TREE REPRESENTATIONS OF NON-SYMMETRIC GROUP-VALUED PROXIMITIES

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ABSTRACT. Let X be a finite set and let d be a function from $X \times X$ into an arbitrary group $\mathcal{G}$. An example of such a function arises by taking a tree T whose vertices include X, assigning two elements of $\mathcal{G}$ to each edge of T (one for each orientation of the edge), and setting $d(i,j)$ equal to the product of the elements along the directed path from i to j. We characterize conditions when an arbitrary function d can be represented in this way, and show how such a representation may be explicitly constructed. We also describe the extent to which the underlying tree and the edge weightings are unique in such a representation. These results generalize a recent theorem involving undirected edge assignments by an Abelian group. The non-Abelian bi-directed case is of particular relevance to phylogeny reconstruction in molecular biology.

1. INTRODUCTION

A classical problem in classification is the following: when can an arbitrary metric on a finite set be realized by embedding the points of the metric space in a positively edge-weighted tree with its associated minimum path-length metric? More precisely, given a metric $d : X \times X \to \mathbb{R}^{\geq 0}$, when does there exist a tree $T = (V, E)$ with $X \subseteq V$ and a weighting $w : E \to \mathbb{R}^{\geq 0}$ such that $d(i,j)$ is the sum of the weights of the edges on the path connecting vertices i and j? Furthermore, if d has such a representation, what can one say concerning the possible choices of T and w?

Both questions have well-known solutions which date back 30 years (see [7], [12], and [14]). Specifically, a tree representation exists for all of X precisely if it exists for every subset of X of size at most 4, and this, in turn, is equivalent to an appropriate "four point condition" involving (in)equalities on sums of pairs of $d(i,j)$ values. Furthermore, when they exist, the pair (T, w) that accommodate a representation of d is uniquely determined, provided T has no vertices in $V - X$ of degree less than 3 and w is strictly positive. Note that the last two provisos can always be imposed.

These classical results, which have become a central tool in classification (particularly in evolutionary biology) have been subsequently generalized in several directions. Hakimi and Patrinos [10] considered two extensions: firstly, to allow for

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edge weightings over $\mathbb{R}$ (rather than just $\mathbb{R}^{\geq 0}$); and, secondly, to consider trees in which each edge is assigned two real numbers (one for each orientation of the edge), with $d(i,j)$ now being defined as the sum of the weights on the directed path from i to j. This second extension allows, but does not necessarily imply, non-symmetry in the function d.

A second line of generalization was adopted by Bandelt and Steel [4] to allow edge weightings to take values in a suitably structured Abelian semigroup. One spin-off of this approach was to provide a tree representation for distance hereditary graphs.

A third line of generalization was provided by Bőcker and Dress [5] who developed a purely combinatorial statement (i.e. involving no algebraic structure) which implied the result of [4]; though, as pointed out in [5], the two results are actually equivalent. The main theorem from [5] will be a central tool here.

This paper represents a continuation of this story. We generalize the approach of [4] by allowing the edge weightings, and hence d, to take values in an arbitrary group, and we follow the approach of Hakimi and Patrinos of allowing each edge to have two weightings, according to its two orientations. This two-step generalization leads to only a slight complication in the statement of the main existence theorem.

A key motivation for considering these generalizations comes from the field of molecular biology, and, in particular, the problem of reconstructing evolutionary trees from aligned genetic sequences. If one assumes that these sequences evolve according to standard Markov models, then to each edge of the underlying tree is associated two transition matrices (depending on the direction along the edge that the process is run). The ordered product of these transition matrices along the path from species i to species j is then the net transition matrix for the pair (i,j) which can be estimated from genetic data (see [2] and [8]). Thus, if we have r-state sequences (for instance $r = 4$ for DNA sequences), we are precisely in the setting of assigning elements of the non-Abelian group $\mathcal{G}$ of $r \times r$ invertible real matrices to each orientation of the edges and taking (directed) products. The results below describe conditions under which the associated tree (and the edge-weightings) can be reconstructed (thereby generalizing the results of [2]). Moreover, these results describe conditions under which such a representation exists over $\mathcal{G}$ (of course, for this particular problem we require more - namely representation over the semigroup of transition matrices, however, representation over $\mathcal{G}$ is certainly a necessary condition).

The structure of the paper is as follows. We begin Section 2 by setting up some terminology and establishing a basic property of tree representations. Several mappings are defined and some important relationships between these mappings are determined. In Section 3, we state the two main (existence and uniqueness) results, Theorems 3.1 and 3.2, and provide proofs. We also derive, as a corollary, the main theorem from [4]. Section 4 makes some concluding remarks.

2. Preliminaries

Throughout this paper, X will denote a finite set, and $\mathcal{G}$ will denote an arbitrary group with identity element $1_{\mathcal{G}}$. We multiply elements of $\mathcal{G}$ from left to right.

Definitions.

