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# RESEARCH REPORT

A CHARACTERIZATION FOR A SET OF PARTIAL PARTITIONS TO DEFINE AN  $X-{\tt TREE}$ 

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### A CHARACTERIZATION FOR A SET OF PARTIAL PARTITIONS TO DEFINE AN X-TREE

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ABSTRACT. Trees whose vertices are partially labelled by elements of a finite set X provide a natural way to represent partitions of subsets of X. The condition under which a given collection of such partial partitions of X can be represented by a tree has previously been characterized in terms of a chordal graph structure on an underlying intersection graph. In this paper, we obtain a related graph-theoretic characterization for the uniqueness of a tree representation of a set of partial partitions of X.

#### 1. Introduction

Throughout this paper, X denotes a non-empty finite set. Let T be a tree with vertex set V, and suppose we have a map  $\phi: X \to V$  with the property that, for all  $v \in V$  with degree at most two,  $v \in \phi(X)$ . Then the ordered pair  $(T; \phi)$ , which we frequently denote by T, is called an X-tree. For example, Figure 1(i) shows an X-tree with  $X = \{1, 2, \ldots, 9\}$ . If  $\phi$  is a bijection from X into the set of pendant vertices of T, then T is a phylogenetic X-tree. In this case, we can view X as the set of pendant vertices of T, and so we frequently denote the pendant vertices of T by the elements of X as  $\phi$  is implicitly determined. A binary phylogenetic X-tree is a phylogenetic X-tree in which every non-pendant (or internal) vertex has degree three. Figure 2(i) shows a binary phylogenetic X-tree with  $X = \{1, 2, \ldots, 7\}$ . Two X-trees  $(T_1; \phi_1)$  and  $(T_2; \phi_2)$ , where  $T_1 = (V_1, E_1)$  and  $T_2 = (V_2, E_2)$ , are isomorphic if there exists a bijection  $\psi: V_1 \to V_2$  which induces a bijection between  $E_1$  and  $E_2$  and satisfies  $\phi_2 = \psi \circ \phi_1$ , in which case,  $\psi$  is unique. We write  $(T_1; \phi_1) \cong (T_2; \phi_2)$  if  $(T_1; \phi_1)$  is isomorphic to  $(T_2; \phi_2)$ .

Phylogenetic trees and X-trees arise in the study of hierarchical classification. For a general overview of X-trees, including a description of the natural equivalence between X-trees and certain set systems due to Buneman [4], see [1, Chapters 1 and 5]. Motivated by two fundamental problems in hierarchical classification, this paper has two main results, Theorem 1.2 and Corollary 1.4. Each result is a graph-theoretic characterization for when, up to isomorphism, there is a unique X-tree satisfying particular properties. In this section, we set up the necessary terminology and notation, and state Theorem 1.2 and Corollary 1.4. The proof of Theorem 1.2

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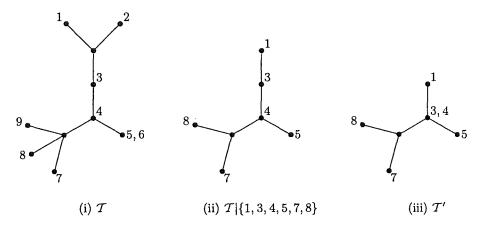


FIGURE 1. (i) T. (ii)  $T|\{1, 3, 4, 5, 7, 8\}$ . (iii) T'.

is delayed until Section 3. The next section contains some known results that will be needed in the proof of Theorem 1.2. Section 4 completes the paper with a brief discussion about the statement of Theorem 1.2 and several further results concerning these two fundamental problems.

A partial partition of X is a partition of a non-empty subset of X into at least two sets (called *cells*), at most one of which may be empty. If these cells are  $A_1, A_2, \ldots, A_n$ , where  $n \geq 2$ , we denote the partial partition by  $A_1|A_2|\cdots|A_n$ . Note that the ordering of the cells in a partial partition is arbitrary. The partial partition is called a partial split if n=2. Furthermore, if n=2 and  $A_1 \cup A_2 = X$ , then  $A_1|A_2$  is called a split of X.

