we have

$$\Delta(G^1) \leqslant N - 1 \quad \text{and} \quad V(G^1) = V(G).$$

Hence, by induction hypothesis, there is a spanning tree T^1 with the same labeling $l\colon V(T^1) \to \mathbb{R}^+$ and satisfying the equality $\rho_l^1 = d_l$ with

$$\rho_l^1(u,v) = \begin{cases} 0, & \text{if } u = v \\ \min\limits_{P \in \mathcal{P}_{u,v}^1} \max\limits_{v^* \in V(P)} l(v^*), & \text{if } u \neq v, \end{cases} \tag{3.19}$$

where $\mathcal{P}_{u,v}^1$ is the set of all paths joining u and v in G^1. To complete the proof it suffices to show that $\rho_l^1 = \rho_l$. Since $\mathcal{P}_{u,v}^1 \subseteq \mathcal{P}_{u,v}$ holds, we have $\rho_l^1(u,v) \geqslant \rho_l(u,v)$ for all u, $v \in V(G)$. Hence, $\rho_l^1 = \rho_l$ if and only if

$$\rho_l^1(u,v) \leqslant \rho_l(u,v) \tag{3.20}$$

holds for all u, $v \in V(G)$. Inequality (3.20) holds if, for every path $P \in \mathcal{P}_{u,v}$, there is a path $P^1 \in \mathcal{P}_{u,v}^1$ such that

$$\max_{v^* \in V(P)} l(v^*) \geqslant \max_{v^* \in V(P^1)} l(v^*). \tag{3.21}$$

The existence of the path $P^1 \in \mathcal{P}_{u,v}^1$ satisfying (3.21) is trivial if $e_1 \notin E(P)$. Let $e_1 \in E(P)$ and let $C \setminus e_1$ and $P \setminus e_1$ be connected graphs obtained from C and, respectively, from P by deleting e_1. Write W for the graph with

$$V(W) = V(P) \cup V(C)$$

and

$$E(W) = E(P \setminus e_1) \cup E(C \setminus e_1).$$

Then we have

$$\begin{aligned} \max_{v^* \in V(W)} l(v^*) &= \max\left\{ \max_{v^* \in V(P \setminus e_1)} l(v^*), \max_{v^* \in V(C \setminus e_1)} l(v^*) \right\} \\ &= \max\left\{ \max_{v^* \in V(P \setminus e_1)} l(v^*), l(v_1) \right\} = \max_{v^* \in V(P \setminus e_1)} l(v^*) = \max_{v^* \in V(P)} l(v^*). \end{aligned} \tag{3.22}$$

Since W is a connected graph, there is a path $P^2 \subseteq W$ joining u and v in W. Consequently,

$$\max_{v^* \in V(P^2)} l(v^*) \leqslant \max_{v^* \in V(W)} l(v^*) \tag{3.23}$$

holds. Inequality (3.21) follows from (3.22) and (3.23) with $P^1 = P^2$. □

Corollary 3.6. *The following statements are equivalent for every finite, connected, labeled graph $G = G(l)$:*

(i) *The function ρ_l is an ultrametric on $V(G)$.*

(ii) *The function ρ_l is a metric on $V(G)$.*

(*iii*) *The inequality*

$$\max\{l(u_1), l(v_1)\} > 0 \tag{3.24}$$

holds for every $\{u_1, v_1\} \in E(G)$.

Proof. Proposition 3.2 and Theorem 3.5 imply that $(i) \Leftrightarrow (ii)$ is valid.

Let $G = G(l)$ be a finite, connected, labeled graph and let $T = T(l)$ be a spanning tree such that $d_l = \rho_l$ holds. Since $E(G) \supseteq E(T)$ holds, statement (iii) of the present corollary implies statement (iii) of Proposition 3.2. Thus, we also have $(iii) \Rightarrow (i)$.

Let us prove the validity $(i) \Rightarrow (iii)$. Let (i) hold. Suppose now that $l(u_1) = l(v_1) = 0$ for some $\{u_1, v_1\} \in E(G)$. Then using (3.17) we obtain $\rho_l(u_1, v_1) = 0$, contrary to (i). □

Example 3.1 gives rise the following problem (cf. Problem 3.1).

Problem 3.2. *Let* $G_1 = G_1(l_1)$ *and* $G_2 = G_2(l_2)$ *be labeled, connected graphs such that*

$$\max\{l_i(u_i), l_i(v_i)\} > 0$$

for every $\{u_i, v_i\} \in E(G_i)$, $i = 1, 2$. *Find conditions under which*

$$(G_1(l_1) \simeq G_2(l_2)) \Leftrightarrow ((V(G_1), \rho_{l_1}) \simeq (V(G_2), \rho_{l_2})) \tag{3.25}$$

is valid. Is the statement

- *Every isometry* $f\colon V(G_1) \to V(G_2)$ *of the ultrametric spaces* $(V(G_1), \rho_{l_1})$ *and* $(V(G_2), \rho_{l_2})$ *is an isomorphism of* $G_1(l_1)$ *and* $G_2(l_2)$

true if (3.25) *is valid?*

In what follows we give a partial solution of Problem 3.2 for labeled rooted trees.

Theorem 3.7. *Let* $T_i = T_i(r_i, l_i)$ *be finite labeled rooted tree such that* $\delta^+(u_i) \neq 1$ *and*

$$(\delta^+(u_i) = 0) \Leftrightarrow (l(u_i) = 0) \tag{3.26}$$

for every $u_i \in V(T_i)$ *and, in addition,* $l(v_i) < l(u_i)$ *holds whenever* v_i *is a direct successor of* u_i, $i = 1, 2$. *Then the following statements hold:*

(*i*) $(T_1(l_1) \simeq T_2(l_2)) \Leftrightarrow ((V(T_1), d_{l_1}) \simeq (V(T_2), d_{l_2}))$ *is valid.*

(*ii*) *If the ultrametric spaces* $(V(T_1), d_{l_1})$ *and* $(V(T_2), d_{l_2})$ *are isometric, then the following conditions are equivalent:*

  (ii_1) $|V(T_1)| = |V(T_2)| = 1$.

  (ii_2) *Every isometry* $f\colon V(T_1) \to V(T_2)$ *of* $(V(T_1), d_{l_1})$ *and* $(V(T_2), d_{l_2})$ *is an isomorphism of* $T_1(l_1)$ *and* $T_2(l_2)$.

In proving this theorem we will use some results describing the structure of balleans $\mathbf{B}_X$ of finite ultrametric spaces (X, d) (see, in particular, Proposition 2.2).

Let A and B be two nonempty bounded subsets of a metric space (X, d). The *Hausdorff distance* $d_H(A, B)$ between A and B is defined by

$$d_H(A, B) = \max\{\sup_{a\in A} \inf_{b\in B} d(a, b), \sup_{b\in B} \inf_{a\in A} d(a, b)\}. \tag{3.27}$$

The definition and some properties of the Hausdorff distance can be found in [4]. See also [23, 24] for properties of Hausdorff distance in ultrametric spaces. We note only that if $\{a\}$ and $\{b\}$ are singular balls in (X, d), then (3.27) implies

$$d_H(\{a\}, \{b\}) = d(a, b).$$

The following lemma is a part of Theorem 2.5 from [7].

Lemma 3.8. *Let (X, d) be a finite nonempty ultrametric space with the representing tree T_X and let B_1 and B_2 be distinct balls in (X, d). If P is the path joining B_1 and B_2 in T_X, then*

$$d_H(B_1, B_2) = \max_{u\in V(P)} l(u).$$

Lemma 3.8 and Proposition 3.2 imply that $(\mathbf{B}_X, d_H)$ is a finite ultrametric space for every finite ultrametric space (X, d). Now we want to describe the structure of the representing tree $T_{\mathbf{B}_X}$.