- Let T be a tree with vertex set V and edge set $E \subseteq \{\{x,y\} : x, y \in V; x \neq y\}$. A vertex $v \in V$ is *interior* if $deg_T(v) > 1$, otherwise v is a *leaf.* An edge $e = \{u, v\} \in E$ is *interior* if both u and v are interior vertices, otherwise we say e is *exterior.*
- Suppose we have a map $\phi : X \to V$ with the property that, for all $v \in V$,
$$\deg_T(v) \leq 2 \Rightarrow v \in \phi(X).$$
The pair $(T; \phi)$ is called an X*-tree*, and we will sometimes write this as the ordered triple $(V, E; \phi)$. If ϕ is a bijection from X into the set V_1 of degree-one vertices of T, then $(V, E; \phi)$ is a *phylogenetic* X*-tree.* In this case, we can view X as a subset of V_1 and so we will frequently just denote a phylogenetic X–tree by just T or (V, E), since ϕ is implicitly determined. An example of a phylogenetic X–tree for $X = \{i, j, k, x\}$ is shown in Figure 1. Two X–trees $(V, E; \phi)$ and $(V', E'; \phi')$ are *isomorphic* if there exists a bijection $\alpha : V \to V'$ which induces a bijection between E and E' and which satisfies $\phi' = \alpha \circ \phi$, in which case α is unique. We denote isomorphism by the symbol $\equiv$.
- For a tree (V, E), let $E^{(2)} = \{(u, v) : \{u, v\} \in E\}$. We can regard $E^{(2)}$ as the set of pairs in which each member consists of an element of E and an orientation of it. Each element of $E^{(2)}$ is called an *arc.* Let w be a function from $E^{(2)}$ into the group $\mathcal{G}$. We refer to $w((u, v))$ as the *weight* of arc (u, v) and, for simplicity, we shall write $w((u, v))$ as $w(u, v)$. Following [2], the *return-trip weights* of an edge $\{u, v\}$ are the elements $w(u, v)w(v, u)$ and $w(v, u)w(u, v)$ of $\mathcal{G}$. We say that an edge e is *properly weighted* if $1_{\mathcal{G}}$ is not a return trip weight for e (or, equivalently, if the return trip weights for e are not both equal to $1_{\mathcal{G}}$).
- Given an X–tree $(T; \phi)$ and vertices $v_1, v_2 \in V$, define $D_{(T;\phi;w)} : V \times V \to \mathcal{G}$ by setting $D_{(T;\phi;w)}(v_1, v_2)$ equal to the (ordered) product of the weights of the arcs on the directed path from v_1 to v_2 if $v_1 \neq v_2$ and $D_{(T;\phi;w)}(v_1, v_2)$ equal to $1_{\mathcal{G}}$ if $v_1 = v_2$. Define $d_{(T;\phi;w)} : X \times X \to \mathcal{G}$ by setting
$$d_{(T;\phi;w)}(i, j) = D_{(T;\phi;w)}(\phi(i), \phi(j)),$$
for all $i, j \in X$. We will sometimes drop or abbreviate the subscripts on $D_{(T;\phi;w)}$ and $d_{(T;\phi;w)}$ and write, for example, $d_T(i, j)$ or even just $d(i, j)$ if there is no chance of ambiguity.
- A *proximity* mapping is any function $\delta : X \times X \to \mathcal{G}$ that satisfies $\delta(i, i) = 1_{\mathcal{G}}$ for all $i \in X$. Furthermore, such a mapping is a *tree proximity* if there is an X–tree $(V, E; \phi)$ with a weight function $w : E^{(2)} \to \mathcal{G}$ such that, for all $i, j \in X$, $d_{(T;\phi;w)}(i, j) = \delta(i, j)$; in which case $(T; \phi; w)$ is said to be a *tree representation* of δ. If, in addition, $(T; \phi)$ is a phylogenetic X–tree and each interior edge is properly weighted, then $(T; \phi; w)$, or more briefly $(T; w)$, is said to be a *standard* tree representation of δ.

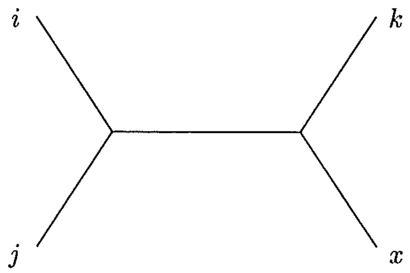

FIGURE 1. A phylogenetic X–tree for $X = \{i, j, k, x\}$.

Before proving Proposition 2.1, we describe how a tree representation $(T; \phi; w)$ of a proximity map δ gives rise to an associated tree representation $(T'; \phi'; w')$ of δ in which $(T'; \phi')$ is a phylogenetic X–tree. For all $v \in V(T)$ (the set of vertices of T), let $S(v) = \{i \in X : \phi(i) = v\}$ and let $s(v) = |S(v)|$. For each interior vertex $v \in V$ with $s(v) > 0$ and for each leaf $v \in V$ with $s(v) > 1$, let us make v the endpoint of $s(v)$ new edges, and modify ϕ so that, instead of mapping $S(v)$ to v, we map $S(v)$ bijectively to the endpoints of the new edges, thereby creating a phylogenetic X–tree $(T'; \phi')$. Let w' denote the extension of w to the arcs of T' by assigning the value $1_{\mathcal{G}}$ to both arcs of each newly-created edge. We will refer to $(T'; \phi'; w')$ as the *phylogenetic expansion* of $(T; \phi; w)$.

Proposition 2.1. *Let $\delta : X \times X \to \mathcal{G}$ be a tree proximity map. Then there exists a standard tree representation of δ.*

Proof. By obtaining the phylogenetic expansion of some tree representation of δ if necessary, we may assume that we have a tree representation $(T; \phi; w)$ of δ for which $(T; \phi)$ is a phylogenetic X–tree. We complete the proof by showing how $(T; \phi; w)$ can be transformed to a standard tree representation of δ. Suppose that u and v are adjacent interior vertices of $(T; \phi; w)$ such that $w(u, v)w(v, u) = 1_{\mathcal{G}}$. Let $(T; \phi; w')$ be obtained from $(T; \phi; w)$ by replacing w with the weight function w' defined, for all distinct v_1 and v_2 of $V(T) - \{u\}$, by $w'(u, v_1) = w(v, u)w(u, v_1)$, $w'(v_1, u) = w(v_1, u)w(v, u)^{-1}$, and $w'(v_1, v_2) = w(v_1, v_2)$. Thus $w'(u, v) = 1_{\mathcal{G}}$ and $w'(v, u) = 1_{\mathcal{G}}$. Using the fact that $(T; \phi)$ is a phylogenetic X–tree, a routine check shows that $(T; \phi; w')$ is a tree representation of δ. Thus the tree $(T'; \phi; w'')$, where

- T' is the tree obtained from T by contracting $\{u, v\}$, and
- the mapping $w'' : E(T')^{(2)} \to \mathcal{G}$ is defined, for all $(v_1, v_2) \in E(T')^{(2)}$, by $w''(v_1, v_2) = w'(v_1, v_2)$,

is also a tree representation of δ. Moreover, it is easily checked that the return-trip weight of every edge in $(T; \phi; w')$ is equal to $1_{\mathcal{G}}$ if and only if it is equal to $1_{\mathcal{G}}$ in $(T; \phi; w)$. Hence, in $(T'; \phi; w'')$, the number of properly weighted interior edges is one less than that for $(T; \phi; w)$. By continuing this process if necessary, we eventually obtain a standard tree representation of δ. $\square$

Remark. In contrast to the classical real-valued symmetric setting, a tree proximity map may not have a tree representation in which the weighting function is proper on *all* edges. In the proof of Theorem 3.1, we outline an explicit polynomial-time construction of a standard tree representation of a tree proximity map.

Before proceeding further, we require the definitions of several maps, each of which are essential to the proofs of the main theorems of this paper.

Definitions.