For a set  $\Sigma$  of partial partitions of X, we denote the set

$$\{(A,\sigma): A \text{ is a non-empty cell of } \sigma \text{ and } \sigma \in \Sigma\}$$

by  $C(\Sigma)$ . Throughout this paper, the only significant part of an element of  $C(\Sigma)$  is the first coordinate. For this reason and for brevity, we denote such an element,  $(A, \sigma)$  say, by just A.

Let  $\mathcal{T}=(T;\phi)$  be an X-tree, let  $\Sigma$  be a set of partial partitions of X, and let  $A_1|A_2|\cdots|A_n$  be an element of  $\Sigma$ , where  $n\geq 2$ . If there is a set F of edges of T such that, for all distinct  $i,j\in\{1,2,\ldots,n\}$ ,  $\phi(A_i)$  and  $\phi(A_j)$  are subsets of the vertex sets of different components of  $T\backslash F$ , then T displays  $A_1|A_2|\cdots|A_n$ ; the edges of F are said to display  $A_1|A_2|\cdots|A_n$  (in T). The X-tree T displays  $\Sigma$  if every element of  $\Sigma$  is displayed by T. If e is an edge of T such that every set of edges that display  $A_1|A_2|\cdots|A_n$  contains e, then e is distinguished by  $A_1|A_2|\cdots|A_n$  (in T). If each edge of T is distinguished by an element of  $\Sigma$ , then we say that T is distinguished by  $\Sigma$  or  $\Sigma$  distinguishes T. The set  $\Sigma$  defines T if T displays  $\Sigma$  and all other X-trees that display  $\Sigma$  are isomorphic to T. An important observation to note is that if  $\Sigma$  defines an X-tree, then this X-tree must be a binary phylogenetic X-tree.

Let  $\Sigma$  be a set of partial partitions of X. The partial partition intersection graph of  $\Sigma$ , denoted int( $\Sigma$ ), is the graph whose vertex set is  $\mathcal{C}(\Sigma)$  and has the property

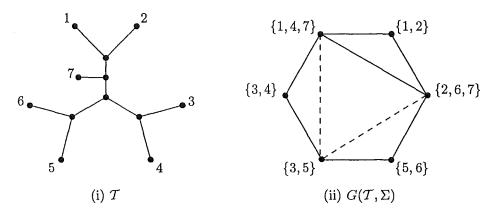


FIGURE 2. (i) A binary phylogenetic X-tree  $\mathcal{T}$  that displays  $\Sigma = \{\{1,2\}|\{3,5\},\{3,4\}|\{2,6,7\},\{5,6\}|\{1,4,7\}\}\}$ . (ii) The graphs int( $\Sigma$ ) (solid edges) and  $G(\mathcal{T},\Sigma)$  (all edges).

that two vertices are joined by an edge precisely if their intersection is non-empty. (A characterization of partition intersection graphs, when every member of  $\Sigma$  is a (full) partition of X, is given in [8].) A graph is *chordal* if every cycle with at least four vertices has an edge connecting two non-consecutive vertices. A *chordalization* (or *triangulation*) of a graph G = (V, E) is a graph G' = (V, E') in which G' is chordal and  $E \subseteq E'$ . A graph G is a restricted chordal completion of  $\operatorname{int}(\Sigma)$  if G is a chordalization of  $\operatorname{int}(\Sigma)$  and the following property holds: if A and A' are non-empty cells of an element of  $\Sigma$ , then A and A' are not adjacent in G. A restricted chordal completion G of  $\operatorname{int}(\Sigma)$  is *minimal* if, for every non-empty subset F of edges in  $E(G) - E(\operatorname{int}(\Sigma))$ ,  $G \setminus F$  is not chordal.