Definition 3.1. *Let T_1 and T_2 be trees and let x be a leaf of T_2. Suppose we have*

$$V(T_2) = V(T_1) \cup \{x\}, \quad x \notin V(T_1), \quad E(T_1) \subseteq E(T_2).$$

In this case we say that T_2 is obtained from T_1 by adding the leaf x to the vertex u.

Remark 3.4. *It is easy to see that if T_2 is obtained from T_1 by adding a leaf x, then there is a unique $u \in V(T_1)$ such that $\{x, y\} \in E(T_2)$.*

In the following lemma we consider an ultrametric space (X, d) with X satisfying the condition

$$\{Y\} \nsubseteq X \tag{3.28}$$

for every $Y \subseteq X$. We note that for every ultrametric space (Z, ρ) there is an ultrametric space (X, d) such that $(X, d) \simeq (Z, \rho)$ and (3.28) holds for every $Y \subseteq X$.

Lemma 3.9. *Let (X, d) be a finite ultrametric space with the representing tree $T_X = T_X(X, l)$, let $\mathbf{B}_X$ be the ballean of (X, d) and let d_H be the Hausdorff distance on $\mathbf{B}_X$. Then the representing tree $T_{\mathbf{B}_X}$ of the ultrametric space $(\mathbf{B}_X, d_H)$ and the labeled rooted tree $T_1 = T_1(r_1, l_1)$, $r_1 = X$, obtained from T_X by adding a leaf to every internal vertex of T_X and labeled such that*

$$l_1(v_1) = \begin{cases} l(v_1), & \text{if } v_1 \in V(T_X) \\ 0, & \text{if } v_1 \notin V(T_X), \end{cases}$$

are isomorphic as labeled rooted trees.

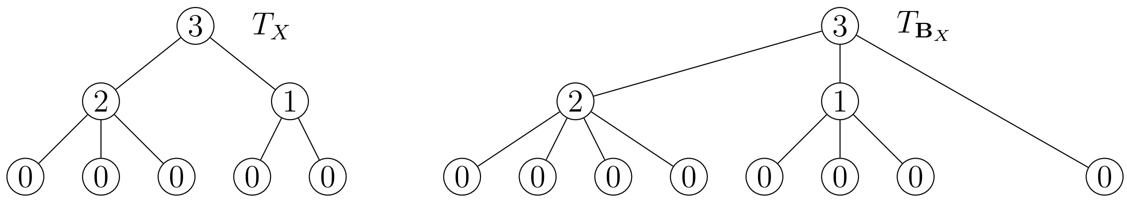

Figure 5: The representing tree T_X of finite ultrametric space (X, d) (from Example 2.1) and the representing tree $T_{\mathbf{B}_X}$ of $(\mathbf{B}_X, d_H)$.

For the proof of this lemma see Theorem 3.10 in [7]. An example of transition from representing tree T_X to representing tree $T_{\mathbf{B}_X}$ is given by Figure 5.

Our next lemma is a direct consequence of Lemma 3.9.

Lemma 3.10. *Let (X_1, d_1) and (X_2, d_2) be finite, nonempty ultrametric spaces. Then the equivalence*

$$(T_{X_1} \simeq T_{X_2}) \Leftrightarrow (T_{\mathbf{B}_{X_1}} \simeq T_{\mathbf{B}_{X_2}})$$

is valid.

In the proof of Theorem 3.7 we also use the next simple fact.

Lemma 3.11. *If $f\colon V(T_1) \to V(T_2)$ is an isomorphism of labeled trees $T_1 = T_1(l_1)$ and $T_2 = T_2(l_2)$, then the equality*

$$d_{l_1}(u_1, v_1) = d_{l_2}(f(u_1), f(v_1))$$

holds for all u_1, $v_1 \in V(T_1)$.

Proof. It follows from the definition of isomorphism of labeled trees and (3.9). □

Proof of Theorem 3.7. (i). By Corollary 3.4 the implication

$$(T_1(l_1) \simeq T_2(l_2)) \Rightarrow ((V(T_1), d_{l_1}) \simeq (V(T_2), d_{l_2}))$$

is valid. Suppose that $(V(T_1), d_{l_1})$ and $(V(T_2), d_{l_2})$ are isometric. Since $(V(T_i), d_{l_i})$ is ultrametric, Theorem 2.2 implies

$$((V(T_1), d_{l_1}) \simeq (V(T_2), d_{l_2})) \Leftrightarrow (T_{V(T_1)} \simeq T_{V(T_2)}),$$

where $T_{V(T_1)}$ and $T_{V(T_2)}$ are the representing trees of $(V(T_1), d_{l_1})$ and $(V(T_2), d_{l_2})$, respectively. Thus,

$$T_{V(T_1)} \simeq T_{V(T_2)} \tag{3.29}$$

is valid. Using Theorem 2.3 we find finite ultrametric spaces (X_1, d_1) and (X_2, d_2) such that

$$T_{X_1} \simeq T(r_1, l_1) \quad \text{and} \quad T_{X_2} \simeq T(r_2, l_2). \tag{3.30}$$

Proposition 2.2, Lemma 3.8 and (3.30) imply

$$(\mathbf{B}_{X_i}, d_{H_i}) \simeq (V(T_i), d_{l_i}), \quad i = 1, 2, \tag{3.31}$$

where d_{H_1} and d_{H_2} are the Hausdorff distances generated by d_1 and d_2, respectively (see (3.27)). By Theorem 2.2, statement (3.31) implies

$$\mathbf{B}_{X_i} \simeq T_{V(T_i)}. \tag{3.32}$$

Now using (3.29) and (3.32) we have $\mathbf{B}_{X_1} \simeq \mathbf{B}_{X_2}$. By Lemma 3.10,

$$T_{X_1} \simeq T_{X_2} \tag{3.33}$$

is valid. From (3.30) and (3.33) it follows that

$$T(r_1, l_1) \simeq T(r_2, l_2),$$

which implies $T(l_1) \simeq T(l_2)$. Statement (i) is proved.

(ii). Let $(V(T_1), d_{l_1})$ and $(V(T_2), d_{l_2})$ be isometric. The implication $(ii_1) \Rightarrow (ii_2)$ is trivially valid. Suppose (ii_2) holds, but (ii_1) is false. Then we have

$$|V(T_1)| = |V(T_2)| \geqslant 2. \tag{3.34}$$

By condition of the theorem, the attitude

$$\delta^+(r_1) \neq 1 \neq \delta^+(r_2) \tag{3.35}$$

satisfied. Using (3.34) and (3.35) we obtain

$$\delta^+(r_1) \geqslant 2 \quad \text{and} \quad \delta^+(r_2) \geqslant 2. \tag{3.36}$$

By statement (i), from $(V(T_1), d_{l_1}) \simeq (V(T_2), d_{l_2})$ it follows that there is an isomorphism $f\colon V(T_1) \to V(T_2)$ of $T_1(l_1)$ and $T_2(l_2)$. Lemma 3.11 implies that the mapping f is also an isometry of $(V(T_1), d_{l_1})$ and $(V(T_2), d_{l_2})$.