- Given a tree $T = (V, E)$, a *discriminating $\mathcal{G}$-dating map* is a function $t : V \to \mathcal{G}$ with the property that if $\{u, v\}$ is an interior edge of T, then $t(u) \neq t(v)$.
- Given a proximity map $\delta : X \times X \to \mathcal{G}$ and an element x in X, there is an important associated map $\delta_x : X \times X \to \mathcal{G}$ defined, for all $i, j \in X$, by
$$\delta_x(i,j) = \delta(x,i)\delta(j,i)^{-1}\delta(j,x).$$
Note that δ_x is not usually a proximity map since we will generally have $\delta_x(i,i) \neq 1_{\mathcal{G}}$.
- Given a phylogenetic X–tree $T = (V, E)$, a discriminating $\mathcal{G}$–dating map $t : V \to \mathcal{G}$, an element x in X, and a proximity map $\delta : X \times X \to \mathcal{G}$, we describe two associated mappings:
  (i) A map $d_x^{(T;t)} : X \times X \to \mathcal{G}$ which is defined as follows. For elements u and v in V, write $u \leq_x v$ if u lies on the path from x to v. For all $i, j \in X$, set
  $$d_x^{(T;t)}(i,j) = t(glb_{\leq_x}(i,j)),$$
  where $glb_{\leq_x}$ denotes the greatest lower bound under the partial order $\leq_x$.
  (ii) An arc weighting function $w = w_{t,x} : E^{(2)} \to \mathcal{G}$ which is defined as follows. To each pair of arcs (u, v) and (v, u), assign the weights $w(u, v)$ and $w(v, u)$, respectively, so that:
    * if $v = i \in X - \{x\}$, set
    $$w(u,i) = t(u)^{-1}t(i)\delta(i,x)^{-1} \text{ and } w(i,u) = \delta(i,x);$$
    * otherwise, if $u \leq_x v$ or $u = x$, set
    $$w(u,v) = t(u)^{-1}t(v) \text{ and } w(v,u) = 1_{\mathcal{G}}.$$
- Lastly, two other mappings are needed. Suppose that $(T; w)$ is a standard tree representation for a tree proximity δ with $T = (V, E)$. Let $x \in X$.
  (i)$'$ Define $t = t^{(T;w;x)} : V \to \mathcal{G}$ as follows. If $(u_1, v_1), (u_2, v_2), \ldots, (u_k, v_k)$ denotes the arcs on the path from x to v (so $u_1 = x$ and $v_k = v$), then set
  $$t(v) = w(u_1,v_1)w(u_2,v_2)\ldots w(u_k,v_k)w(v_k,u_k)\ldots w(v_2,u_2)w(v_1,u_1).$$
  In other words, for all $v \in V$, $t(v)$ is the ordered product of the weights of the arcs on the directed path from x to v multiplied by the ordered product of the weights on the directed path from v back to x. Since $(T; w)$ is a standard tree representation (and so each interior edge is properly weighted), it follows that $t^{(T;w;x)}$ is a discriminating $\mathcal{G}$–dating map.
  (ii)$'$ The second map $t_{\delta,x} : V \to \mathcal{G}$ is defined as follows: for each $v \in V$, select elements i and j of X so that v is the greatest lower bound (under the partial order $\leq_x$) of i and j, and set
  $$t_{\delta,x}(v) = \delta(x,i)\delta(j,i)^{-1}\delta(j,x).$$

That $t_{\delta,x}$ is well-defined (i.e. independent of the choice of i and j) and, moreover, a discriminating $\mathcal{G}$–dating map, follows from the first part of Lemma 2.2.

Lemma 2.2 establishes some important relationships between the above mappings.

Lemma 2.2. *Let $\delta : X \times X \to \mathcal{G}$ be a proximity map and let x be an element of X.*

1. *If $(T; w)$ is a standard tree representation of δ, then*
$$t_{\delta,x} = t^{(T;w;x)}$$
and
$$\delta_x = d_x^{(T;t')},$$
where $t' = t^{(T;w;x)}$ $(= t_{\delta,x})$.
2. *Conversely, if $\delta_x = d_x^{(T;t)}$ for some phylogenetic X–tree T and discriminating $\mathcal{G}$–dating map t, then $(T; w_{t,x})$ is a standard tree representation of δ.*

Proof. **Part 1.** To prove the first half of Part 1, let v be an element of $V(T)$, and choose elements i and j of X so that $v = glb_{\leq_x}(i, j)$ in T. Let p_v (resp. q_v) be the ordered product of arc weights on the path from x to v (resp. v to x) in T. Furthermore, let p_i (resp. q_j) be the ordered product of arc weights on the path from v to i (resp. j to v) in T. Since $(T; w)$ is a tree representation of δ, it follows that
$$t_{\delta,x}(v) = \delta(x, i)\delta(j, i)^{-1}\delta(j, x) = p_v p_i (q_j p_i)^{-1} q_j q_v = p_v q_v = t^{(T;w;x)}(v),$$
as required.

For the second half of Part 1, set $t' = t_{\delta,x}$. Since $t_{\delta,x} = t^{(T;w;x)}$ and since $t^{(T;w;x)}$ is a discriminating $\mathcal{G}$–dating map, $t_{\delta,x}$ is a discriminating $\mathcal{G}$–dating map. Now, for all $i, j \in X$, we have
$$d_x^{(T;t')}(i, j) = t_{\delta,x}(glb_{\leq_x}(i, j)) = \delta(x, i)\delta(j, i)^{-1}\delta(j, x) = \delta_x(i, j),$$
as required.

Part 2. Suppose that $\delta_x = d_x^{(T;t)}$, for some phylogenetic X–tree T and discriminating $\mathcal{G}$–dating map t. Firstly, note that, by the definition of $w_{t,x}$ and the fact that $t(u) \neq t(v)$ for each interior edge $\{u, v\}$ of T, we see that each interior edge of T is properly weighted. We complete the proof of Part 2 by verifying that $d_{(T;w_{t,x})}(i, j) = \delta(i, j)$, for all $i, j \in X$. Let I denote the cardinality of $\{x, i, j\}$. Depending on the value of I, there are three cases to consider:

- $I = 1$. In this case, $d_{(T;w_{t,x})}(x, x) = 1_{\mathcal{G}} = \delta(x, x)$, as required.
- $I = 2$. In this case, we may assume that $i = x$. Since $\delta_x = d_x^{(T;t)}$, we deduce that $t(x) = 1_{\mathcal{G}}$ and so, by the definition of $w_{t,x}$, we have $d_{(T;w_{t,x})}(x, j) = t(j)\delta(j, x)^{-1}$. Therefore, as $t(j) = t(glb_{\leq_x}(j, j)) = d_x^{(T;t)}(j, j) = \delta_x(j, j) = \delta(x, j)\delta(j, x)$, it follows that $d_{(T;w_{t,x})}(x, j) = \delta(x, j)$. Furthermore, from the definition of $w_{t,x}$, we directly get $d_{(T;w_{t,x})}(j, x) = \delta(j, x)$, as required.

