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Recovering Symbolically Dated, Rooted Trees from Symbolic Ultrametrics

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A well known result from cluster theory states that there is a 1-to-1 correspondence between dated, compact, rooted trees and ultrametrics. In this paper, we generalize this result yielding a canonical 1-to-1 correspondence between symboli-

holds. In the second part of the paper, we use our main result to derive, as a corollary, a theorem by H. J. Bandelt and M. A. Steel regarding a canonical 1-to-1 correspondence between additive trees and metrics satisfying the 4-point condition, both taking their values in abelian monoids. © 1998 Academic Press

All (di-)graphs $G=(V, E \subseteq V^2)$ studied in this paper will be finite (and—by definition—without multiple edges). For a vertex v, let

$$d_-(v) := \sharp\{w \in V : (w, v) \in E\}$$

denote its in-degree, and

$$d_+(v) := \sharp\{w \in V : (v, w) \in E\}$$

its out-degree. A *path* $u_0 u_1 \cdots u_l$ of length $l \geqslant 0$ is a sequence of vertices $u_0, u_1, ..., u_l \in V$, such that $(u_{j-1}, u_j) \in E$ for $j=1, ..., l$. A *rooted tree* $T=(V, E)$ is a connected digraph (that is, the associated undirected graph is connected) such that there exists exactly one vertex $r \in V$ (the *root*) with $d_-(r)=0$ while we have $d_-(v)=1$ for all $v \in V-\{r\}$. The *leaves* of a rooted tree are the vertices v of out-degree 0, all other vertices are called *inner vertices*. A rooted tree is called *compact* if $d_+(v) \geqslant 2$ holds for all

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inner vertices v. In a rooted tree $T=(V, E)$, the *last common ancestor* $\mathrm{lca}(u, v)=\mathrm{lca}_T(u, v)$ of $u, v \in V$ is defined as follows: if $r=: u_0, u_1, ..., u_k := u$ is the (unique!) path from r to u, and $r =: v_0, v_1, ..., v_l := v$ the path from r to v, then $\mathrm{lca}(u, v) := u_j$ if $j := \max\{i \in \{0, ..., \min\{k, l\}\}: u_i = v_i\}$. So $\mathrm{lca}(u, v) = u$ holds if $k \leqslant l$ and $u = v_k$, $\mathrm{lca}(u, v) = v$ if $l \leqslant k$ and $v = u_l$, and $\mathrm{lca}(u, v) = u_j$ if $u_j = v_j$ and $u_{j+1} \neq v_{j+1}$ holds for some $j < \min\{k, l\}$. Note also that a rooted tree is compact if and only if every (inner) vertex is the last common ancestor of two (distinct) leaves in which case we can even find, for every ancestor $v \in V$ of any leaf $x \in V$, some leaf $y \in X$ with $v = \mathrm{lca}(x, y)$. Moreover, given any three leaves $x, y, z \in V$, one has necessarily

$$\sharp\{\mathrm{lca}(x, y), \mathrm{lca}(x, z), \mathrm{lca}(y, z)\} \leqslant 2. \tag{1}$$

Let X be a finite set. A (strict) *X-hierarchy* is a subset $C \subseteq \mathscr{P}(X)$ with $\varnothing, X \in \mathscr{C}$, $\{x\} \in \mathscr{C}$ for all $x \in X$, and

$$C_1 \cap C_2 \in \{C_1, C_2, \varnothing\} \tag{2}$$

for all $C_1, C_2 \in \mathscr{C}$. The subsets $C \in \mathscr{C}$ will also be called ($\mathscr{C}$-)*clusters*. For $x, y \in X$, we denote by $C(x, y) = C_{\mathscr{C}}(x, y)$ the (unique!) minimal cluster in $\mathscr{C}$ (with respect to inclusion) that contains both, x and y.

Given a rooted tree $T=(V, E)$ with leaf set X and a vertex $v \in V$, we denote by $C(v) = C_T(v)$ the subset of X consisting of exactly all those leaves $x \in X$ for which there exists a path from v to x. We will also say that v *induces* $C(v)$. Given $x, y, z \in X$, then obviously $z \in C(\mathrm{lca}(x, y))$ is equivalent to $\mathrm{lca}(x, y) \in \{\mathrm{lca}(x, z), \mathrm{lca}(y, z)\}$ because the path from $v := \mathrm{lca}(x, y)$ to any given $z \in C(\mathrm{lca}(x, y))$ cannot start by simultaneously following the path to x and to y.

A rooted tree $T=(V, E)$ is *dated* by a map $t: V \to \mathbb{R}$ if $t(x) = 0$ for all leaves $x \in V$, and $t(u) > t(v)$ for all $(u, v) \in E$. It is well known or—at least—folklore (cf. Gordon [9] and also Theorem 1 below) that there is a 1-to-1 correspondence between

(a) (isomorphism classes of) dated, compact, rooted trees $(V, E; t)$ with leaf set $X \subseteq V$,

(b) *dated hierarchies*, that is, pairs $(\mathscr{C}, t)$ consisting of an X-hierarchy $\mathscr{C}$ and a strictly monotonously increasing map $t: \mathscr{C} \setminus \{\varnothing\} \to \mathbb{R}$ with $t(\{x\}) = 0$ for all $x \in X$, and

(c) *ultrametrics* defined on X, that is, maps $d: X \times X \to \mathbb{R}$ with

- $d(x, y) = 0 \Leftrightarrow x = y$,
- $d(x, y) = d(y, x)$ and
- $d(x, z) \leqslant \max\{d(x, y), d(y, z)\}$ for all $x, y, z \in X$.

The correspondence between (a) and (c) is given by associating to any such tree $(V, E; t)$ the map

$$d\colon X \times X \to \mathbb{R}: \qquad (x, y) \mapsto t(\mathrm{lca}(x, y)).$$

Similarly, the correspondence between (b) and (c) is given by associating to any such dated hierarchy $(\mathscr{C}, t)$ the map

$$d\colon X \times X \to \mathbb{R}: \qquad (x, y) \mapsto t(C(x, y)).$$

What we want to do in this note is to remove the restrictions regarding the *values* of t and d as far as possible. But first, we recall the relevant result from cluster theory regarding non-dated structures (see for instance [7]).

THEOREM 1. *Given a finite set X, there exists a canonical* 1-*to*-1 *correspondence between*

(i) (*isomorphism classes of*) *compact, rooted trees $T = (V, E)$ with leaf set X,*

(ii) *X-hierarchies $\mathscr{C}$, and*

(iii) *ternary relations $\wr$ defined on X (with $(a, b, c) \in \wr$ denoted by $ab \wr c$, for $a, b, c \in X$) satisfying the following assertions for all $a, b, c, d \in X$:*

(H1) $aa \wr b \Leftrightarrow a \neq b$ (H2) $ab \wr c \Rightarrow ba \wr c$

(H3) $ab \wr d$ and $bc \wr d \Rightarrow ac \wr d$ (H4) $ab \wr c$ and $bc \wr d \Rightarrow ac \wr d.$

More precisely, the correspondence between (i) and (ii) is as follows: Given a compact, rooted tree $T = (V, E)$, the associated hierarchy $\mathscr{C}_T$ is defined by

$$\mathscr{C}_T := \{ C_T(v) : v \in V \} \cup \{ \emptyset \},$$

while for an X-hierarchy $\mathscr{C}$, a corresponding tree $T = (V, E)$ can be defined by

$$V := \mathscr{C} - \{ \emptyset \}$$

and

$$E := \{ (C_1, C_2) \in V^2 : C_2 \subsetneq C_1, \text{ and there exists no } C \in \mathscr{C} \text{ with } C_2 \subsetneq C \subsetneq C_1 \}.$$