Let v_1^* be a leaf of T_1 and let u_1^* be the unique vertex of T_1 such that $\{v_1^*, u_1^*\} \in E(T_1)$. Since f is an isomorphism of $T_1(l_1)$ and $T_2(l_2)$, the vertex $v_2^* = f(v_1^*)$ is a leaf of T_2 and $\{v_2^*, u_2^*\} \in E(T_2)$ holds with $u_2^* = f(u_1^*)$. Using (3.26) we also see that

$$l_1(v_1^*) = l_2(v_2^*) = 0 \quad \text{and} \quad l_1(u_1^*) = l_2(u_2^*) > 0.$$

Let us define the bijection $g\colon V(T_2) \to V(T_2)$ as

$$g(v_2) = \begin{cases} v_2^*, & \text{if } v_2 = u_2^* \\ u_2^*, & \text{if } v_2 = v_2^* \\ v_2, & \text{otherwise.} \end{cases} \tag{3.37}$$

Then the composition

$$V(T_1) \xrightarrow{f} V(T_2) \xrightarrow{g} V(T_2) \tag{3.38}$$

is not an isomorphism T_1 and T_2 because v_1^* is a leaf of T_1, but $g(f(v_1^*))$ is an inner node of T_2, $g(f(v_1^*)) = g(v_2^*) = u_2^*$.

Since f is an isometry, mapping (3.38) is an isometry if and only if g is an isometry. Using (3.37) and Definition 2.1 we can simply prove that g is an isometry if and only if

$$d_{l_2}(x, u_2^*) = d_{l_2}(x, v_2^*) \tag{3.39}$$

holds whenever

$$u_2^* \neq x \neq v_2^* \tag{3.40}$$

and $x \in V(T_2)$.

Let $x \in V(T_2)$ satisfy (3.40). Let us consider the path $P_1 = (v_1, \ldots, v_n)$ joining $v_2^* = v_1$ and $x = v_n$, and the path $P_2 = (u_1, \ldots, u_m)$ joining $u_2^* = u_1$ and $x = u_m$. Since v_2^* is a leaf of T_2, $\{u_2^*, v_2^*\} \in E(T_2)$ (because $\{u_1^*, v_1^*\} \in E(T_1)$ and f is an isomorphism of T_1 and T_2), we obtain the equalities

$$m + 1 = n \quad \text{and} \quad v_2 = u_1,\ v_3 = u_2,\ \ldots,\ v_n = u_{m-1} = u_m.$$

Now equality (3.39) follows from (3.9) and the equality $l_2(v_2^*) = 0$. □

We conclude this section with a simple example of connected labeled graph $G(l)$ for which the group of isomorphisms of $G(l)$ coincides with the group isometries of $(V(G), \rho_l)$.

Example 3.2. *Let $G = G(l)$ be the labeled graph shown in Figure 6. Then every isometry $f\colon V(G) \to V(G)$ from $(V(G), \rho_l)$ to $(V(G), \rho_l)$ is an isomorphism from $G(l)$ to $G(l)$.*

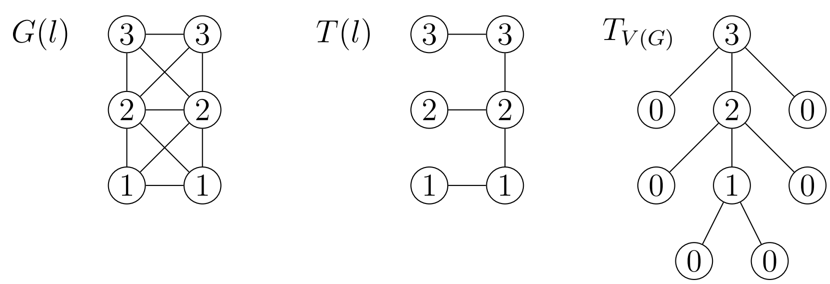

Figure 6: Here $T = T(l)$ is a spanning tree for $G(l)$ satisfying the equality $\rho_l = d_l$ and $T_{V(G)}$ is the representing tree for the ultrametric space $(V(G), \rho_l)$.

4 Isomorphisms of monotone trees and of equidistant trees

Let $T = T(r)$ be a rooted tree. Write

$$V_0^+(T) = \{v \in V(T)\colon \delta^+(v) = 0\}. \tag{4.1}$$

It is clear that $V_0^+(T) \subseteq L(T)$ and $V_0^+(T) = L(T)$ if and only if $r \notin L(T)$ or $V(T) = \{r\}$.

Now, following [27, Definition 19.30], we introduce the concept of equidistant tree.

Definition 4.1. *Let $T = T(r, w)$ be a finite weighted rooted tree with strictly positive w. The weight w is* equidistant *if there is a constant K such that, for every $u \in V_0^+(T)$,*

$$K = \sum_{i=1}^{n-1} w(\{v_i, v_{i+1}\}), \tag{4.2}$$

where $(v_1, \dots, v_n)$ is the path joining the root $r = v_1$ with the leaf $u = v_n$ in T. In this case we say that $T(r, w)$ is equidistant.

Note that the root r of an equidistant tree $T = T(r, w)$ can be a leaf of T (see Figure 7).

We will also say that a labeling $l\colon V(T) \to \mathbb{R}^+$ of a labeled rooted tree $T = T(r, l)$ is *monotone* if

$$l^{-1}(0) = V_0^+(T)$$

and, in addition, the inequality

$$l(v) < l(u) \tag{4.3}$$

holds whenever v is a direct successor of u.

A tree is *monotone* if it is a labeled rooted tree with monotone labeling. By Theorem 2.3, the tree T_X is monotone for every finite ultrametric space (X, d).

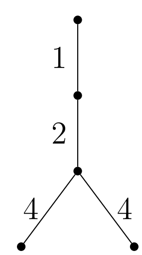

Figure 7: The rooted trees in which the root has degree 1 are known as planted trees. It is an example of planted, equidistant tree satisfying equality (4.2) with $K = 7$.

The following proposition gives us a tool for the investigation of a duality between equidistant trees and monotone trees.

Proposition 4.1. *Let $T = T(r)$ be a finite, nonempty rooted tree. Then the following statements hold:*

(i) For every monotone labeling $l\colon V(T) \to \mathbb{R}^+$ there is the unique equidistant weight $w\colon E(T) \to \mathbb{R}^+$ such that

$$w(\{u, v\}) = \frac{1}{2}(l(u) - l(v)) \tag{4.4}$$

holds whenever v is a direct successor of u.

(ii) For every equidistant weight $w\colon E(T) \to \mathbb{R}^+$ there is the unique monotone labeling $l\colon V(T) \to \mathbb{R}^+$ such that (4.4) holds whenever v is a direct successor of u.

Proof. (*i*) Let $l\colon V(T) \to \mathbb{R}^+$ be monotone. Since for every $\{u, v\} \in E(T)$ either u is a direct successor of v or v is a direct successor of u, there is the unique weight $w\colon E(T) \to \mathbb{R}^+$ for which (4.4) holds whenever v is a direct successor of u. We must prove that w is equidistant.

Equality (4.4) implies that $w(e) > 0$ for every $e \in E(T)$, i.e., w is strictly positive. Let $v \in V_0^+(T)$ and let $(v_1, \ldots, v_n)$ be a path in T such that $v_1 = r$ and $v_n = v$. Then using (4.4) and the equality $l(v) = 0$ we obtain

$$\begin{aligned}\sum_{i=1}^{n-1} w(\{v_i, v_{i+1}\}) &= \sum_{i=1}^{n-1} \frac{1}{2}(l(v_i) - l(v_{i+1})) \\ &= \frac{1}{2}(l(v_1) - l(v_n)) = \frac{1}{2}(l(r) - l(v)) = \frac{1}{2}l(r).\end{aligned}$$

Hence (4.2) holds with $K = \frac{1}{2}l(r)$. Thus w is equidistant.