- $I = 3$. By the definition of $w_{t,x}$, we have

$$d_{(T;w_{t,x})}(i,j) = \delta(i,x)t(glb_{\leq_x}(i,j))^{-1}t(j)d(j,x)^{-1}.$$

Now

$$t(glb_{\leq_x}(i,j)) = d_x^{(T;t)}(i,j) = d_x^{(T;t)}(j,i) = \delta_x(j,i) = \delta(x,j)\delta(i,j)^{-1}\delta(i,x),$$

which also implies that $t(j) = t(glb_{\leq_x}(j,j)) = \delta(x,j)\delta(j,x)$. Therefore $d_{(T;w_{t,x})}(i,j) = \delta(i,j)$, as required.

□

Combining Proposition 2.1 with the last lemma, we get Corollary 2.3.

Corollary 2.3. **1.** *A proximity map $\delta : X \times X \to \mathcal{G}$ is a tree proximity if and only if $\delta_x = d_x^{(T;t)}$ for some phylogenetic X–tree T and discriminating $\mathcal{G}$–dating map t.*

2. *Suppose that δ is a tree proximity. If T is the phylogenetic tree involved in a standard tree representation of δ, then $(T; w_{t,x})$ is a standard tree representation of δ, where $t = t_{\delta,x}$.*

The next proposition is an immediate consequence of [5, Theorem 2], the main theorem of [5].

Proposition 2.4. *Let $\delta : X \times X \to \mathcal{G}$ be a proximity map and let x be an element of X. Then there exists a phylogenetic X–tree T and a discriminating $\mathcal{G}$–dating map t such that $\delta_x = d_x^{(T;t)}$ if and only if δ_x satisfies the following conditions:*

(U1) *$\delta_x(i,j) = \delta_x(j,i)$, for all $i, j \in X$;*
(U2) *$|\{\delta_x(i,j), \delta_x(i,k), \delta_x(j,k)\}| \leq 2$, for all $i, j, k \in X$; and*
(U3) *there exist no pairwise distinct elements i, j, k, and l of X with*

$$\delta_x(i,j) = \delta_x(j,k) = \delta_x(k,l) \neq \delta_x(j,l) = \delta_x(l,i) = \delta_x(i,k).$$

Furthermore, up to canonical isomorphism, T is unique.

Combining Corollary 2.3 with Proposition 2.4, we get Corollary 2.5.

Corollary 2.5. *A proximity map $\delta : X \times X \to \mathcal{G}$ is a tree proximity map if and only if δ_x satisfies* (U1), (U2), *and* (U3) *for some $x \in X$.*

The existence part of Theorem 3.1 is proved via Corollary 2.5.

3. Main Results

We are now ready to state and prove our two main (existence and uniqueness) results, Theorems 3.1 and 3.2. Note that an explanation for the slight complication concerning "H_δ" in the statement of Theorem 3.1 is given in the remark immediately following the proof of Theorem 3.1.

Theorem 3.1. *Let $\delta : X \times X \to \mathcal{G}$ be a proximity map. Let H_δ denote the following (finite) subset of $\mathcal{G}$:*

$$\{\delta(i,k)\delta(j,k)^{-1}\delta(j,l)\delta(i,l)^{-1} : i,j,k,l \in X\}.$$

Suppose that H_δ has no elements of order 2. Then δ is a tree proximity map if and only if δ satisfies the following two conditions:

(P1) *For all distinct elements i,j and k of X,*

$$\delta(i,j)\delta(k,j)^{-1}\delta(k,i) = \delta(i,k)\delta(j,k)^{-1}\delta(j,i).$$

(P2) *For all four distinct elements of X, we can order these elements as i, j, k, and l so that*

$$\delta(i,k)\delta(j,k)^{-1} = \delta(i,l)\delta(j,l)^{-1}.$$

Furthermore, a standard tree representation of δ, if one exists, can be constructed in polynomial time from δ.

Proof. If δ is a tree proximity map, then it is straightforward to check that (P1) and (P2) must hold by cancelling the products of the appropriate arc weights in $\mathcal{G}$.

Before establishing the converse, note that if $\delta(i,k)\delta(j,k)^{-1} = \delta(i,l)\delta(j,l)^{-1}$, for some elements i, j, k, and l of X, then it is easily checked using (P1) that

$$\delta(k,i)\delta(l,i)^{-1} = \delta(k,j)\delta(l,j)^{-1}$$

also holds. We freely use this observation in the proof that follows.

Let x be an element of X. To prove the converse, it suffices to show, by Corollary 2.5, that δ_x satisfies conditions (U1), (U2), and (U3) as listed in the statement of Proposition 2.4. We now show that this is indeed the case.

For all $i,j \in X$, (P1) shows that δ_x satisfies (U1). Furthermore, for all $i,j,k \in X$, (P2) together with (U1) shows that δ_x satisfies (U2). The proof that (U3) holds for δ_x is as follows.

3.1.1. *δ_x satisfies* (U3).

Proof. Suppose that i, j, k, and l are pairwise distinct elements of X with

$$\delta_x(i,j) = \delta_x(j,k) = \delta_x(k,l)$$

and

$$\delta_x(j,l) = \delta_x(l,i) = \delta_x(i,k).$$

We prove (3.1.1) by showing that $\delta_x(i,j)$, $\delta_x(j,k)$, $\delta_x(k,l)$, $\delta_x(j,l)$, $\delta_x(l,i)$, and $\delta_x(i,k)$ are all equal.

If $|\{x,i,j,k,l\}| = 4$, then it is clear that (3.1.1) holds. Therefore assume that $|\{x,i,j,k,l\}| = 5$. Depending on the relationship between i, j, k, and l given by (P2) and noting the observation above, there are three cases to consider:

(i) $\delta(i,k)\delta(j,k)^{-1} = \delta(i,l)\delta(j,l)^{-1}$;
(ii) $\delta(i,j)\delta(k,j)^{-1} = \delta(i,l)\delta(k,l)^{-1}$; and
(iii) $\delta(i,j)\delta(l,j)^{-1} = \delta(i,k)\delta(l,k)^{-1}$.

We shall denote the above equations as (i), (ii), and (iii), respectively. Moreover, in the analysis of Cases (i)–(iii), we freely use the fact that (U1) holds for δ_x.