Given any such tree T and the associated X-hierarchy $\mathscr{C} := \mathscr{C}_T$, we have

$$C_T(\mathrm{lca}_T(x, y)) = C_{\mathscr{C}}(x, y)$$

for all $x, y \in X$, while

$$z \in C_{\mathscr{C}}(x, y) \quad \text{implies}$$
$$\mathrm{lca}(x, y) = \mathrm{lca}(x, z) \quad \text{or} \quad \mathrm{lca}(x, y) = \mathrm{lca}(y, z). \tag{3}$$

To discuss the correspondence between (ii) and (iii), let $\mathscr{C}$ denote an X-hierarchy. The associated ternary relation $\wr$ is simply defined by $ab \wr c$ if and only if there exists some cluster $C \in \mathscr{C}$ with $a, b \in C$ and $c \in X - C$. Vice versa, for a ternary relation $\wr$, the associated hierarchy $\mathscr{C} = \mathscr{C}(\wr)$ is defined by

$$\mathscr{C} := \{C \subseteq X : ab \wr c \text{ holds for all } a, b \in C \text{ and } c \in X - C\} \tag{4}$$

or—equivalently[1]—by

$$\mathscr{C} := \{C \subseteq X : \text{there exist } a, b \in X \text{ with "}ab \wr c \Leftrightarrow c \notin C\text{", for all } c \in X\}.$$

Finally, given an arbitrary compact, rooted tree $T = (V, E)$, the corresponding ternary relation $\wr$ is defined by

$$ab \wr c \qquad \text{if and only if} \quad \mathrm{lca}(a, b) \neq \mathrm{lca}(a, c), \mathrm{lca}(b, c) \qquad (a, b, c \in X) \tag{5}$$

which in turn is obviously equivalent with $\mathrm{lca}(a, b) \neq \mathrm{lca}(a, c) = \mathrm{lca}(b, c)$.

Remark 1. Given a ternary relation $ab \wr c$ on a finite set X such that (H2), (H3) and (H4) hold, but instead of (H1) only

$$\text{(H1}'\text{)} \quad aa \wr b \Rightarrow a \neq b$$

holds for all $a, b \in X$, we can extend $\wr$ to a relation $\wr'$ defined by

$$ab \wr' c \quad \Leftrightarrow \quad ab \wr c \text{ or } a = b \neq c$$

which surely satisfies (H1) to (H4). Consequently, we can define an X-hierarchy corresponding to $\wr$ by

$$\mathscr{C}(\wr) := \mathscr{C}(\wr') = \{C \subseteq X : ab \wr c \text{ holds for all } a, b \in C \text{ and } c \in X - C\}$$
$$\cup \bigcup_{x \in X} \{\{x\}\} \tag{6}$$

so that, for all $a, b, c \in X$, we have $a, b \in C$ and $c \in X - C$ for some $C \in \mathscr{C}(\wr)$ if and only if we have $a = b \neq c$ or $ab \wr c$.

[1] Of course, if a ternary relation $\wr$ does not satisfy the above assertions (H1) to (H4), the two systems may differ from each other considerably.

Now, let $T=(V, E)$ denote a finite, compact, rooted tree, and let $X \subseteq V$ denote the set of leaves of T. Any map $t\colon V \to M$ into an *arbitrary* set M will be called a *symbolic dating map*. Given such a map, we can define a "symbolic ultrametric" on X by

$$D_{(V, E; t)}\colon X \times X \to M; \quad (x, y) \mapsto xy := t(\operatorname{lca}(x, y)). \tag{7}$$

Clearly, isomorphic symbolically dated trees with the same leaf set X give rise to the same map D. In addition, the following three assertions are easily verified (regarding (U3), cf. the lower row in Fig. 1, where M equals the set $\{\bullet, ⊘, \circ\}$):

(U1) $xy = yx$ for all $x, y \in X$,

(U2) $\sharp\{xy, xz, yz\} \leqslant 2$ for all $x, y, z \in X$,

(U3) there exist no pairwise distinct $a, b, c, d \in X$ with $ab = bc = cd \neq bd = da = ac$.

We would like to show that, vice versa, for any given map $D\colon X \times X \to M$ which satisfies conditions (U1) to (U3), there exists a unique triple $(V, E; t)$ as above with $D = D_{(V, E; t)}$—where, of course, uniqueness is claimed relative to "canonical isomorphism." Yet, all trees in Fig. 2 lead to the same map $D_{(V, E; t)}$. So, to achieve uniqueness, we somehow have to restrict the set of dating maps:

To this end, consider a finite, compact, rooted tree $T=(V, E)$ together with a symbolic dating map $t\colon V \to M$, for some set M of symbols. Let $\mathring{E} := \{(u, v) \in E : d_+(v) > 0\}$ denote the set of *inner edges* of T. Clearly, if $t(u) = t(v)$ holds for an inner edge (u, v), then contracting this edge leads to a "smaller" tree with the same leaf set and inducing the same map D. Consequently, to exclude such a case, we define a map t to be *discriminating* if $t(u) \neq t(v)$ holds for all inner edges $(u, v) \in \mathring{E}$. Such triples $(V, E; t)$ where $T = (V, E)$ is a finite, compact, rooted tree and t is a discriminating symbolic dating map will be henceforth called *SDR trees*. We denote the set of isomorphism classes $[V, E; t]$ of M-dated SDR trees $(V, E; t)$ with leaf set X by $\mathrm{SDR}(X, M)$.

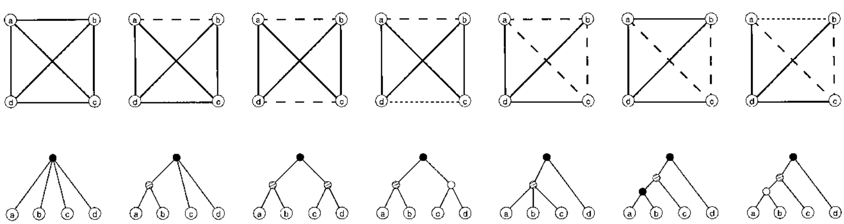

FIG. 1. All admissible 4-point configurations and the associated trees.

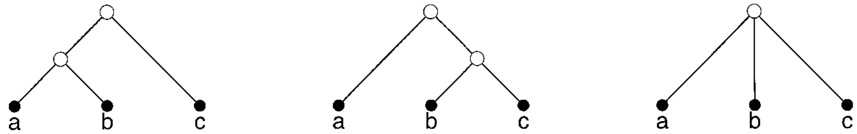

FIG. 2. Three SDR trees with equal symbolic ultrametric.

Next, a map $D: X \times X \to M$ is called a *symbolic ultrametric* if the conditions (U1), (U2) and (U3) above are satisfied for $xy := D(x, y)$, where $x, y \in X$. We denote the set of M-valued symbolic ultrametrics on X by $\mathrm{SU}(X, M)$. Now we can state the main result of our paper:

THEOREM 2. *Let X, M denote two finite sets. For any symbolic ultrametric $D: X \times X \to M$, there exists (up to canonical isomorphism) a unique SDR tree $(V, E; t)$ with leaf set X and discriminating symbolic dating map $t: V \to M$ such that $D = D_{(V, E; t)}$ holds, that is, the map*

$$\varphi: \mathrm{SDR}(X, M) \to \mathrm{SU}(X, M):$$

$$[V, E; t] \mapsto \left(D_{(V, E; t)}: X \times X \to M : (x, y) \mapsto t(\mathrm{lca}(x, y))\right) \tag{8}$$

is a bijection.