(*ii*) Let $w\colon E(T) \to \mathbb{R}^+$ be equidistant. For every $u \in V(T)$ we define $l(u)$ by

$$2l(u) = \begin{cases} K, & \text{if } u = r \\ K - \sum_{j=1}^{n-1} w(\{u_j, u_{j+1}\}), & \text{if } u \neq r, \end{cases} \tag{4.5}$$

where $u_1 = r$, $u_n = u$ and $(u_1, \ldots, u_n)$ is the unique path joining the root r and the node u in T and K is the constant defined by (4.2). Then (4.2) and (4.5) imply that $l(v_0) = 0$ holds for every $v_0 \in V_0^+(T)$. Moreover, if v is a direct successor of u, then using (4.5) we obtain

$$2l(v) = 2l(u) - w(\{u, v\}),$$

which implies (4.4).

Suppose that $l_1\colon V(T) \to \mathbb{R}^+$ is a monotone labeling such that $l_1 \neq l$ but

$$w(\{u, v\}) = \frac{1}{2}(l_1(u) - l_1(v)) \tag{4.6}$$

holds whenever v is a direct successor of u. Since l_1 and l are monotone, we have $l_1(v) = l(v)$ for every $v \in V_0^+(T)$. Hence, there is

$$u^* \in V(T) \setminus V_0^+(T) \tag{4.7}$$

such that $l_1(u^*) \neq l(u^*)$ but $l_1(v) = l(v)$ for every successor of u^*. Condition (4.7) implies that the set of all successors of u^* is nonempty. Let v^* be a direct successor of u^*. Then using (4.4) and (4.6) we obtain

$$\begin{aligned}\frac{1}{2}(l_1(u^*) - l_1(v^*)) = w(\{u^*, v^*\}) &= \frac{1}{2}(l(u^*) - l(v^*)), \\ l_1(u^*) - l_1(v^*) &= l(u^*) - l(v^*), \\ l_1(u^*) &= l(u^*),\end{aligned}$$

contrary to $l_1(u^*) \neq l(u^*)$. Statement (*ii*) is proved. □

Figure 8 gives us an example of equidistant tree and the corresponding monotone tree.

In what follows we write $\hat{l} * w$ and $\hat{w} * l$ for the monotone labeling and, respectively, for equidistant weight obtained from the equidistant $w\colon E(T) \to \mathbb{R}^+$ and, respectively, from the monotone $l\colon V(T) \to \mathbb{R}^+$ by (4.4).

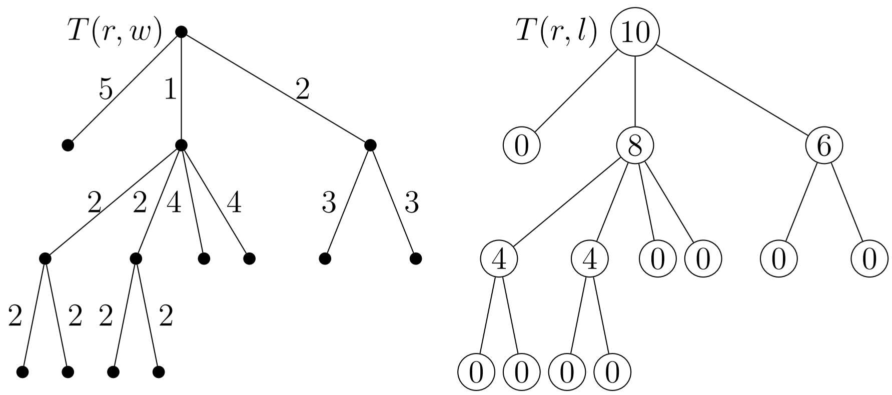

Figure 8: The weight w and labeling l satisfy (4.4) whenever v is a direct successor of u.

Proposition 4.2. *Let $T_1 = T_1(r_1)$ and $T_2 = T_2(r_2)$ be finite, nonempty rooted trees. Then the following statements hold:*

(i) $(T_1(r_1, \hat{l} * w_1) \simeq T_2(r_2, \hat{l} * w_2)) \Leftrightarrow (T_1(r_1, w_1) \simeq T_2(r_2, w_2))$ *is valid for all equidistant weights* $w_1 \colon E(T_1) \to \mathbb{R}^+$ *and* $w_2 \colon E(T_2) \to \mathbb{R}^+$.

(ii) $(T_1(r_1, \hat{w} * l_1) \simeq T_2(r_2, \hat{w} * l_2)) \Leftrightarrow (T_1(r_1, l_1) \simeq T_2(r_2, l_2))$ *is valid for all monotone labelings* $l_1 \colon V(T_1) \to \mathbb{R}^+$ *and* $l_2 \colon V(T_2) \to \mathbb{R}^+$.

(iii) The equalities

$$\hat{w} * (\hat{l} * w_1) = w_1 \quad \text{and} \quad \hat{l} * (\hat{w} * l_1) = l_1 \tag{4.8}$$

are satisfied for every equidistant weight $w_1 \colon E(T_1) \to \mathbb{R}^+$ *and every monotone labeling* $l_1 \colon V(T_1) \to \mathbb{R}^+$.

Proof. Statements (i) and (ii) follow directly from Proposition 4.1 and the definitions of isomorphic weighted graphs and of isomorphic labeled graphs.

(iii) Let $w_1 \colon E(T_1) \to \mathbb{R}^+$ be an equidistant weight. By statement (i) of Proposition 4.1, $l = \hat{l} * w_1$ is the unique monotone labeling satisfying

$$\frac{1}{2}(\hat{l} * w_1(u) - \hat{l} * w_1(v)) = w_1(\{u, w\}) \tag{4.9}$$

whenever v is a direct successor of u. By statement (ii) of Proposition 4.1, $\hat{w} * (\hat{l} * w_1)$ is the unique equidistant weight satisfying

$$\frac{1}{2}(\hat{l} * w_1(u) - \hat{l} * w_1(v)) = \hat{w} * (\hat{l} * w_1)(\{u, w\}) \tag{4.10}$$

whenever v is a direct successor of u. Equalities (4.9) and (4.10) imply the first equality in (4.8). The second one can be proved similarly. □

The constant K in Definition 4.1 of equidistant trees has a simple geometric interpretation. It is the distance between the root r and arbitrary $v_0 \in V_0^+(T)$ in the metric space $(V(T), d_w)$, where d_w is the metric defined by rule (3.1) with $G = T$ and equidistant w.

Analogously, if $l = \hat{l} * w$, then, for every $v \in V(T)$, the value $\frac{1}{2}l(v)$ is the distance in $(V(T), d_w)$ between v and arbitrary $v_0 \in V_0^+(T_v)$, where T_v is the rooted subtree of $T(r, w)$ lying below v (see (2.2), (2.3)).

Remark 4.1. *Let C be an arbitrary strictly positive real number. Proposition 4.1 remains valid if we replace formula (4.4) with the formula*

$$w(\{u, w\}) = C(l(u) - l(v)),$$

but the following two lemmas are valid only in the case $C = \frac{1}{2}$.

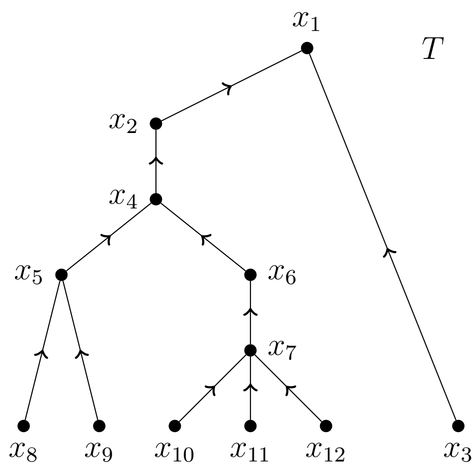

Figure 9: Let x be a root of T, $u_1 = x_8$ and $u_2 = x_{12}$. Then $P = (u_1, v_1, v_2, v_3, v_4, u_2) = (x_8, x_5, x_4, x_6, x_7, x_{12})$ and $v_{i^*} = x_4$. Vertex x_4 is the first common vertex of two paths which join x_8 and x_{12} with the root $r = x_1$.