Case (i). Since $\delta_x(l,i) = \delta_x(k,i)$, we have $\delta(x,l)\delta(i,l)^{-1} = \delta(x,k)\delta(i,k)^{-1}$, which implies that

$$\delta(x,l)\delta(i,l)^{-1}\delta(i,k) = \delta(x,k). \tag{1}$$

Now, by (i), $\delta(j,l)^{-1} = \delta(i,l)^{-1}\delta(i,k)\delta(j,k)^{-1}$ and so

$$\begin{aligned}
\delta_x(j,l) = \delta_x(l,j) &= \delta(x,l)\delta(j,l)^{-1}\delta(j,x) \\
&= \delta(x,l)\delta(i,l)^{-1}\delta(i,k)\delta(j,k)^{-1}\delta(j,x) \\
&= \delta(x,k)\delta(j,k)^{-1}\delta(j,x), && \text{by (1)}, \\
&= \delta_x(k,j) = \delta_x(j,k),
\end{aligned}$$

completing the proof of (U3) for Case (i).

Case (ii). The proof of (U3) for Case (ii) is analogous to that of Case (i). We omit the details and just remark that we first deduce $\delta(x,k)\delta(j,k)^{-1}\delta(j,i) = \delta(x,i)$ via the fact that $\delta_x(i,j) = \delta_x(k,j)$, and then show $\delta_x(k,l) = \delta_x(l,i)$.

Case (iii). Since $\delta_x(j,i) = \delta_x(k,l)$ and since $\delta_x(j,l) = \delta_x(k,i)$, we have

$$\delta(x,j)\delta(i,j)^{-1}\delta(i,x) = \delta(x,k)\delta(l,k)^{-1}\delta(l,x) \tag{2}$$

and

$$\delta(x,j)\delta(l,j)^{-1}\delta(l,x) = \delta(x,k)\delta(i,k)^{-1}\delta(i,x), \tag{3}$$

respectively. By combining (2) and (3), we deduce that

$$\delta(l,k)^{-1}\delta(l,x)\delta(i,x)^{-1}\delta(i,j) = \delta(i,k)^{-1}\delta(i,x)\delta(l,x)^{-1}\delta(l,j),$$

which in turn implies that

$$\delta(i,k)\delta(l,k)^{-1}\delta(l,x)\delta(i,x)^{-1} = \delta(i,x)\delta(l,x)^{-1}\delta(l,j)\delta(i,j)^{-1}. \tag{4}$$

Substituting (iii) into (4), we get

$$\delta(i,j)\delta(l,j)^{-1}\delta(l,x)\delta(i,x)^{-1} = \delta(i,x)\delta(l,x)^{-1}\delta(l,j)\delta(i,j)^{-1}.$$

Since H_δ has no elements of order 2, the last equation implies that

$$\delta(i,x)\delta(l,x)^{-1}\delta(l,j)\delta(i,j)^{-1} = 1_G. \tag{5}$$

Having established (5), we complete the proof of (U3) for Case (iii) as follows. By (iii), $\delta(i,k)^{-1} = \delta(l,k)^{-1}\delta(l,j)\delta(i,j)^{-1}$, and so

$$\begin{aligned}
\delta_x(i,k) = \delta_x(k,i) &= \delta(x,k)\delta(i,k)^{-1}\delta(i,x) \\
&= \delta(x,k)\delta(l,k)^{-1}\delta(l,j)\delta(i,j)^{-1}\delta(i,x) \\
&= \delta(x,k)\delta(l,k)^{-1}\delta(l,x), && \text{by (5)}, \\
&= \delta_x(k,l),
\end{aligned}$$

as required. □

We conclude that δ_x satisfies (U1), (U2), and (U3) and so, by Corollary 2.5, δ is a tree proximity map.

Lastly, we describe a polynomial time algorithm for finding a standard tree representation of δ. Firstly, we provide a construction of a phylogenetic X–tree that turns out to be isomorphic to the underlying phylogenetic X–tree of a standard tree representation of δ. For a tree proximity map δ and an element x in X, let $R(\delta, x)$ denote the set of x–rooted phylogenetic trees (that is, trees rooted on leaf x) which is constructed as follows. For each pairwise disjoint triple $i, j, k \in X$, if

$$\delta_x(i,j) \neq \delta_x(i,k) = \delta_x(j,k),$$

then place the x–rooted tree $ij|kx$, as shown in Figure 1, into $R(\delta, x)$. Let $A[R(\delta, x)]$ denote the x–rooted tree constructed from $R(\delta, x)$ by applying the algorithm of Aho et al. [1] (see also [6] and [11]). Briefly, in this algorithm, one first constructs a graph G having vertex set $X - \{x\}$ and with an edge between any two vertices i and j precisely if there exists $k \in X - \{x\}$ such that $ij|kx \in R(\delta, x)$. One then takes the connected components of this graph, which form the top "clusters" of the tree, and continues this process recursively on the vertices of each component. For further details see [6] or [11].

We now show that if $(T; w)$ is a standard tree representation of δ, then

$$A[R(\delta, x)] \equiv T. \tag{6}$$

To prove (6), we argue by induction based on the number of interior vertices in the longest path of T that starts at x, when one considers T as an x–rooted tree. Let $h(T)$ denote this number. If $h(T) = 1$, then, as T is part of a standard tree representation of δ, it follows by the first part of Lemma 2.2 that $R(\delta, x)$ is empty and so (6) holds.

Now assume that $h(T) > 1$ and that (6) holds for all trees in a standard tree representation of δ with fewer interior vertices in the longest path starting at x. For $r > 1$, let $V_1, V_2, \ldots, V_r$ denote the vertex sets of the subtrees of T, other than the isolated vertex x, incident with the vertex of T adjacent to x. For all $p \in \{1, 2, \ldots, r\}$, let $X_p = \phi^{-1}(V_p)$. Thus $X_1, X_2, \ldots, X_r$ forms a partition of $X - \{x\}$.

Let G be the graph described above in the brief description of the algorithm. To prove the induction step of the proof, it suffices to show that $X_1, X_2, \ldots, X_r$ are precisely the vertex sets of the connected components of G. That is, for some $p \in \{1, 2, \ldots, r\}$, elements i and j are both in X_p if and only if there exists $k \in X - \{x\}$ such that $ij|kx \in R(\delta, x)$. We now show that this is indeed the case.