First, we can easily prove that φ is injective:

LEMMA 1. *Given two SDR trees $(V_1, E_1; t_1)$ and $(V_2, E_2; t_2)$ representing elements from* $\mathrm{SDR}(X, M)$, *then $D_{(V, E_1; t_1)} = D_{(V_2, E_2; t_2)}$ if and only if $[V_1, E_1; t_1] = [V_2, E_2; t_2]$.*

Proof. Let $T = (V, E)$ be a compact rooted tree with leaf set X and assume that $t_1, t_2: V \to M$ are two symbolic dating maps. Suppose that $(V, E; t_1)$ and $(V, E; t_2)$ induce the same symbolic ultrametric on X. Then clearly, t_1 and t_2 must coincide—even if they are not supposed to be discriminating—because, as T is compact, one can find $x, y \in X$ with $\mathrm{lca}(x, y) = v$ for any $v \in V$ which then implies

$$t_1(v) = t_1(\mathrm{lca}(x, y)) = D(x, y) = t_2(\mathrm{lca}(x, y)) = t_2(v).$$

So, in view of Theorem 1, the following lemma completes the proof of Lemma 1:

LEMMA 2. *For an SDR tree $(V, E; t)$ from* $\mathrm{SDR}(X, M)$, *let $D := D_{(V, E; t)}$ denote the induced ultrametric. Let $\wr$ denote the ternary relation on X*

induced by (V, E) *as defined in* (5). *Then, for all* $a, b, c \in X$, *we have* $ab \wr c$ *if and only if one of the following two conditions holds*:

- $D(a, b) \neq D(a, c) = D(b, c)$, *or*
- $D(a, b) = D(a, c) = D(b, c)$, *and there is some* $x \in X$ *with* $D(a, x) = D(b, x) \neq D(c, x) = D(a, b)$.

So, in particular, we can recover the relation $\wr$ *and, hence, the tree* (*up to isomorphism*) *from* D.

Proof. First note that due to Theorem 1, the relation $\wr$ satisfies conditions (H1) to (H4). With $D(x, y) = t(\mathrm{lca}(x, y))$, we infer that $D(a, b) \neq D(a, c) = D(b, c)$ implies $\mathrm{lca}(a, b) \neq \mathrm{lca}(a, c), \mathrm{lca}(b, c)$ and, hence (cf. (5)), $ab \wr c$. Next, suppose that the second condition holds; then we conclude analogously from $D(a, b) \neq D(a, x) = D(b, x)$ and from $D(a, x) \neq D(a, c) = D(c, x)$ that $ab \wr x$ and $ax \wr c$ hold, so (H4) implies $ab \wr c$.

Now, suppose that $ab \wr c$ holds for some $a, b, c \in X$ and, hence,

$$w := \mathrm{lca}(a, b) \neq u := \mathrm{lca}(a, c) = \mathrm{lca}(b, c).$$

Furthermore, suppose that $D(a, b) \neq D(a, c) = D(b, c)$ does not hold. Then, clearly, we must have $D(a, b) = D(a, c) = D(b, c)$. As u is a common ancestor of both, a and b, and as w is the last common ancestor of a and b, we infer that $u \neq w$ must be an ancestor of w, too. Let

$$u =: u_0, u_1, \ldots, u_l := w$$

denote the path of length $l \geqslant 1$ from u to w. Then

$$t(u) = t(\mathrm{lca}(a, b)) = D(a, b) = D(a, c) = t(\mathrm{lca}(a, c)) = t(w)$$

together with our assumption that t is discriminating implies $l \geqslant 2$. Since t is compact, there exists some $x \in X$ with $v := u_1 = \mathrm{lca}(a, x)$. We easily conclude $\mathrm{lca}(b, x) = v$, $\mathrm{lca}(x, c) = u$ and, finally,

$$D(a, x) = D(b, x) = t(v) \neq t(u) = D(x, c) = D(a, c) = D(b, c) = t(w) = D(a, b).$$

This proves the equivalence. ∎

Next, given a symbolic ultrametric $D : X \times X \to M : (x, y) \mapsto xy$ from $\mathrm{SU}(X, M)$, Lemma 2 suggests to define two ternary relations on X:

- We say that a and b are *separated* from c, denoted by $ab \mid c$, if $ab \neq ac = bc$ holds.
- We say that a and b are *paired with respect to c*, denoted by $ab \parallel c$, if either $ab \mid c$ holds, or one has $ab = bc = ac$ and there exists some $x \in X$ with $ax = bx \neq cx = ab$. In the latter case, we will also say that a and b are paired with respect to c *via* x or, for short, that $ab \parallel c$ holds *via* x.

Remark 2. Given $a, b, c \in X$, then $ab|c \Leftrightarrow ba|c$, and $ab\|c \Leftrightarrow ba\|c$. If $ab\|c$, then $a \neq c \neq b$. If $ab|c$ does not hold, then $ab\|c$ holds if and only if there exists some $x \in X$ with $ab|x$, $ax|c$ and $bx|c$ in which case $ab\|c$ holds via x.

As the forthcoming proofs will become a bit technical, we introduce a different point of view regarding these ternary relations: For the complete graph $\Gamma_X = (X, \binom{X}{2})$, we consider the map $D: X \times X \to M$ as an edge coloring $D: \binom{X}{2} \to M$, $\{x, y\} \mapsto D(x, y)$. Figure 3 illustrates the ternary relations $ab|c$ and $ab\|c$ in this context. Regarding this edge coloring, our assumptions (U2) and (U3) state that there exists no 3-colored triangle (see Fig. 3, (U2)), and that there is no induced subgraph K_4 on a, b, c, d with $ab = bc = cd \neq bd = da = ac$ as depicted in Fig. 3, (U3) and (U3'). To simplify the forthcoming proofs, we deduce two further simple rules in the following

LEMMA 3. *Assume we are given two finite sets X, M and a symbolic ultrametric $D: X \times X \to M : (x, y) \mapsto xy$. Then, for $a, b, c, d \in X$, the following two assertions hold*:

(U4) *If $ab|c$ and $bc|d$, then $ad = cd$ and, hence, $ac|d$.*

(U5) *If $ac|b$ and $bd|c$, then $ab = bc = cd = da$.*

Proof. (The graph representation of our rules (U4) and (U5) is given in Fig. 3 as well: Note that for (U4) and (U5), the colors represented by the dashed and the dotted lines may or may not be distinct.) To prove (U4), we assume $ad \neq cd$. By applying (U2) twice, we get $ad = ac$ and $ab = bd$ in contradiction to (U3). So (U4) must hold. To prove (U5), we note that our assumptions surely imply $ab = bc = cd$, and we assume $ad \neq ab$. By applying (U2) twice, we get $ad = ac = bd$, again in contradiction to (U3). So (U5) must hold, too. ∎

Remark 3. Note that a, b, c, d do not necessarily have to be pairwise distinct in the assertions depicted in Fig. 3: rule (U2) is trivial if at least two points coincide, while the configuration of rule (U3) can only appear for four pairwise distinct points; the conditions of rule (U4) imply that $a \neq c$, $a \neq d$, $b \neq c$, $b \neq d$ and $c \neq d$, while the rule is trivial for $a = b$; the conditions of rule (U5) imply that $a \neq b$, $a \neq d$, $b \neq c$ and $c \neq d$, while the rule is trivial for $a = c$ or $b = d$.

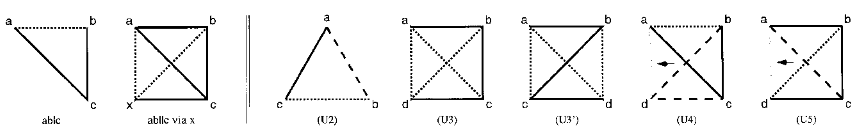

FIG. 3. Graph representations of $ab|c$, $ab\|c$ and the four rules.

We leave it as an exercise to the reader to establish that the rules allow exactly the seven types of edge colorings of K_4 depicted in the first row of Fig. 1, and that these correspond exactly to the seven distinct types of SDR trees with four leaves and discriminating dating map depicted in the second row (where ● is associated to the solid line, ▨ to the dashed line and ○ to the dotted line). We will now show that our terminology "paired with respect to c" is in conformity with the situation in a rooted tree where two leaves a, b are paired with respect to another leaf c if their last common ancestor is further away from the root (and hence closer to a and b) than the last common ancestor of a and c—which, of course, then coincides with that of b and c. (cf. (5))

LEMMA 4. *For $a, b, c, d \in X$, if $ab \| d$ and $bc \| d$, then $ac \| d$.*

Proof. We must distinguish four cases.