Lemma 4.1. *Let $T = T(r, w)$ be an equidistant tree, let $l = \hat{l} * w$ be the corresponding monotone labeling, let u_1, u_2 be two different points of the set $V_0^+(T)$ and P be the path joining u_1 and u_2 in T. Then*

$$d_w(u_1, u_2) = \max_{v \in V(P)} l(v) \tag{4.11}$$

holds.

Proof. Let $P = (v_0, v_1, \ldots, v_n, v_{n+1})$ and $v_0 = u_1$, $v_{n+1} = u_2$ hold. It can be shown (see Figure 9) that there is $i^* \in \{1, \ldots, n\}$ such that:

- v_i is a direct successor of v_{i+1} if $i + 1 \leqslant i^*$;
- v_{i+1} is a direct successor of v_i if $i + 1 > i^*$.

Since $\delta^+(u_1) = \delta^+(u_2) = 0$, it is clear also that v_0 is a direct successor of v_1 and v_{n+1} is a direct successor of v_n. Now from (3.1) and (4.4) it follows that

$$2d_w(u_1, u_2) = 2d_w(v_0, v_{n+1}) = (l(v_1) - l(v_0)) + \sum_{i=1}^{i^*-1}(l(v_{i+1}) - l(v_i))$$
$$+ \sum_{i=i^*}^{n-1}(l(v_i) - l(v_{i+1})) + (l(v_n) - l(v_{n+1})) = 2l(v_{i^*}) - (l(u_1) + l(u_2)). \quad (4.12)$$

The labeling $l = \hat{l} * w$ is monotone. Hence we have

$$l(v^*) = \max_{1 \leqslant i \leqslant n} l(v_i) \quad \text{and} \quad l(u_1) = l(u_2) = 0. \quad (4.13)$$

Equality (4.11) follows from (4.12) and (4.13). □

A dual form of Lemma 4.1 can be formulated as follows (cf. Theorem 2.4).

Lemma 4.2. *Let $T = T(r, l)$ be a finite monotone rooted tree, let $w = \hat{w} * l$ and let u_1, $u_2 \in V_0^+(T)$ be different. Then (4.11) holds for the path P joining u_1 and u_2 in T.*

It is well known that, for phylogenetic equidistant trees, the restriction of d_w on the set of leaves of T is an ultrametric (see Theorem 7.2.5 in [25]). Lemma 4.1 and Proposition 3.2 imply the following generalization of this result.

Theorem 4.3. *Let $T = T(w)$ be a finite weighted tree with strictly positive weight and let*

$$d_w \colon V(T) \times V(T) \to \mathbb{R}^+$$

be the corresponding shortest-path metric. If there is $r \in V(T)$ such that $T(r, w)$ is an equidistant tree, then the restriction $d_w|_{V_0^+(T) \times V_0^+(T)}$ is an ultrametric on $V_0^+(T)$.

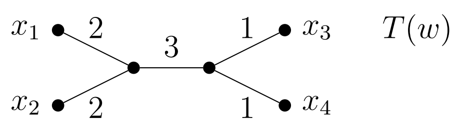

Figure 10: The restriction of d_w on the set $X = \{x_1, x_2, x_3, x_4\}$ of the leaves of $T(w)$ is an ultrametric.

There is a weighted tree $T = T(w)$ such that the restriction of shortest-path metric d_w on the set $L = L(T)$ of all leaves of T is an ultrametric but the tree $T(r, w)$ is not equidistant for any choice of the root $r \in V(T)$. (See Figure 10.) Since, for every $r \in V(T)$, we have

$$V_0^+(T) \subseteq L(T),$$

the restriction $d_w|_{V_0^+(T) \times V_0^+(T)}$ is also an ultrametric on $V_0^+(T)$. Thus, the converse theorem to Theorem 4.3 does not hold in general.

Let $T = T(r, w)$ be a weighted rooted tree. In what follows we will use the denotation

$$V_1^+(T) = \{v \in V(T) \colon \delta^+(v) = 1\}. \quad (4.14)$$

Proposition 4.3. *Let $T = T(r, w)$ be an equidistant tree and let $\delta^+(v) \geqslant 2$ hold for some $v \in V(T)$. Then there is an equidistant tree $T' = T'(r', w')$ such that*

$$V_1^+(T') = \varnothing, \quad V_0^+(T) = V_0^+(T'), \quad V(T') \subseteq V(T),$$
$$|V(T')| + |V_1^+(T)| = |V(T)|, \tag{4.15}$$

and

$$d_w|_{V_0^+(T)\times V_0^+(T)} = d_{w'}|_{V_0^+(T')\times V_0^+(T')}.$$

Proof. The proposition is evident if $|V_0^+(T)| = 1$ or $V_1^+(T) = \varnothing$. Let $V_1^+(T) \neq \varnothing$ and $|V_0^+(T)| \geqslant 2$ hold. The last inequality holds if and only if the set

$$V_2^{++}(T) = \{v \in V(T) \colon \delta^+(v) \geqslant 2\}$$

is nonempty. Since $\delta^+(r)$ is strictly positive, we have either $r \in V_2^{++}(T)$, or $r \in V_1^+(T)$. We first do the case $r \in V_2^{++}(T)$. Starting from the tree $T(r, w)$ we define an equidistant tree $T' = T'(r', w')$ by the following inductive rule.

We choose an arbitrary $v^* \in V_1^+(T)$ and consider the weighted rooted tree $T_1 = T_1(r_1, w_1)$ such that

$$r_1 = r \quad \text{and} \quad V(T_1) = V(T) \setminus \{v^*\} \quad \text{and} \tag{4.16}$$
$$E(T_1) = \Big(E(T) \cup \big\{\{u_1, u_2\}\big\}\Big) \setminus \big\{\{u_1, v^*\}, \{u_2, v^*\}\big\}, \tag{4.17}$$

and

$$w_1(e) = \begin{cases} w(e), & \text{if } e \in E(T) \\ w(\{u_1, v^*\}) + w(\{v^*, u_2\}), & \text{if } e = \{u_1, u_2\}, \end{cases} \tag{4.18}$$

where u_1 and u_2 are the neighbors of v^* in T. If $V_1^+(T_1) = \varnothing$, then we set

$$T'(r', w') = T_1(r_1, w_1).$$

Otherwise, by repeating the above-described procedure with $T_1(r_1, w_1)$ instead of $T(r, w)$, we obtain the weighted rooted tree $T_2(r_2, w_2)$, etc. Since $V_1^+(T)$ is finite and

$$|V_1^+(T)| = |V_1^+(T_1)| + 1 = |V_1^+(T_2)| + 2 = \dots$$

holds, we have $V_1^+(T_k) = \varnothing$ for some $k \geqslant 1$. Thus $T'(r', w') = T_k(r_k, w_k)$ and the construction of T' is completed.