Suppose that $i, j \in X_p$, for some $p \in \{1, 2, \ldots, r\}$. Let $v = glb_{\leq_x}(i, j)$ in T. Since $i, j \in X_p$, there exists an interior vertex u in T and a k in X such that, in T, vertices u and v are adjacent and $u = glb_{\leq_x}(i, k) = glb_{\leq_x}(j, k)$. By Part 1 of Lemma 2.2, the map $t_{\delta,x} : V(T) \rightarrow \mathcal{G}$ is a discriminating $\mathcal{G}$–dating map and so

$t_{\delta,x}(u) \neq t_{\delta,x}(v)$. Therefore

$$d_x^{(T;t)}(i,j) \neq d_x^{(T;t)}(i,k) = d_x^{(T;t)}(j,k),$$

where $t = t_{\delta,x}$. By Part 1 of Lemma 2.2, $\delta_x = d_x^{(T;t)}$ and so $ij|kx \in R(\delta, x)$.

Now suppose that there is no p in $\{1, 2, \ldots, r\}$ such that $i, j \in X_p$. An argument similar to that used in the last paragraph, shows that there is no $k \in X - \{x\}$ such that $ij|kx \in R(\delta, x)$. This establishes (6).

Having established (6), we see that $A[R(\delta, x)]$ is part of a standard tree representation of δ. By Part 2 of Corollary 2.3, the pair $(A[R(\delta, x)]; w_{t,x})$, for $t = t_{\delta,x}$, provides a standard tree representation of δ. Furthermore, the tree $A[R(\delta, x)]$ can be constructed in polynomial time (see [1], [6], or [11]), and once this tree is constructed, the arc function $w_{t,x}$ can also be constructed in polynomial time. This completes the proof of Theorem 3.1. □

Remark. The condition on H_δ in the statement of Theorem 3.1 is necessary as there exists a group $\mathcal{G}$ with elements of order 2 and a proximity map $\delta : X \times X \to \mathcal{G}$ such that (P1) and (P2) are satisfied, but in which there is no tree representation of δ. An example is provided by the construction in [4] used to illustrate the "necessary part" of [4, Proposition 1(2)].

Given a standard tree representation $(T; w)$ of a tree proximity map δ our second main result shows that, up to isomorphism, T is determined by δ, and the arc weighting $w : E^{(2)} \to \mathcal{G}$ is partially determined. More precisely, although w is not completely determined (as pointed out by [2], [8], and [10]), the return-trip weights of every exterior edge as well as, up to conjugacy, the return-trip weights of every interior edge of $(T; w)$ can be obtained (this was established for the particular group analysed in [2]). Moreover, we show that the arc weights can be arbitrarily specified on a certain subset of arcs, but once this is done, then all the remaining arc weights are determined.

Before stating Theorem 3.2, we note the following. If T and T' are two isomorphic trees, then one can identify the set of vertices (resp. edges) of T' as being equal to the set of vertices (resp. edges) of T. For the sake of simplicity and without ambiguity, we shall treat the vertices (resp. edges) of two such trees in the statement and proof of Theorem 3.2 as equivalent.

Theorem 3.2. *Let $\delta : X \times X \to \mathcal{G}$ be a tree proximity map. Suppose that $(T; w)$ and $(T'; w')$ are both standard tree representations of δ. Then:*

1. *T is isomorphic to T'.*
2. *Let $e = \{u, v\}$ be an edge of T.*
   (i) *If e is an exterior edge, then*

$$w(u, v)w(v, u) = w'(u, v)w'(v, u).$$

   (ii) *If e is an interior edge, then*

$$w(u, v)w(v, u) \cong w'(u, v)w'(v, u),$$

where $\alpha \cong \beta$ denotes conjugacy in $\mathcal{G}$, that is, there exists an element γ in $\mathcal{G}$ such that $\alpha = \gamma\beta\gamma^{-1}$.

3. *Select an interior (resp. exterior) edge, $\{u, v\}$ say, of T. For all $\xi, \zeta \in \mathcal{G}$ such that $\xi\zeta \cong w(u, v)w(v, u)$ (resp. $\xi\zeta = w(u, v)w(v, u)$), there exists a standard tree representation $(T; w'')$ with*

$$w''(u, v) = \xi \text{ and } w''(v, u) = \zeta.$$

4. *Let $\mathring{E}$ denote the set of interior edges of T. Then there exists a subset A of $E^{(2)}$, with $|A| = 1 + |\mathring{E}|$, such that*

$$w_{|A} = w'_{|A} \Rightarrow w = w'.$$

Furthermore, provided $|\mathring{E}| \geq 1$, one can extend an arbitrary assignment of elements of $\mathcal{G}$ to the members of A to a weight function from $E^{(2)}$ into $\mathcal{G}$ which, together with T, gives a standard tree representation of δ. Moreover, all standard tree representations of δ can be obtained in this way.

Proof. **Part 1.** Equation (6) shows that T is determined by δ, and provides, moreover, a polynomial time constructive algorithm. Alternatively, the result may be deduced from Proposition 2.4 as follows. From the proof of Theorem 3.1, δ_x satisfies (U1), (U2), and (U3). Therefore, by combining the first part of Lemma 2.2 with Proposition 2.4, we deduce that T is isomorphic to T'.

Part 2. Here we freely use the fact, from the previous part, that T is isomorphic to T'.

To prove (i), suppose that $e = \{i, u\}$ is an exterior edge of T, where $i \in X$. If i and u are the only vertices of T, then (i) holds. Therefore assume that T has at least three vertices. Let j and k be elements of $X - \{i\}$ such that the path from j to k in T is incident with u. It follows that

$$\delta(i, j)\delta(k, j)^{-1}\delta(k, i) = w(i, u)w(u, i),$$

completing the proof of (i).

To prove (ii), suppose that $e = \{u, v\}$ is an interior edge of T. Now let i and j be elements of X such that the path from i to j is incident with u, but not with v. Similarly, let k and l be elements of X such that the path from k to l is incident with v, but not with u. Then

$$\delta(i, l)\delta(k, l)^{-1}\delta(k, j)\delta(i, j)^{-1} = D_{(T;w)}(i, u)w(u, v)w(v, u)D_{(T;w)}(i, u)^{-1}$$

and

$$\delta(i, l)\delta(k, l)^{-1}\delta(k, j)\delta(i, j)^{-1} = D_{(T';w')}(i, u)w'(u, v)w'(v, u)D_{(T';w')}(i, u)^{-1}.$$

By equating the right-hand-sides of the last two equations, and then multiplying the resulting equation on the left by $D_{(T;w)}(i, u)^{-1}$ and on the right by $D_{(T;w)}(i, u)^{-1}$, we get the desired result. This completes the proof of (ii).