Case $ab | d$ and $bc | d$ (cf. Fig. 4). We know $ab \neq ad = bd = cd \neq bc$. If $ac \neq ad = cd$, then $ac | d$. If $ac = ad = cd$, then we apply (U2) to a, b, c and conclude $ab = bc$, hence $ab = cb \neq db = ac = ad = cd$, so $ac \| d$ holds via b.

Case $ab | d$ and $bc \| d$ via x (cf. Fig. 5). We have $ab \neq ad = bd = bc = cd = dx \neq bx = cx$. If $ac \neq ad = cd$, then $ac | d$. If $ac = ad = cd$, then we apply (U4) to a, b, c, x and get $ax = cx$, hence $ax = cx \neq dx = ac = ad = cd$, so we have $ac \| d$ via x.

Case $ab \| d$ via x and $bc | d$. This is proved by analogy to the last case, exchanging a and c.

Case $ab \| d$ via x and $bc \| d$ via y (cf. Fig. 6). For $m := ab$, $p := bx$ and $q := by$ we have $p \neq m \neq q$ and $ab = ad = bd = bc = cd = dx = dy = m$, $ax = bx = p$, $by = cy = q$. If $ac \neq m = ad = cd$, we are done. So suppose $ac = m$. Since $cx = p = ax$ would then imply $ac \| d$ via x, we may also suppose $cx \neq p$, which in view of $cx \in \{ac, ax\} = \{m, p\}$ implies $cx = m$. Similarly, replacing x by y and exchanging the role of a and c, we see that

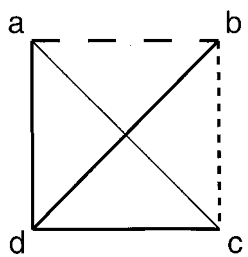

FIG. 4. Lemma 4, Case $ab | d$ and $bc | d$.

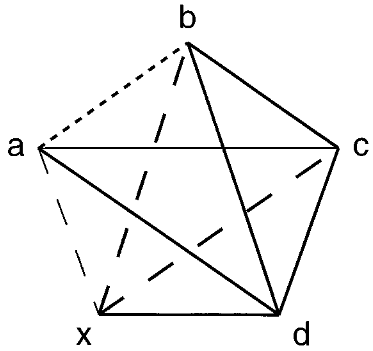

FIG. 5. Lemma 4, Case $ab|d$ and $bc\|d$ via x.

we may also assume $ay=m$. But this leads to a contradiction: applying rule (U4) to x, b, c, y leads to $xy=cy=q$ while applying rule (U5) to x, c, a, y leads to $xy=ay=m$. So, $ac\|d$ must hold also in this last case. ∎

LEMMA 5. *For $a, b, c, d \in X$, if $ab\|c$ and $bc\|d$, then $ac\|d$.*

Proof. Again, we distinguish four cases.

Case $ab|c$ and $bc|d$. Here, our claim follows directly from (U4).

Case $ab\|c$ via x and $bc|d$ (cf. Fig. 7). We have $ax=bx\neq cx=ab=ac=bc\neq bd=cd$. We apply (U4) to x, b, c, d and get $dx=bd$. Next, we apply (U4) to a, x, c, d and get $ad=cd$, hence $ac\neq cd=ad$, that is $ac|d$.

Case $ab|c$ and $bc\|d$ via y (cf. Fig. 8). We have $ab\neq ac=bc=bd=cd=dy\neq by=cy$. We apply (U4) to a, b, c, y and get $ay=by$. Next, we apply (U4) to a, c, y, d and get $ad=cd$. So, we have $ac=ad=cd=dy\neq ay=cy$, hence $ac\|d$ holds via y.

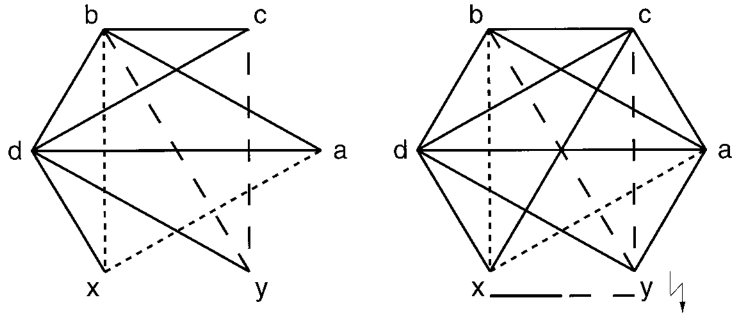

FIG. 6. Lemma 4, Case $ab\|d$ via x and $bc\|d$ via y.

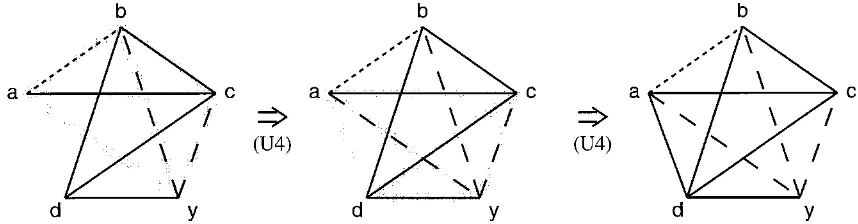

FIG. 7. Lemma 5, Case $ab \| c$ via x and $bc | d$.

Case $ab \| c$ via x and $bc \| d$ via y (cf. Fig. 9). We have $ax = bx \neq cx = ab = ac = bc = bd = cd = dy \neq by = cy$. Obviously $bx \neq cx$ and $by = cy$ implies $x \neq y$. We apply (U4) three times: For x, b, c, y we get $xy = cy$, for a, x, c, y we infer $ay = cy$ and, finally, for a, b, y, d we conclude $ad = dy$. So $ay = cy \neq dy = ac = ad = cd$, hence $ac \| d$ follows via y.

So, $ac \| d$ must hold in all four cases.

Proof of the main theorem. Given a symbolic ultrametric

$$D: X \times X \to M : (x, y) \mapsto xy$$

and the associated ternary relations $|$ and $\|$, it follows from Remark 2, Lemma 4, Lemma 5 and the symmetry of D that the conditions (H1′) to (H4) of Remark 1 hold for the relation $\|$. So, Theorem 1 states that the set of clusters

$$\mathscr{C}_D := \mathscr{C}(\|) = \{C \subseteq X : ab \| c \text{ holds for all } a, b \in C, c \in X - C\} \cup \bigcup_{x \in X} \{\{x\}\}. \tag{9}$$

is an X-hierarchy, and there exists a unique compact, rooted tree $T = (V, E)$ with $\mathscr{C}_T = \mathscr{C}_D$.