It follows from (4.16)–(4.18), that

$$r' = r, \quad V(T') = V_0^+(T) + V_2^{++}(T), \quad V_1^+(T') = \varnothing$$

and $V_0^+(T') = V_0^+(T) = L(T')$, where $L(T')$ is the set of leaves of T'. Moreover, the equality

$$d_w(u', v') = d_{w'}(u', v')$$

holds for all u', $v' \in V(T')$. Hence $T'(r', w')$ is equidistant and

$$d_w|_{V_0^+(T)\times V_0^+(T)} = d_{w'}|_{V_0^+(T)\times V_0^+(T)} = d_{w'}|_{V_0^+(T')\times V_0^+(T')}. \tag{4.19}$$

In the case $r \in V_1^+(T)$ we define the weighted rooted tree $T_1(r_1, w_1)$ such that r_1 is the unique direct successor of r,

$$V(T_1) = V(T) \setminus \{r\}, \quad E(T_1) = E(T) \setminus \{\{r_1, r\}\}$$

and $w_1 = w|_{E(T_1)}$. Repeating this procedure, we find the smallest positive integer k_0 such that $r_{k_0} \in V_2^{++}(T)$. The weighted rooted tree $T_{k_0} = T_{k_0}(r_{k_0}, w_{k_0})$ is equidistant and

$$d_w|_{V(T_{k_0}) \times V(T_{k_0})} = d_{w_{k_0}} \quad \text{and} \quad V_0^+(T) = V_0^+(T_{k_0}).$$

Now using (4.16)–(4.18) with $T_{k_0}(r_{k_0}, w_{k_0})$ instead of $T(r, w)$ we can construct $T'(r', w')$ such that $V_1^+(T') = \varnothing$ and (4.19) hold. □

Remark 4.2. *The condition*

- *there is $v \in V(T)$ such that $\delta^+(v) \geqslant 2$*

cannot be dropped in Proposition 4.3. If the inequality $\delta^+(v) \leqslant 1$ holds for all $v \in V(T)$, then $T = T(r, w)$ is a weighted path joining the root r with the unique vertex belonging to the one-point set $V_0^+(T)$. In this case we have the equality

$$|V_1^+(T)| + 1 = |V(T)|,$$

which together with (4.15) *implies $|V(T')| = 1$. Thus, T' is empty, contrary to Definition 2.2*

An example of transition from $T(r, w)$ to $T'(r', w')$ is given by Figure 11.

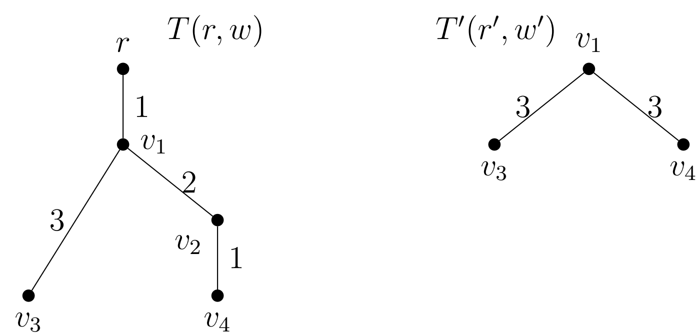

Figure 11: Here $T(r, w)$ and $T'(r', w')$ are equidistant, $r' = v_1$ and $w'(\{u, v\}) = d_w(u, v)$ holds for every $\{u, v\} \in E(T')$.

Remark 4.3. *The set $V_2^{++}(T')$ has the following nice geometric interpretation:*

- *A point x of the metric space $(V(T), d_w)$ belongs to $V_2^{++}(T')$ if and only if*

$$d_w(y, x) = d_w(x, z) = \frac{1}{2} d_w(y, z)$$

holds for some distinct y, $z \in V_0^+(T)$.

The following proposition can be considered as a generalization of Theorem 7.2.8 from [25].

Proposition 4.4. *Let $T_1(r_1, w_1)$ and $T_2(r_2, w_2)$ be equidistant trees. Then*

$$\Big(T_1'(r_1', w_1') \simeq T_2'(r_2', w_2')\Big) \Leftrightarrow \Big(\Big(V_0^+(T_1), d_{w_1}|_{V_0^+(T_1)\times V_0^+(T_1)}\Big) \simeq \Big(V_0^+(T_2), d_{w_2}|_{V_0^+(T_2)\times V_0^+(T_2)}\Big)\Big)$$

is valid

Proof. It follows from Proposition 4.2 and Theorem 2.2. □

Theorem 4.4. *Let $T = T(r)$ be a finite rooted tree. Then the following statements are equivalent:*

(i) *The set $V_1^+(T)$ is empty.*

(ii) *The logical equivalence*

$$\big(T(r, w_1) \simeq T(r, w_2)\big) \Leftrightarrow \Big(\Big(V_0^+(T), d_{w_1}|_{V_0^+(T)\times V_0^+(T)}\Big) \simeq \Big(V_0^+(T), d_{w_2}|_{V_0^+(T)\times V_0^+(T)}\Big)\Big)$$

is valid whenever $w_1 \colon E(T) \to \mathbb{R}^+$ and $w_2 \colon E(T) \to \mathbb{R}^+$ are equidistant.

Proof. The equivalence $(i) \Leftrightarrow (ii)$ is trivially valid if $E(T) = \varnothing$. Let $E(T) \neq \varnothing$ hold.

$(i) \Rightarrow (ii)$. Let (i) hold. Then we have the equality

$$T'(r', w_i') = T'(r, w_i')$$

for $i = 1$, 2 and the validity of (ii) follows from Proposition 4.4.

$(ii) \Rightarrow (i)$. This implication is true if and only if

$$\neg(i) \Rightarrow \neg(ii),$$

where $\neg$ is the logical negation symbol. Suppose there is $v^* \in V^+(T)$ such that $\delta^+(v^*) = 1$. If $v^* \neq r$, then we have $\delta(v^*) = 1$ and, consequently, there are exactly two nodes v_1 and v_2 such that v^* is a direct successor of v_1 and v_2 is the unique direct successor of v^*.

Let $w \colon E(T) \to \mathbb{R}^+$ be an equidistant weight. Then we can find strictly positive, pairwise distinct real numbers t_1, t_2, s_1, s_2 such that

$$t_1 + t_2 = s_1 + s_2 = w(\{v_1, v^*\}) + w(\{v^*, v_2\}) \tag{4.20}$$

and

$$(w(e) - t_1)(w(e) - t_2)(w(e) - s_1)(w(e) - s_2) \neq 0 \tag{4.21}$$

holds for every $e \in E(T)$.

Let us define the weights $w_1 \colon E(T) \to \mathbb{R}^+$ and $w_2 \colon E(T) \to \mathbb{R}^+$ as

$$w_1(e) = \begin{cases} s_1, & \text{if } e = \{v_1, v^*\}, \\ s_2, & \text{if } e = \{v^*, v_2\}, \\ w(e), & \text{otherwise} \end{cases} \quad \text{and} \quad w_2(e) = \begin{cases} t_1, & \text{if } e = \{v_1, v^*\}, \\ t_2, & \text{if } e = \{v^*, v_2\}, \\ w(e), & \text{otherwise.} \end{cases}$$

Then w_1 and w_2 are equidistant and, moreover, using formula (4.18) we obtain the equalities

$$w' = w_1' = w_2'.$$

Now Proposition 4.3 implies

$$d_{w_1}|_{V_0^+(T) \times V_0^+(T)} = d_{w_2}|_{V_0^+(T) \times V_0^+(T)}.$$

Since t_1, t_2, s_1, s_2 are pairwise distinct, from condition (4.21) it follows that $T(r, w_1)$ and $T(r, w_2)$ are not isomorphic. Thus, (ii) is false. Hence, $\neg(i) \Rightarrow \neg(ii)$ is valid if $v^* \neq r$.

The case $v^* = r$ is more simple and can be considered similarly. □

The following result is a dual form of Theorem 4.4 and it is a partial generalization of Theorem 2.2.