Part 3. Suppose that $\{u, v\}$ is an interior edge of T. Let $\alpha = w(u, v)$ and $\beta = w(v, u)$, and suppose that $\xi\zeta \cong \alpha\beta$, that is, $\xi\zeta = \gamma\alpha\beta\gamma^{-1}$ for some $\gamma \in \mathcal{G}$. Let $\{u_1, u_2, \ldots, u_r\}$ be the set of vertices in T adjacent u other than v, and let $\{v_1, v_2, \dots, v_s\}$ be the set of vertices in T adjacent to v other than u. Let $w'' : E^{(2)} \to \mathcal{G}$ denote the arc weighting function defined as follows:

- $w''(u,v) = \xi$ and $w''(v,u) = \zeta$;
- $w''(u,u_i) = \gamma w(u,u_i)$ and $w''(u_i,u) = w(u_i,u)\gamma^{-1}$, for all $i \in \{1,2,\dots,r\}$;
- $w''(v,v_j) = \xi^{-1}\gamma\alpha w(v,v_j)$ and $w''(v_j,v) = w(v_j,v)\beta\gamma^{-1}\zeta^{-1}$, for all $j \in \{1,2,\dots,s\}$; and
- w'' agrees with w on all other arcs.

It is easily checked that each edge of T is properly weighted under the arc weighting w''. Furthermore, for all $i,j \in X$, a case analysis (depending on which of the above arcs are crossed in the path from i to j) using elementary cancellation of products in the group $\mathcal{G}$ shows that $\delta_{(T;w'')}(i,j) = \delta_{(T;w)}(i,j)$, as required.

Now suppose that $\{x,u\}$ is a exterior edge of T, with $x \in X$, $w(x,u) = \alpha$, and $w(u,x) = \beta$. Suppose that $\xi\zeta = \alpha\beta$ and let $\{u_1, u_2, \dots, u_r\}$ be the set of vertices in T adjacent to u other than x. Let $w'' : E^{(2)} \to \mathcal{G}$ denote the arc weighting function defined as follows:

- $w''(x,u) = \xi$ and $w''(u,x) = \zeta$;
- $w''(u,u_i) = \xi^{-1}\alpha w(u,u_i)$ and $w''(u_i,u) = w(u_i,u)\beta\zeta^{-1}$, for all $i \in \{1,\dots,s\}$; and
- w'' agrees with w on all other arcs.

Again it is easily checked that each edge of T is properly weighted under the new arc weighting w'', and that, for all $i,j \in X$, $\delta_{(T;w'')}(i,j) = \delta_{(T;w)}(i,j)$, as required.

Part 4. We begin the proof of Part 4 by constructing the desired subset of $E^{(2)}$. Select an element, x say, of X. Let e be the edge of T incident with x. Set A to be a subset of $E^{(2)}$ such that $(u,v) \in A$ if and only if $(v,u) \notin A$ and $\{u,v\} \in \mathring{E} \cup \{e\}$. We now show that A has the properties claimed in the statement of Part 4.

Firstly, to each member of A assign an arbitrary element of $\mathcal{G}$. Let $w^* : E^{(2)} \to \mathcal{G}$ denote the arc weight function that extends this arbitrary assignment of elements of $\mathcal{G}$ to the members of $E^{(2)}$ and is constructed as follows:

- For each arc (u,v) in A, set $w^*(v,u)$ so that, if $u \leq_x v$ (resp. $v \leq_x u$) holds, the ordered product of the weights of the arcs from x to v (resp. u) and back to x is equal to $t_{\delta,x}(v)$ (resp. $t_{\delta,x}(u)$). It is not difficult to see that this can be done recursively (and furthermore uniquely) based on the number of edges separating v (resp. u) from x.
- For the remaining arcs in $E^{(2)}$, if $v = i \in X$, then set $w^*(u,v) = p^{-1}\delta(x,i)$ and $w^*(v,u) = \delta(i,x)q^{-1}$, where p is the ordered product of the arc weights from x to u under w^* and q is the ordered product of the arc weights from u to x under w^*.

Note that w^* is well-defined. We next show that $(T;w^*)$ is a tree representation of δ by showing that, for all $i,j \in X$, $d_{(T;w^*)}(i,j) = d_{(T;w)}(i,j)$.

Set $d = d_{(T;w)}$. Clearly, we have $d_{(T;w^*)}(x,i) = \delta(x,i) = d(x,i)$ and, similarly, $d_{(T;w^*)}(i,x) = d(i,x)$, for all $i \in X$. So assume that i, j, and x are pairwise distinct. Let $v = glb_{\leq_x}(i,j)$, and let p_v and q_v be the ordered products of arc weights from x to v and from v to x, respectively, in $(T;w^*)$. Furthermore, let q_i and p_j be the ordered products of arc weights from i to v and from v to j, respectively, in $(T;w^*)$. By the definition of w^*, we have

$$p_v q_v = t_{\delta,x}(v) = \delta(x,j)\delta(i,j)^{-1}\delta(i,x) = d(x,j)d(i,j)^{-1}d(i,x).$$

Therefore

$$\begin{aligned} d(i,j) &= [d(x,j)^{-1}p_v q_v d(i,x)^{-1}]^{-1} \\ &= [(p_v p_j)^{-1} p_v q_v (q_i q_v)^{-1}]^{-1}, \qquad \text{since } d = d_{(T;w^*)} \text{ when } x \in \{i,j\}, \\ &= q_i p_j = d_{(T;w^*)}(i,j). \end{aligned}$$

Hence $(T;w^*)$ is a tree representation of δ. Furthermore, $(T;w^*)$ must be a standard tree representation of δ, for otherwise, the phylogenetic X–tree associated with the standard tree representation of δ obtained from $(T;w^*)$, by the method described in Proposition 2.1, has fewer internal vertices than T, contradicting Part 1.

Since $w^*_{|A}$ and δ determines the weight of each arc under w^* and since T is isomorphic to T', it follows that all standard tree representations of δ can be obtained in this way by making the appropriate assignment of elements of $\mathcal{G}$ to the members of A and that if $w_{|A} = w'_{|A}$, then $w = w'$. This completes the proof of Part 4 and so Theorem 3.2 is proved. □

We complete this section of the paper by showing that the main theorem of [4] can be deduced from Theorems 3.1 and 3.2.

Suppose $\mathcal{S}$ is an Abelian semigroup with identity (we will denote the binary operation by addition $+$, the identity by 0, and write $2x$ as shorthand for $x + x$). In [4], the authors considered two further conditions on $\mathcal{S}$, namely, cancellation ($x + y = x + z \Rightarrow y = z$) and uniqueness of halves ($2x = 2y \Rightarrow x = y$). These two conditions are easily seen to be equivalent to the condition that $\mathcal{S}$ embeds in an Abelian group $\mathcal{G}$ that has no elements of order 2. Thus the following corollary immediately gives the main theorem of [4].