To define the symbolic dating map $t: V \to M$, we consider the diagram of maps

$$\begin{tikzcd} & V \arrow[dd, dashed, "t"] \\ X^2 \arrow[ur, two heads, "\mathrm{lca}"] \arrow[dr, "D"'] & \\ & M \end{tikzcd} \tag{10}$$

and show that the map $D: X^2 \to M : (x, y) \mapsto xy$ factors through the map lca: $X^2 \to V$ via a map $t: V \to M$. Note that, in this case, the map t is necessarily uniquely determined by this property in view of the fact that T is compact and that, consequently, lca is surjective. To show the existence of t, assume that $\mathrm{lca}(x, y) = \mathrm{lca}(x', y')$ holds for some leaves $x, y, x', y' \in X$. We have to show that $xy = x'y'$ holds, too. As $\mathrm{lca}(x, y) = \mathrm{lca}(x', y')$ implies $x' \in C(\mathrm{lca}(x, y))$ and, hence, $\mathrm{lca}(x, y) = \mathrm{lca}(x', y) = \mathrm{lca}(x', y')$ or $\mathrm{lca}(x, y) = \mathrm{lca}(x', x) = \mathrm{lca}(x', y')$ (cf. (3)), we can assume without loss of generality

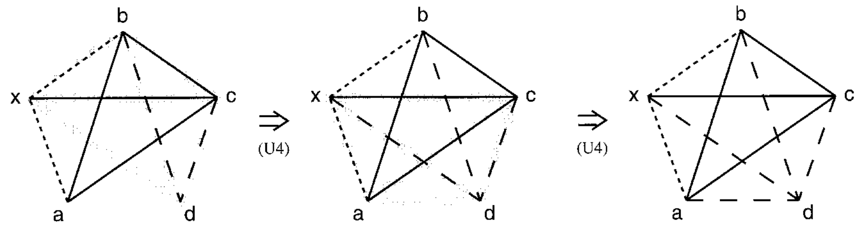

FIG. 8. Lemma 5, Case $ab|c$ and $bc\|d$ via y.

that $\{x, y\} \cap \{x', y'\} \neq \varnothing$. So suppose $x = x'$ and let $z := y'$. From $\mathrm{lca}(x, y) = \mathrm{lca}(x, z)$, we infer $z \in C(\mathrm{lca}(x, y))$ and $y \in C(\mathrm{lca}(x, z))$. Now suppose $xy \neq xz$; then $xy|z$ or $xz|y$ must hold, and we conclude $z \notin C(\mathrm{lca}(x, y))$ or $y \notin C(\mathrm{lca}(x, z))$, a contradiction in either case.

Finally, we show that t is discriminating: given an inner edge $(u, v) \in \mathring{E}$, there exist pairwise distinct $a, b, c \in X$ with $\mathrm{lca}(a, b) = v$ and $\mathrm{lca}(a, c) = \mathrm{lca}(b, c) = u$, because T is compact. We know $a, b \in C(v)$ and $c \notin C(v)$, so we can infer $ab \| c$. Suppose $t(u) = t(v)$, that is $ab = bc = ac$. Then there would exist some $x \in X$ with $ax = bx \neq cx = ab$. From $t(\mathrm{lca}(a, x)) = ax \neq t(u) = t(v)$, we infer $\mathrm{lca}(a, x) \notin \{u, v\}$. Similarly, we get $\mathrm{lca}(b, x) \notin \{u, v\}$. This leads to a contradiction in each of the following, mutually exclusive three cases: If $x \in C(v)$, then $\mathrm{lca}(a, x) = v$ or $\mathrm{lca}(b, x) = v$. If $x \in C(u) - C(v)$, then $\mathrm{lca}(a, x) = \mathrm{lca}(b, x) = u$, and for $x \in X - C(u)$ we infer $\mathrm{lca}(a, x) = \mathrm{lca}(c, x)$, hence $ax = cx$. So, no such $x \in X$ can exist and, hence, $ab|c$ must hold which implies $t(u) = ab \neq bc = ac = t(v)$.

Consequently, $(V, E; t)$ is an SDR tree, and it follows immediately from our construction that $D_{(V, E; t)}(x, y) = t(\mathrm{lca}(x, y)) = D(x, y)$ holds for all $x, y \in X$. So, the map φ: $\mathrm{SDR}(X, M) \to \mathrm{SU}(X, M)$ must be surjective and, hence (cf. Lemma 1), bijective. ∎

Now, let $(\Gamma, +)$ denote a 2-divisible abelian group. A (Γ)-*weighted tree* $(V', E'; w)$ is an (unrooted) finite tree $T' = (V', E' \subseteq \binom{V'}{2})$ together with a weighting function $w: E' \to \Gamma$. In the following, we will consider only weighted trees $(V', E'; w)$ with leaf set $Y \subseteq V'$ such that there is no vertex $v \in V'$ of degree two, and $w(e) \neq 0$ holds for all inner edges $e \in E' := \{\{u, v\} \in E' : u, v \in V' - Y\}$. We denote the set of isomorphism classes $[T'; w]$

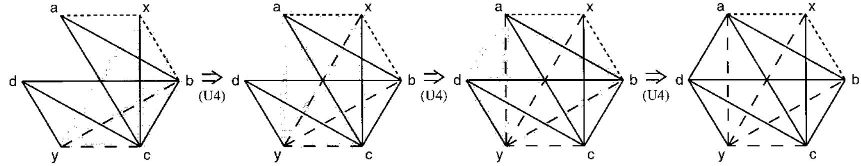

FIG. 9. Lemma 5, Case $ab\|c$ via x and $bc\|d$ via y

of Γ-weighted trees $(T'; w)$ with leaf set Y that satisfy these conditions by $\mathrm{WT}(Y, \Gamma)$.

Let Y denote a finite set. A map d: $Y \times Y \to \Gamma$ is said to satisfy the 4-*point condition* if, for any four elements $x, y, x', y' \in Y$, one has

$$\sharp\{d(x, y) + d(x', y'), d(x, y') + d(x', y), d(x, x') + d(y, y')\} \leqslant 2. \quad (11)$$

We denote the set of Γ-valued symmetric maps d: $Y \times Y \to \Gamma$ with $d(x, x) = 0$ for all $x \in Y$ that satisfy the 4-point condition by $\mathrm{SM}_4(Y, \Gamma)$.

We can construct a canonical map Φ: $\mathrm{WT}(Y, \Gamma) \to \mathrm{SM}_4(Y, \Gamma)$ as follows: given an arbitrary weighted tree $(V', E'; w)$ from $\mathrm{WT}(Y, \Gamma)$ and $x, y \in Y$, there exists a unique path $x =: u_0, u_1, ..., u_l := y$ from x to y such that $\{u_{i-1}, u_i\} \in E'$ for all $i = 1, ..., l$ and $u_{i-1} \neq u_{i+1}$ for all $i = 1, ..., l-1$ hold. So, by putting

$$d_w(x, y) := \sum_{j=1}^{l} w(\{u_{j-1}, u_j\}), \quad (12)$$

we get a map d_w: $Y \times Y \to \Gamma$ induced by $(V', E'; w)$. Obviously, $d_w(x, x) = 0$ and $d_w(x, y) = d_w(y, x)$ holds for all $x, y \in Y$ by definition of d_w. That d_w also satisfies the 4-point condition follows easily from the fact that there are only four trees with four leaves (cf. Fig. 10). So we define $\Phi((V', E'; w)) := d_w$. Clearly, d_w depends only on the isomorphism class of $(V', E'; w)$, that is, associating d_w to $(V', E'; w)$ via Φ defines indeed a map from $\mathrm{WT}(Y, \Gamma)$ into $\mathrm{SM}_4(Y, \Gamma)$ that we will also denote by Φ.

In addition, d_w does not only satisfy the 4-point condition: for any edge $\{u, v\} \in E'$, there exist leaves $x, y, x', y' \in Y$ such that the path from x to y is incident with u but not v, and the path from x' to y' is incident with v but not u. Then

$$d(x, y) + d(x', y') + 2w(\{u, v\}) = d(x, x') + d(y, y')$$

holds (cf. Fig. 10 again). This establishes

Remark 4. Let Φ: $\mathrm{WT}(Y, \Gamma) \to \mathrm{SM}_4(Y, \Gamma)$ denote the canonical map described in (12). Given a tree $(V', E'; w)$ from $\mathrm{WT}(Y, \Gamma)$ and a map d: $Y \times Y \to \Gamma$ from $\mathrm{SM}_4(Y, \Gamma)$ such that $d = \Phi((V', E'; w))$ holds, then

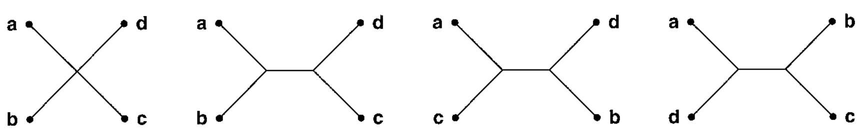

FIG. 10. The four trees with four leaves.

$$w(E') \subseteq w(d) := \{\xi \in \Gamma : \text{there exist } x, x', y, y' \in Y \text{ with}$$
$$2\xi = d(x, x') + d(y, y') - d(x, y) - d(x', y')\}.$$

The following theorem is a simple consequence of—and actually equivalent with–the main result of H.-J. Bandelt and M. A. Steel in [2].