Theorem 4.5. *The following statements are equivalent for every finite rooted tree $T = T(r)$.*

(i) *The set $V_1^+(T)$ is empty.*

(ii) *The logical equivalence*

$$\big(T(r, l_1) \simeq T(r, l_2)\big) \Leftrightarrow \Big(\Big(V_0^+(T), d_{l_1}|_{V_0^+(T) \times V_0^+(T)}\Big) \simeq \Big(V_0^+(T), d_{l_2}|_{V_0^+(T) \times V_0^+(T)}\Big)\Big)$$

is valid whenever $l_1 \colon V(T) \to \mathbb{R}^+$ and $l_2 \colon V(T) \to \mathbb{R}^+$ are monotone.

Proposition 4.5. *Let (X, d) be a finite ultrametric space with $|X| \geqslant 2$, let T_X be the representing tree of (X, d) and let $T = T(r, w)$ be an equidistant tree such that*

$$(V_0^+(T), d_w|_{V_0^+(T) \times V_0^+(T)}) \simeq (X, d).$$

Then the inequality

$$|V(T)| \geqslant |\mathbf{B}_X| \tag{4.22}$$

holds, where $\mathbf{B}_X$ is the set of balls of (X, d). Moreover, the equality $|V(T)| = |\mathbf{B}_X|$ holds if and only if $T_X \simeq T(r, w)$.

Proof. Let us consider $l \colon V(T_X) \to \mathbb{R}^+$ defined by (2.1). The weight $\hat{w} * l \colon E(T_X) \to \mathbb{R}^+$ is equidistant by Proposition 4.1. Using Lemma 4.1 we obtain

$$(X, d) \simeq (V_0^+(T), d_{\hat{w} * l}|_{V_0^+(T_X) \times V_0^+(T_X)}).$$

Consequently,

$$\Big(V_0^+(T_X), d_{\hat{w} * l}|_{V_0^+(T_X) \times V_0^+(T_X)}\Big) \simeq \Big(V_0^+(T), d_w|_{V_0^+(T) \times V_0^+(T)}\Big)$$

is valid. Now the equality

$$T'(r', w') = T_X(X, \hat{w} * l) \tag{4.23}$$

follows from Proposition 4.4. (Note that $T'_X = T_X$ holds because $V_1^+(T_X) = \varnothing$.) Since

$$V(T', r', w') \subseteq V(T, r, w)$$

and $|V(T_X)| = |\mathbf{B}_X|$ hold (see Proposition 2.2), inequality (4.22) follows.

Suppose that $T_X \simeq T(r, w)$. Then we have

$$|V(T(r, w))| = |V(T_X)| = |\mathbf{B}_X|.$$

Now, to complete the prove we note that $|V(T_X)| = |\mathbf{B}_X|$ holds if and only if

$$T'(r', w') = T(r, w),$$

so the isomorphism of T_X and $T(r, w)$ as rooted trees follows from (4.23). □

5 Planted equidistant trees and ultrametrics

Recall that a rooted tree $T = T(r)$ is planted if $\delta^+(r) = 1$ holds.

The following propositions clarify the "ultrametric" meaning of the constant K from the definition of equidistant trees (see formula (4.2)).

Proposition 5.1. *Let $T = T(r, w)$ be an equidistant tree and let d_1 be the restriction of the shortest-path metric d_w on the set $V_1^+(T) \times V_1^+(T)$. Then the diameter $\operatorname{diam}(V_1^+(T))$ of ultrametric space $(V_1^+(T), d_1)$ satisfies the inequality*

$$\operatorname{diam}(V_1^+(T)) \leq 2K. \tag{5.1}$$

This inequality is strict if and only if T is planted.

Proposition 5.2. *Let $T = T(w)$ be a finite weighted tree with $|V(T)| \geqslant 2$ and let $L = L(T)$ be the set of leaves of T. Suppose the restriction $\rho = d_w|_{L\times L}$ is an ultrametric on L. Then the following conditions are equivalent:*

- *(i) There is $r \in L$ such that the weighted rooted tree $T(r, w)$ is equidistant.*
- *(ii) The ultrametric space (L, ρ) is a sphere with an added center, i.e., there are $c \in L$ and $t > 0$ such that the equality $L = S_t(c) \cup \{c\}$ holds, where $S_t(c) = \{x \in L \colon \rho(x, c) = t\}$.*
- *(iii) There is $r \in V(T)$ such that $T(r, w)$ is planted and equidistant.*

The proofs of these propositions are straightforward and we omit it here.

It should be noted that for some planted equidistant trees $T = T(r, w)$ the restriction $d_w|_{L\times L}$ on the set L of the leaves of T is not an ultrametric (see Figure 7). The following proposition describes the geometry of planted equidistant trees $T(r, w)$ for which $d_w|_{L\times L}$ is an ultrametric.

Proposition 5.3. *Let $T = T(r, w)$ be planted and equidistant and let*

$$V_2^{++}(T) = \{v \in V(T) \colon \delta^+(v) \geqslant 2\} \neq \varnothing.$$

Then the following conditions are equivalent:

(*i*) *The metric $\rho = d_w|_{L\times L}$ is an ultrametric on L.*

(*ii*) *The inequality*

$$2\,\mathrm{dist}(r, V_2^{++}(T)) \geqslant \mathrm{dist}(r, V_0^+(T)) \tag{5.2}$$

holds, where, for every nonempty $A \subset V(T)$,

$$\mathrm{dist}(r, A) = \min\{d_w(r, a) \colon a \in A\}.$$

Proof. $(i) \Rightarrow (ii)$ Suppose (i) holds. We must prove inequality (5.2). Let $v^* \in V_2^{++}(T)$ such that

$$d_w(r, v^*) = \mathrm{dist}(r, V_2^{++}(T)). \tag{5.3}$$

Let $P = (v_0, \ldots, v_n)$ be the path in T with $v_0 = r$ and $v_n = v^*$. Since P is a path, the inequality $\delta^+(v_i) \geqslant 1$ holds for every $i \in \{1, \ldots, n-1\}$. If there is $i_1 \in \{1, \ldots, n-1\}$ such that $\delta^+(v_{i_1}) \geqslant 2$, then $v_{i_1} \in V_2^{++}(T)$ and we have

$$\begin{aligned} d_w(r, v^*) = \sum_{j=0}^{n-1} w(\{v_j, v_{j+1}\}) &= \sum_{j=0}^{i_1-1} w(\{v_j, v_{j+1}\}) + \sum_{j=i_1}^{n-1} w(\{v_j, v_{j+1}\}) \\ &= d_w(r, v_{i_1}) + d_w(v_{i_1}, v^*) > d_w(r, v_{i_1}), \end{aligned}$$

contrary to (5.3).

Inequality $\delta^+(v^*) \geqslant 2$ implies that there exist two distinct direct successors u_1 and u_2 of v^*. Let $x_i \in V_0^+(T)$ be a successor of u_i, $i = 1, 2$. It follows from the definition of d_w that

$$d_w(r, x_i) = d_w(r, v^*) + d_w(v^*, x_i) \tag{5.4}$$

for $i = 1, 2$, and, in addition,

$$d_w(x_1, x_2) = d_w(x_1, v^*) + d_w(v^*, x_2). \tag{5.5}$$

Since $T(r, w)$ is equidistant, we have

$$d_w(r, x_1) = d_w(r, x_2) = \mathrm{dist}(r, V_0^+(T)). \tag{5.6}$$

Equalities (5.4), (5.5) and (5.6) imply

$$d_w(x_1, x_2) = 2(\mathrm{dist}(r, V_0^+(T)) - d_w(r, v^*)). \tag{5.7}$$

From the ultrametricity (L, ρ) and (5.6) it follows that

$$d_w(x_1, x_2) \leqslant \max_{i=1,2} d_w(r, x_i) = \mathrm{dist}(r, V_0^+(T)). \tag{5.8}$$

Now using (5.3), (5.7) and (5.8) we obtain

$$d_w(x_1, x_2) = 2(\operatorname{dist}(r, V_0^+(T)) - \operatorname{dist}(r, V_2^{++}(T))) \leqslant \operatorname{dist}(r, V_0^+(T)).$$

Inequality (5.2) follows.