To illustrate some of these notions, take  $X = \{1, 2, ..., 7\}$  and let

$$\Sigma = \{\{1,2\} | \{3,5\}, \{3,4\} | \{2,6,7\}, \{5,6\} | \{1,4,7\}\}.$$

Let  $\mathcal{T}$  be the binary phylogenetic X-tree shown in Figure 2(i). Then  $\mathcal{T}$  displays  $\Sigma$ . A (unique) restricted chordal completion of  $\operatorname{int}(\Sigma)$  is shown in Figure 2(ii), where  $\operatorname{int}(\Sigma)$  is the graph induced by the solid lines of this graph.

We can now describe the first of the two fundamental problems mentioned earlier. Suppose that X is a set of objects. In evolutionary biology, X may be a set of species. A particular character (or attribute) of a subset of the objects induces a partial partition of X so that the states of this character correspond to the cells of this partial partition and an element of X is in some cell precisely if it takes this state for this character. Suppose that T is a phylogenetic X-tree representing the historical "evolution" of the members in X, and suppose that  $A_1|A_2|\cdots|A_n$ , where  $n \geq 2$ , is a partial partition of X. If we make the assumption that the states of a character evolve along the edges of T so that a change to some particular state occurs at most once, then T displays  $A_1|A_2|\cdots|A_n$ . Let  $\Sigma$  be a set of partial partitions of X. In the more general setting of X-trees, the first problem is to determine if there exists an X-tree that displays  $\Sigma$  and, if there is such an X-tree, determine whether it is unique up to isomorphism. Deciding the first part is an NP-complete problem [3, 10]. However, Theorem 1.1 (indicated in [5] and [9], and

formally proved in [10]) is a graph-theoretic characterization for when there exists such an X-tree.

Theorem 1.1. Let  $\Sigma$  be a set of partial partitions of X. Then there exists an X-tree that displays  $\Sigma$  if and only if there exists a restricted chordal completion of  $int(\Sigma)$ .

Our first main result, Theorem 1.2, is the uniqueness analogue of Theorem 1.1. Let  $\mathcal{T}$  be an X-tree and let X' be a subset of X. We denote the minimal subtree of  $\mathcal{T}$  containing X' by  $\mathcal{T}(X')$ . (Observe that  $\mathcal{T}(X')$  may not be an X'-tree.) Now let A and A' be subsets of X. If the intersection of the vertex sets of  $\mathcal{T}(A)$  and  $\mathcal{T}(A')$  is non-empty, then  $\mathcal{T}(A) \cap \mathcal{T}(A')$  is said to be non-empty; otherwise,  $\mathcal{T}(A) \cap \mathcal{T}(A')$  is empty. Note that if  $A_1|A_2|\cdots|A_n$  is a partial partition of X and X' is an X'-tree that displays  $A_1|A_2|\cdots|A_n$ , then  $\mathcal{T}(A_i) \cap \mathcal{T}(A_j) = \emptyset$  for all distinct i and j in  $\{1,2,\ldots,n\}$ . Let  $\Sigma$  be a set of partial partitions of X. The subtree intersection graph of  $\mathcal{T}$  induced by  $\Sigma$  is the graph whose vertex set is  $\mathcal{C}(\Sigma)$  and which has the property that two vertices, A and A' say, are joined by an edge precisely if  $\mathcal{T}(A) \cap \mathcal{T}(A')$  is non-empty. This graph is denoted by  $G(\mathcal{T}, \Sigma)$ . As an example, consider the binary phylogenetic X-tree  $\mathcal{T}$  and the set  $\Sigma$  of partial partitions of X shown in Figure 2. Then  $G(\mathcal{T}, \Sigma)$  is the graph, with dashed lines included, in Figure 2(ii).

**Theorem 1.2.** Let  $\Sigma$  be a set of partial partitions of X. Then  $\Sigma$  defines an X-tree if and only if the following two conditions are satisfied:

- (i) there is a binary phylogenetic X-tree that displays  $\Sigma$  and is distinguished by  $\Sigma$ ; and
- (ii) there is a unique minimal restricted chordal completion of  $int(\Sigma)$ .