THEOREM 3. *Given a finite set* Y *and a* 2-*divisible group* Γ, *there exists a canonical* 1-*to*-1 *correspondence between* $\mathrm{WT}(Y, \Gamma)$ *and* $\mathrm{SM}_4(Y, \Gamma)$.

This is obviously true for $\sharp Y = 1$, because $\sharp\,\mathrm{WT}(Y, \Gamma) = \sharp\,\mathrm{SM}_4(Y, \Gamma) = 1$ holds in this case. In case $\sharp\, Y > 1$, we can choose a non-empty set X and an element $* \notin X$ so that $X^* := X \dot\cup \{*\}$ coincides with Y. Hence, Theorem 3 follows easily from

THEOREM 4. *Given a finite set* X *and a* 2-*divisible group* Γ, *there exist canonical* 1-*to*-1 *correspondences between* $\mathrm{SDR}(X, \Gamma)$, $\mathrm{SU}(X, \Gamma)$, $\mathrm{WT}(X^*, \Gamma)$ *and* $\mathrm{SM}_4(X^*, \Gamma)$. (cf. Fig. 11).

Proof. Note that we have constructed already a canonical bijection φ: $\mathrm{SDR}(X, \Gamma) \to \mathrm{SU}(X, \Gamma)$ (cf. (8)) and a canonical map Φ: $\mathrm{WT}(X^*, \Gamma) \to \mathrm{SM}_4(X^*, \Gamma)$. Next, we observe that there exists a canonical bijection

$$\psi\colon \mathrm{WT}(X^*, \Gamma) \to \mathrm{SDR}(X, \Gamma).$$

Suppose that we are given a tree $(V', E'; w)$ from $\mathrm{WT}(X^*, \Gamma)$ and denote by r the unique vertex in V' which forms an edge $\{r, *\} \in E'$ together with $*$. We construct a rooted tree $T = (V, E)$ by putting

$$V := V' - \{*\} \qquad \text{and}$$
$$E := \{(u, v) : \{u, v\} \in E' - \{\{r, *\}\},$$
$$\text{and the path from } * \text{ to } v \text{ is incident with } u\}.$$

Furthermore, we construct[2] a symbolic dating map $t\colon V \to \Gamma$: we put $t(r) := w(\{r, *\})$, and we define iteratively $t(v) := t(u) + w(\{u, v\})$ for all $(u, v) \in E$. We infer $t(u) \neq t(v)$ for all inner edges $\{u, v\} \in \mathring{E}'$ from $w(\{u, v\}) \neq 0$, and we have $d_+(v) \geqslant 2$ for an arbitrary inner vertex $v \in V - X$ since the degree of v in (V', E') is greater than or equal to three. In addition, we have $d_-(r) = 0$ and $d_-(v) = 1$ for all $v \in V - \{r\}$ as there can be only one $u \in V$ with $\{u, v\} \in E$ separating v from $*$. So we have constructed for any weighted tree an associated SDR tree, and it is very easy to verify that this establishes in fact a map from the set of isomorphism classes of weighted trees to the set of isomorphism classes of SDR trees.

[2] In fact, this construction is a rather unorthodox discrete version of the fundamental construction in elementary calculus, the map t: $V \to \Gamma$ denoting the *integral* of the map w: $E' \to \Gamma$, and w denoting the *derivative* of t.

$$
\begin{tikzcd}
\mathrm{SDR}(X,\Gamma) \arrow[r, hook, two heads, "\varphi"] & \mathrm{SU}(X,\Gamma) \\
\mathrm{WT}(X^*,\Gamma) \arrow[u, hook, two heads, "\psi"] \arrow[ur, hook, two heads] \arrow[r, hook, "\Phi"] & \mathrm{SM}_4(X^*,\Gamma) \arrow[u, two heads, "\Psi"']
\end{tikzcd}
$$

FIG. 11. The commutative diagram.

To show that ψ is bijective, we construct its inverse: suppose we are given an SDR tree $(V, E; t)$ from $\mathrm{SDR}(X, \Gamma)$. Let $r \in V$ denote the root of (V, E), and suppose $* \notin X$. We construct a tree (V', E') by putting

$$V' := V \mathbin{\dot\cup} \{*\} \qquad \text{and} \qquad E' := \{\{u, v\} : (u, v) \in E\} \cup \{\{*, r\}\}.$$

Finally, we define the "derivative" w of t in terms of a weighting function w: $E' \to \Gamma$, defined by $w(\{*, r\}) := t(r)$ and $w(\{u, v\}) := t(v) - t(u)$ for all $(u, v) \in E$. Again, it is very easy to see that this construction induces a map from $\mathrm{SDR}(X, \Gamma)$ into $\mathrm{WT}(X^*, \Gamma)$ which is just reversing the above procedure and, hence, forms the inverse of ψ.

Next, we want to establish a map Ψ: $\mathrm{SM}_4(X^*, \Gamma) \to \mathrm{SU}(X, \Gamma)$. Given a map d: $X^* \times X^* \to \Gamma$ from $\mathrm{SM}_4(X^*, \Gamma)$, we define D: $X \times X \to \Gamma$ by

$$D(x, y) := \tfrac{1}{2}(d(x, *) + d(y, *) - d(x, y)). \tag{13}$$

We claim that $D \in \mathrm{SU}(X, \Gamma)$ holds: As the distance function d is symmetric, so is D, hence D satisfies (U1). Given $x, y, z \in X$, we may suppose that x, y, z are ordered in such a way that

$$d(x, y) + d(z, *) = d(x, z) + d(y, *)$$

holds which implies $\sharp\{D(x, y), D(x, z), D(y, z)\} \leqslant 2$ because of

$$\begin{aligned} D(x, y) &= \tfrac{1}{2}(d(x, *) + d(y, *) - d(x, y)) \\ &= \tfrac{1}{2}(d(x, *) + d(z, *) - d(x, z)) = D(x, z). \end{aligned}$$

So D satisfies (U2). In addition, if $x_1, x_2, x_3, x_4 \in X$ are ordered so that $d(x_1, x_2) + d(x_3, x_4) = d(x_1, x_3) + d(x_2, x_4)$ holds, then we also have

$$\begin{aligned} D(x_1, x_2) + D(x_3, x_4) &= \tfrac{1}{2} \sum_{j=1}^{4} d(x_j, *) - \tfrac{1}{2}(d(x_1, x_2) + d(x_3, x_4)) \\ &= \tfrac{1}{2} \sum_{j=1}^{4} d(x_j, *) - \tfrac{1}{2}(d(x_1, x_3) + d(x_2, x_4)) \\ &= D(x_1, x_3) + D(x_2, x_4), \end{aligned}$$

so D satisfies the 4-point condition as well. Now suppose there exist x_1, x_2, x_3, $x_4 \in X$ with

$$\alpha := D(x_1, x_2) = D(x_2, x_3) = D(x_3, x_4)$$

and

$$\beta := D(x_1, x_3) = D(x_1, x_4) = D(x_2, x_4).$$

We distinguish three cases: if

$$D(x_1, x_2) + D(x_3, x_4) = D(x_1, x_3) + D(x_2, x_4)$$

holds, then $\alpha + \alpha = \beta + \beta$. If

$$D(x_1, x_2) + D(x_3, x_4) = D(x_1, x_4) + D(x_2, x_3),$$

then $\alpha + \alpha = \beta + \alpha$, and in case of

$$D(x_1, x_3) + D(x_2, x_4) = D(x_1, x_4) + D(x_2, x_3)$$

we conclude $\beta + \beta = \beta + \alpha$. So $\alpha = \beta$ holds in every case. This proves that D also satisfies (U3), hence D is a symbolic ultrametric in $\mathrm{SU}(X, \Gamma)$, and we can define $\Psi(d) := D$.