$(ii) \Rightarrow (i)$ Let inequality (5.2) hold. By Theorem 4.3 the metric $d_w|_{V_0^+(T)\times V_0^+(T)}$ is an ultrametric. Consequently $\rho = d_w|_{L(T)\times L(T)}$ is an ultrametric on $L(T)$ if and only if the strong triangle inequalities

$$d_w(x_1, x_2) \leqslant \max\{d_w(r, x_1), d_w(r, x_2)\} \tag{5.9}$$

and

$$d_w(r, x_1) \leqslant \max\{d_w(x_1, x_2), d_w(r, x_2)\} \tag{5.10}$$

and

$$d_w(r, x_2) \leqslant \max\{d_w(x_1, x_2), d_w(r, x_1)\} \tag{5.11}$$

hold. Inequalities (5.10) and (5.11) are trivial because $T(r, w)$ is equidistant. Let v^* be a point of $V_2^{++}(T)$ satisfying (5.3). The triangle inequality implies

$$d_w(x_1, x_2) \leqslant d_w(x_1, v^*) + d_w(v^*, x_2). \tag{5.12}$$

The induced rooted subtree T_{v^*} of $T(r)$ is equidistant with the weight $w|_{E(T_{v^*})}$. It implies

$$\begin{aligned} d_w(x_1, v^*) + d_w(v^*, x_2) &= 2 \min_{v\in V_0^+(T_{v^*})} d_w(v^*, v) \\ &= 2(\min_{v\in V_0^+(T(r))} d_w(r, v) - d_w(r, v^*)) = 2(\operatorname{dist}(r, V_0^+(T)) - \operatorname{dist}(r, V_2^{++}(T))) \end{aligned} \tag{5.13}$$

Moreover, we have

$$\max\{d_w(r, x_1), d_w(r, x_2)\} = \min_{v\in V_0^+(T(r))} d_w(r, v) = \operatorname{dist}(r, V_0^+(T)). \tag{5.14}$$

Consequently it suffices to show that

$$2(\operatorname{dist}(r, V_0^+(T)) - \operatorname{dist}(r, V_2^{++}(T))) \leqslant \operatorname{dist}(r, V_0^+(T)).$$

The last inequality is equivalent to inequality (5.2). □

Let $T = T(w)$ be a weighted tree. We say that a node $v^* \in V(T)$ is a *center* of T if the rooted tree $T(r, w)$ is equidistant with $r = v^*$. The following example (see Figure 12) shows that several distinct nodes of T can be centers of T.

Proposition 5.4. *Let T be a finite, nonempty tree. Then the following statements are equivalent:*

(i) T is star.

(ii) There is a strictly positive weight $w\colon E(T) \to \mathbb{R}^+$ such that the weighted rooted tree $T(r, w)$ is equidistant for every $r \in V(T)$.

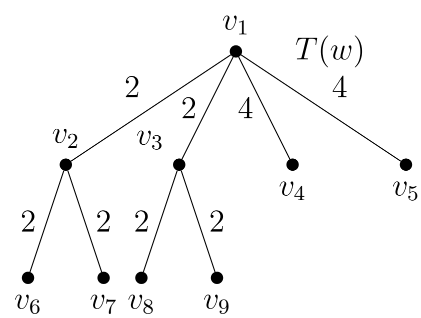

Figure 12: $T(r, w)$ is equidistant if and only if $r \in \{v_1, v_4, v_5\}$.

Proof. $(i) \Rightarrow (ii)$. Let T be a star and let c be a strictly positive real number. Then $T(r, w)$ is equidistant for every $r \in V(T)$ if we define $w \colon E(T) \to \mathbb{R}^+$ as

$$w(e) = c$$

for every $e \in E(T)$.

$(ii) \Rightarrow (i)$. Let statement (ii) hold. It is clear that (ii) holds if $|V(G)| = 2$. Suppose $|V(G)| \geqslant 3$. Then there is $v^* \in V(T)$ such that $\delta(v^*) \geqslant 2$ holds. We claim that, for every $u \in V(T)$, the inequality $\delta(u) \geqslant 2$ implies the equality $v^* = u$. Indeed, if $u \neq v^*$ and u, $v^* \in V(T)$, then there is a path $P_0 = \{v_1, \ldots, v_m\}$ in T with $v_1 = u$ and $v_m = v^*$. The inequalities $\delta(u) \geqslant 2$ and $\delta(v^*) \geqslant 2$ imply that there is v_{-1} and v_{m+1} such that v_{-1}, $v_{m+1} \notin V(P_0)$ and

$$\{v_{-1}, v_1\}, \{v_m, v_{m+1}\} \in E(T).$$

Since T is an acyclic graph, we have $v_{-1} \neq v_{m+1}$. Consequently,

$$P_1 = \{v_{-1}, v_1, \ldots, v_m, v_{m+1}\}$$

is a path in T and $P_1 \supseteq P_0$. If $\delta(v_{-1}) \geqslant 2$ or $\delta(v_m + 1) \geqslant 2$ holds, then we can find a path $P_2 \supseteq P_1$ such that $P_2 \subseteq T$ and $V(P_1)$ is a proper subset of $V(P_2)$. Since T is a finite tree, there is a path $P \supseteq P_0$, $P \subseteq T$, joining some leaves a, $b \in L(T)$,

$$P = (a, \ldots, u \ldots, v^*, \ldots, b).$$

The rooted trees $T(u, w)$ and $T(v^*, w)$ are equidistant. Hence, the equalities

$$d_w(a, u) = d_w(u, b) \quad \text{and} \quad d_w(a, v^*) = d_w(v^*, b)$$

hold. Using these equalities and the definition of shortest-path metric d_w we obtain

$$\begin{aligned} d_w(a, u) + d_w(v^*, b) &= d_w(u, b) + d_w(a, v^*) \\ &= (d_w(u, v^*) + d_w(v^*, b)) + (d_w(a, u) + d_w(u, v^*)). \end{aligned}$$

That implies $d(u, v^*) = 0$. Hence, $u = v^*$ holds, contrary to $u \neq v^*$.

A finite connected graph G is a tree if and only if

$$|V(G)| = |E(G)| + 1 \tag{5.15}$$

([5, Corollary 1.5.3]). Moreover, for every finite graph G, we have

$$\sum_{v \in V(G)} \delta(v) = 2|E(G)| \tag{5.16}$$

([2, Theorem 1.1]).

It was shown above that $\delta(v) = 1$ holds for every $v \in V(T)$ whenever $v \neq v^*$. Consequently, using (5.15) we can rewrite (5.16) as

$$\delta(v^*) + |V(G)| - 1 = 2(|V(G)| - 1).$$

Thus,

$$\delta(v^*) = |V(G)| - 1$$

holds. Consequently, the vertexes v^*, v are adjacent for every $v \neq v^*$ and $\{v_1, v_2\} \notin E(T)$ if $v_1 \neq v^*$ and $v_2 \neq v^*$. Thus, T is a star. □

Remark 5.1. *Other curious characterizations of stars are given by Corollary 4.9 in [8] and by Corollary 8 in [9]. These characterizations as well as Proposition 5.4 describe some extremal properties of weighted stars.*

The results of this paper have some natural analogies in the case when weights and labelings of rooted trees are some functions whose range is the positive cone E_+ of an ordered vector space E and the ultrametrics are replaced by some "generalized ultrametrics" taking their values in E_+.

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