Corollary 3.3. *Suppose $\mathcal{G}$ is an Abelian group, with no elements of order 2, and $\mathcal{S} \subseteq \mathcal{G}$ forms a semigroup. Suppose further that $\delta : X \times X \to \mathcal{S}$ is symmetric (i.e. $\delta(i,j) = \delta(j,i)$, for all $i, j \in X$). Then δ can be realized by a symmetric edge weighting $w : E^{(2)} \to \mathcal{S}$ of an X-tree $(T;\phi)$ if and only if the following four point condition applies:*

For all (not necessarily distinct) four points in X, there exists an ordering of these points, i, j, k, and l say, and an element ξ in $\mathcal{S}$ such that

$$\delta(i,j) + \delta(k,l) + 2\xi = \delta(i,k) + \delta(j,l) = \delta(i,l) + \delta(j,k). \tag{7}$$

Furthermore, the triple $(T;\phi;w)$ is uniquely determined by δ, provided we insist that no arc of T has weighting zero.

Proof. Regarding the existence of a tree representation of δ the "only if" direction is clear. For the "if" part, we note that (P1) and (P2) in the statement of Theorem 3.1 clearly apply, and thus, by Theorem 3.1, there exists a tree representation $(T;\phi;w')$ of δ, where $(T;\phi)$ is a phylogenetic X–tree and $w' : E^{(2)} \to \mathcal{G}$. We wish to show that w' can be replaced by a function w that (i) maps into $\mathcal{S}$ and (ii) is symmetric. To this end, we first establish the following claim: For each edge $e = \{u,v\}$ of T, there exists $\xi \in \mathcal{S}$ such that

$$w'(u,v) + w'(v,u) = 2\xi. \tag{8}$$

To establish (8), there are two cases to consider depending upon e being either an interior edge of T or an exterior edge of T. We will consider just the former, since the proof of the latter is similar. Select $i',j',k',l' \in X$ in a such a way that in T the path between leaves i' and j' is incident with u, but not with v, while the path between k' and l' is incident with v, but not with u. Then, as G is Abelian and denoting $d_{(T;\phi;w')}$ as d', we get

$$d'(i',j') + d'(l',k') + w'(u,v) + w'(v,u) = d'(i',k') + d'(l',j').$$

Since $d' \equiv \delta$, the condition described by Equation (7) (plus the symmetry of δ) guarantees the existence of $\xi \in \mathcal{S}$ such that

$$d'(i',j') + d'(l',k') + 2\xi = d'(i',k') + d'(l',j'),$$

which in view of the previous equation implies that $w'(u,v) + w'(v,u) = 2\xi$, as required to establish the claim.

Now, referring to Equation (8), set $w(u,v)$ and $w(v,u)$ both equal to ξ, for each edge $\{u,v\}$ of T. Let $d = d_{(T;\phi;w)}$. Then, for each $i,j \in X$,

$$2d(i,j) = d(i,j) + d(j,i) = d'(i,j) + d'(j,i) = \delta(i,j) + \delta(j,i) = 2\delta(i,j)$$

and so $2[d(i,j) - \delta(i,j)] = 0$. Since $\mathcal{G}$ has no elements of order 2, it follows that $d \equiv \delta$, and so $(T;\phi;w)$ provides the desired tree representation of δ.

Regarding the uniqueness of the tree representation, suppose that $(T_1;\phi_1;w_1)$ and $(T_2;\phi_2;w_2)$ both provide tree representations of δ, where w_1 and w_2 are both symmetric functions taking values in $\mathcal{S} - \{0\}$.

For all $i \in \{1,2\}$, let $(T_i';w_i')$ denote the phylogenetic expansion of the tree representation $(T_i;\phi_i;w_i)$. Then $(T_1';w_1')$ and $(T_2';w_2')$ are both standard tree representations of δ. Consequently, by Theorem 3.2, T_1' and T_2' are isomorphic. Therefore, by noting that, for an Abelian group, two elements are conjugates precisely if they are identical, the second part of Theorem 3.2 shows that $w_1'(u,v) + w_1'(v,u) = w_2'(u,v) + w_2'(v,u)$ for each (isometrically equivalent) edge $\{u,v\}$ in T_1 and T_2. But, since w_1' and w_2' are both symmetric, this implies that $2[w_1'(u,v) - w_2'(u,v)] = 0$ and, since $\mathcal{G}$ has no elements of order 2, this in turn implies that $w_1'(u,v) = w_2'(u,v)$. In particular, $w_1'(u,v) = 0$ precisely if $w_2'(u,v) = 0$, which together with the isomorphism between T_1' and T_2' and the way in which these trees were constructed from $(T_1;\phi_1)$ and $(T_2;\phi_2)$ implies that $(T_1;\phi_1)$ and $(T_2;\phi_2)$ are isomorphic, and $w_1 \equiv w_2$ as required. $\square$

4. Remarks

- We return to the problem that motivated our analysis, namely, the case where $\mathcal{G}$ is the group of $r \times r$ invertible real matrices and we have a general r-state Markov process on a tree ([2], [8], and [13]). In this setting, each arc has an associated transition matrix, and $\delta(i,j)$ is the net transition matrix of states at j conditional on the states at i. The conditions (P1) and (P2) translate into a collection of polynomial function identities between the joint distribution of states at the leaves of the tree - such functions are examples of "phylogenetic invariants" [9] and we note that the invariants described by (P1) are independent of the underlying tree T (so called "model invariants"). To date, most investigation of phylogenetic invariants has been for submodels of this general model (obtained by restricting the transition matrices assigned to the arcs), although a phylogenetic invariant has been described for this general model ([13] - essentially by taking determinants of the equation in (P2)). We point out here that phylogenetic invariants are, in fact, abundant for this general model since each triple or quadruple gives rise (via (P1) and (P2), respectively) to r^2 polynomial identities.

  Referring to Theorem 3.1, note that, in this setting, H_δ would not be expected to have elements of order 2, however $\mathcal{G}$ clearly does, which is why we did not impose the simpler restriction in Theorem 3.1 that $\mathcal{G}$ have no elements of order 2.
- Suppose $\mathcal{G}$ is a group, and $\mathcal{S} \subseteq \mathcal{G}$ is a semigroup. An interesting extension of Theorem 3.1 would be to characterize when a proximity map $\delta : X \times X \to \mathcal{S}$ is a tree proximity map with arc weights lying in $\mathcal{S}$.

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