Now consider the diagram in Fig. 11. We claim that the diagram is commutative, that is, one has $\varphi \circ \psi = \Psi \circ \Phi$. Let $(V', E'; w)$ be a weighted tree from $\mathrm{WT}(X^*, \Gamma)$, and put $(V, E; t) := \psi((V', E'; w))$ and $D_t := \varphi((V, E; t)) = \varphi \circ \psi((V', E'; w))$. Furthermore, let $d_w := \Phi((V', E'; w))$

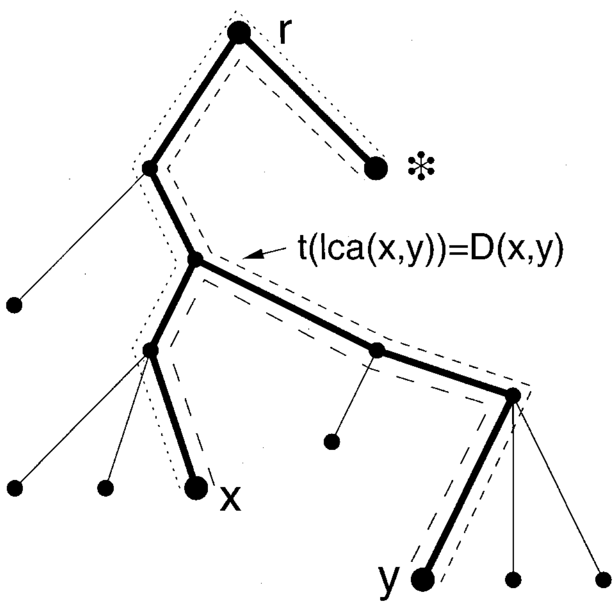

FIG. 12. To Eq. (14).

denote the induced map from $X^* \times X^*$ into Γ according to (12). It is easy to verify (cf. Fig. 12) that

$$D_t(x, y) = \tfrac{1}{2}(d_w(x, *) + d_w(y, *) - d_w(x, y)) \tag{14}$$

holds for all $x, y \in X$. But this implies $D_t = \Psi(d_w)$ in view of (13) and therefore $\varphi \circ \psi = \Psi \circ \Phi$.

As ψ and φ are bijective, it is obvious that Ψ must be surjective and Φ must be injective as depicted in Fig. 11. To show that both maps are indeed bijections, it is enough to show that Ψ is injective. Yet, from (13) we infer

$$D(x, x) = \tfrac{1}{2}(d(x, *) + d(x, *) - d(x, x)) = d(x, *)$$

for all $x \in X$, so we can calculate d from D as well by

$$d(x, y) = 2D(x, y) - D(x, x) - D(y, y) \tag{15}$$

for all $x, y \in X$. So Ψ is indeed injective, and Theorem 4 is established. ∎

It is well known that if we want to check whether a given symmetric map $d: X^* \times X^* \to \mathbb{R}$ with $d(x, x) = 0$ for all $x \in X^*$ satisfies the 4-point condition in the (considerably stronger) form

$$d(x, y) + d(x', y') \leqslant \max\{d(x, x') + d(y, y'), d(x, y') + d(y, x')\} \tag{16}$$

for all $x, y, x', y' \in X^*$, it is sufficient to show that d satisfies Condition (16) for all $x, y, x', y' \in X^*$ with $* \in \{x, y, x', y'\}$ (cf. Corollary 7 and Remark 5 below). Yet, if we replace $\mathbb{R}$ by an arbitrary 2-divisible abelian group Γ and (16) by (11), we need an additional condition. To this end, given a symmetric map $d: X^* \times X^* \to \Gamma$ and $x, y, x', y' \in X^*$, we say that x, y are *separated* from x', y', denoted by $xy|x'y'$, if $d(x, y) + d(x', y') \neq d(x, x') + d(y, y') = d(x, y') + d(y, x')$ holds.

Lemma 6. *If $d: X^* \times X^* \to \Gamma$ is a symmetric map with $d(x, x) = 0$ for all $x \in X^*$, then the following two conditions are equivalent*:

(i) *d satisfies the 4-point condition,*

(ii) *d satisfies Condition (11) for all $x, y, x', y' \in X^*$ with $* \in \{x, y, x', y'\}$, and there exist no $x_1, x_2, x_3, x_4 \in X$ such that $*x_1|x_3x_4$, $*x_2|x_1x_3$, $*x_3|x_2x_4$ and $*x_4|x_1x_2$ hold.*

Proof. Let $D: X \times X \to \Gamma$ be defined as in (13). We know from Theorem 4 that d satisfies the 4-point condition if and only if D satisfies conditions (U1) to (U3). Clearly, for $x, y, z \in X$ we have $d(*, x) + d(y, z) = d(*, z) + d(x, y)$ if and only if

$$D(x, y) = \tfrac{1}{2}(d(*, x) + d(*, y) - d(x, y))$$
$$= \tfrac{1}{2}(d(*, y) + d(*, z) - d(y, z)) = D(y, z).$$

So $*x \mid yz$ holds if and only if $D(y, z) \neq D(x, y) = D(x, z)$.

Suppose d satisfies the 4-point condition. If there exist $x_1, x_2, x_3, x_4 \in X$ such that $*x_1 \mid x_3 x_4$, $*x_2 \mid x_1 x_3$, $*x_3 \mid x_2 x_4$ and $*x_4 \mid x_1 x_2$ hold, then we get $D(x_1, x_2) = D(x_2, x_3) = D(x_3, x_4) \neq D(x_1, x_3) = D(x_1, x_4) = D(x_2, x_4)$ in contradiction to (U3).

Now suppose d satisfies condition (ii). We conclude that D satisfies (U1) and (U2) as in the proof of Theorem 4 (note that we only used the 4-point condition for $*, x, y, z$ in this part of the proof). If there exist $x_1, x_2, x_3, x_4 \in X$ with $D(x_1, x_2) = D(x_2, x_3) = D(x_3, x_4) \neq D(x_1, x_3) = D(x_1, x_4) = D(x_2, x_4)$, then we can directly infer $*x_1 \mid x_3 x_4$, $*x_2 \mid x_1 x_3$, $*x_3 \mid x_2 x_4$ and $*x_4 \mid x_1 x_2$. So no such $x_1, x_2, x_3, x_4 \in X$ can exist, and D must also satisfy (U3). ▮

COROLLARY 7. *A symmetric map $d: X^* \times X^* \to \mathbb{R}$ with $d(x, x) = 0$ for all $x \in X^*$ satisfies the four-point condition if it satisfies Condition* (16) *for all $x, y, x', y' \in X^*$ with $* \in \{x, y, x', y'\}$.*

Proof. Suppose there exist $x_1, x_2, x_3, x_4 \in X$ such that $*x_1 \mid x_3 x_4$, $*x_2 \mid x_1 x_3$, $*x_3 \mid x_2 x_4$ and $*x_4 \mid x_1 x_2$ hold. We infer $d(*, x_1) + d(x_3, x_4) < d(*, x_4) + d(x_1, x_3)$, $d(*, x_2) + d(x_1, x_3) < d(*, x_3) + d(x_1, x_2)$, $d(*, x_3) + d(x_2, x_4) < d(*, x_2) + d(x_3, x_4)$ and $d(*, x_4) + d(x_1, x_2) < d(*, x_1) + d(x_2, x_4)$. But this implies

$$\begin{aligned} d(*, x_1) &+ d(x_3, x_4) + d(*, x_2) + d(x_1, x_3) + d(*, x_3) \\ &+ d(x_2, x_4) + d(*, x_4) + d(x_1, x_2) \\ &< d(*, x_4) + d(x_1, x_3) + d(*, x_3) + d(x_1, x_2) + d(*, x_2) \\ &+ d(x_3, x_4) + d(*, x_1) + d(x_2, x_4), \end{aligned}$$

a contradiction. ▮

Remark 5. Of course, as is well known, the map d will also satisfy condition (16) in this case which is most easily shown in the standard way by establishing directly that both assertions, condition (16) for all $x, y, x', y' \in X^*$ <u>and</u> condition (16) for all $x, y, x', y' \in X^*$ with $* \in \{x, y, x', y'\}$, are equivalent with the assertion that the corresponding map $D\colon X^2 \to \mathbb{R}$ satisfies the condition

$$D(x, z) \geqslant \min\{D(x, y), D(y, z)\}$$

for all $x, y, z \in X$.

Now, let $(\Lambda, +)$ be an abelian monoid with neutral 0 satisfying

$$\alpha + \xi = \alpha + \zeta \quad \text{implies} \quad \xi = \zeta \qquad \text{(cancellation)},$$

$$\alpha + \alpha = \beta + \beta \quad \text{implies} \quad \alpha = \beta \qquad \text{(uniqueness of halves)}$$

for all $\alpha, \beta, \xi, \zeta \in \Lambda$. Canonical choices for Λ are $\Lambda = \mathbb{R}$, $\Lambda = \mathbb{R}_{\geqslant 0}$, $\Lambda = \mathbb{Z}$, or $\Lambda = \mathbb{N}_0$, under addition. More generally, any additively closed subset Λ of a 2-divisible abelian group Γ with $0 \in \Lambda$ satisfies these conditions, and any abelian monoid satisfying these conditions is an additively closed subset of some abelian 2-divisible group containing its neutral element. A map $d\colon X \times X \to \Lambda \subseteq \Gamma$ satisfies the 4-*point condition with respect* to Λ if, for any subset $A \subseteq X$ of cardinality at most four, there exists some $\xi \in \Lambda$ and some labeling $A = \{x, x', y, y'\}$ such that

$$d(x, y) + d(x', y') + 2\xi = d(x, x') + d(y, y') = d(x, y') + d(y, x'), \tag{17}$$

that is, the values of d are in Λ, d satisfies the 4-point condition as a map from X into Γ, and one has $w(d) \subseteq \Lambda$.[3] Clearly, this holds for any map $d = d_w$, where d_w is the induced map of some weighted tree $(V', E'; w)$ with $w(E') \subseteq \Lambda$.

Note that in a 2-divisible abelian group Γ, a map $d\colon X \times X \to \Gamma$ satisfies the 4-point condition with respect to Γ if and only if (11) holds, so (17) generalizes (11). For an additively closed subset $\Lambda \subseteq \Gamma$ with $0 \in \Lambda$, we denote by $\mathrm{SM}_4(Y, \Lambda)$ the set of Λ-valued symmetric maps $d\colon Y^2 \to \Lambda$ with $d(x, x) = 0$ for all $x \in Y$ that satisfy the 4-point condition with respect to Λ. It follows immediately from these definitions and Remark 4 that the bijection $\Phi\colon \mathrm{WT}(Y, \Gamma) \to \mathrm{SM}_4(Y, \Gamma)$ induces a bijection from $\mathrm{WT}(Y, \Lambda)$ onto $\mathrm{SM}_4(Y, \Lambda)$. In other words, the above results imply the main result of H.-J. Bandelt and M. A. Steel from [2]:

THEOREM 5 (Bandelt and Steel). *Let $d\colon X \times X \to \Lambda$ be a symmetric map with $d(x, x) = 0$ for all $x \in X$, where Λ is a cancellative abelian monoid that has uniqueness of halves. Then d satisfies the* 4-*point condition with respect to Λ if and only if there exists a Λ-weighted tree $T = (V, E; w)$ with leaf*

[3] Note that in case $d(x, x) = 0$ holds for all $x \in X$, the assumption $w(d) \subseteq \Lambda$ actually implies $d(x, y) \in \Lambda$ for all $x, y \in X$.

set $X \subseteq V$ that has no vertices of degree two while all inner edges have non-zero weight, that realizes d. In this case, such a tree T is necessarily unique.

More generally, if N is an *arbitrary* subset of Γ with $0 \in N$, then Φ induces a bijection from

$$\mathrm{WT}(Y, N) := \{(V', E'; w) \in \mathrm{WT}(Y, \Gamma) : w(E') \subseteq N\} \tag{18}$$

onto a subset of $\mathrm{SM}_4(Y, \Gamma)$ denoted—in accordance with the notations introduced above—by $\mathrm{SM}_4(Y, N)$ which consists exactly of those maps $d \in \mathrm{SM}_4(Y, \Gamma)$ for which the set

$$\begin{aligned} \Delta(d) := \{\xi \in \Gamma\text{: there exists } & x, x', y, y' \in Y \text{ with } xy \mid x'y', \\ & 2\xi = d(x, x') + d(y, y') - d(x, y) - d(x', y') \\ & \text{and } \{z \in Y : xz \mid x'y' \text{ and } xy \mid zx'\} = \emptyset\} \end{aligned} \tag{19}$$

is contained in N.

Although one might think that Theorem 2 presents a considerable generalization of Theorem 5, both theorems are in fact equivalent: we could also use Theorem 5 to prove the crucial step in Theorem 2. We do not give this proof in detail, but the idea is as follows: We consider the $\mathbb{Q}$-vector space $\Gamma = \mathbb{Q}^M$ and the canonical injective embedding of M into this vector space given by associating to any $m \in M$ the map $\iota_m: M \to \mathbb{Q}$ defined by $\iota_m(n) := \delta_{m,n}$ $(m, n \in M)$. Next, given a symbolic ultrametric D: $X \times X \to M$, we use (15) to construct a map d: $X^* \times X^* \to \Gamma$ that satisfies the 4-point condition, we then use Theorem 5 to find a corresponding weighted tree $T' = (V', E')$ with leaf set X^*, and from that tree, we construct a rooted, symbolically dated tree $T = (V, E)$ with leaf set X for which we finally verify that the dating map actually takes its values in M (as embedded in $\mathbb{Q}^M$).

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Note added in proof. Some historical remarks: The first to observe that an integer-valued metric defined on a finite set can be realized by a tree if and only if this holds for every four-point submetric was Zaretskii (cf. [12]). This was generalized later by Simões Pereira [11] and, independently, by Buneman [4] who studied the realizability of real-valued metrics by trees with edges of arbitrary positive length.

As we learned only after finishing this paper, Patrinos and Hakimi were then the first to include into consideration trees whose edges were of arbitrary, positive, or negative length. In [P], they actually established Theorem 3 for the particularly relevant case $\Gamma := \mathbb{R}$.

Unaware of this, Bandelt and Steel then proceeded to study the still more general case where the lengths of edges were allowed to take their values in (almost) arbitrary abelian groups—a simple yet decisive generalization of Patrinos' and Hakimi's result if it comes to derive Theorem 2 as a consequence of Theorem 3 along the way described just above.

Zaretskii was probably also the first to study the transformation from tree metrics to ultrametrics as defined in (13), employed later—and partly independent—also by Farris *et al.* [8], Brossier [3], and many others.

With our approach, bringing this line of evolution to a (temporary) close by allowing symbolic dating maps taking their values in completely arbitrary sets, we hope to eventually bridge the gap between distance- and sequence-based methods in sequence analysis (cf. [H]) as it allows to treat symbols—e.g., amino acid classes—attached to pairs of objects in almost the same way distances have been used so far.

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