Furthermore, if  $\mathcal{T}$  is the X-tree defined by  $\Sigma$ , then  $\mathcal{T}$  is a binary phylogenetic X-tree that displays  $\Sigma$  and is distinguished by  $\Sigma$ , and  $G(\mathcal{T}, \Sigma)$  is the unique minimal restricted chordal completion of  $\operatorname{int}(\Sigma)$ .

The proof of Theorem 1.2 is the substance of Section 3. In Section 4, we highlight, with two examples, that conditions (i) and (ii) in the statement of Theorem 1.2 cannot be weakened. We remark here that a different type of combinatorial characterization has recently been given in [2] for when a minimum sized set of partial X-splits, where each cell of every partial X-split has size two, defines an X-tree.

We next describe two basic operations on X-trees. Let  $\mathcal{T}=(T;\phi)$  be an X-tree and let X' be a subset of X. The restriction of  $\mathcal{T}$  to X', denoted  $\mathcal{T}|X'$ , is the X'-tree obtained from  $\mathcal{T}(X')$  by suppressing all vertices of degree two that are not in  $\phi(X')$ . The operation of restriction is illustrated by (i) and (ii) in Figure 1. Now let e be an edge of f with end-vertices f and f and let f be the vertex of f that identifies f and f and f and f by contracting f is f and f where f is the map from f to the vertex set of f defined by

$$\phi_e(x) = \begin{cases} \phi(x) & \text{if } x \notin \phi^{-1}(u) \cup \phi^{-1}(v), \\ v_e & \text{if } x \in \phi^{-1}(u) \cup \phi^{-1}(v). \end{cases}$$

The X-tree  $(T/e; \phi_e)$  is denoted by T/e. An X-tree T' is said to be obtained from T by contraction if T' can be obtained from T by contracting a sequence of edges. It is easily checked that the ordering of the edges in such a sequence is arbitrary. Note that if  $\Sigma$  is a set of partial partitions of X and T is an X-tree that is distinguished by  $\Sigma$ , then no contraction of T displays  $\Sigma$ .

Let  $X_1$  and  $X_2$  be subsets of X. An  $X_1$ -tree  $\mathcal{T}_1$  resolves an  $X_2$ -tree  $\mathcal{T}_2$  if  $\mathcal{T}_2$  can be obtained from a restriction of  $\mathcal{T}_1$  by contraction (or, equivalently,  $\mathcal{T}_2$  is a restriction of a contraction of  $\mathcal{T}_1$ ), in which case,  $\mathcal{T}_1$  is said to be a resolution of  $\mathcal{T}_2$ . This provides a convenient partial order on the set of X'-trees which we denote by  $\leq$ , where X' is a subset of X. In the case above, we write  $\mathcal{T}_2 \leq \mathcal{T}_1$ . As an example, in Figure 1 we have  $\mathcal{T}' \leq \mathcal{T}$ .

We now state the second fundamental problem. For  $i \in \{1, 2, ..., n\}$ , let  $\mathcal{T}_i$  be an  $X_i$ -tree, where  $X_i$  is a subset of X. A basic task in hierarchical classification is to combine all of the members (the input trees) of  $\bigcup_{i=1}^n \{\mathcal{T}_i\}$  into a single X-tree (the output tree) so that, for each i, the output tree is a resolution of  $\mathcal{T}_i$ . Informally, this means that, for each i, the output tree contains all of the "branching" information of  $\mathcal{T}_i$ . Of course, this may not be possible, and so we have our second fundamental problem: determine if there exists an X-tree  $\mathcal{T}$  such that, for each i,  $\mathcal{T}_i \leq \mathcal{T}$  and, if there is such an X-tree, determine whether it is unique up to isomorphism. Like the first fundamental problem, deciding the first part of this problem is an NP-complete problem [10], but again there is a graph-theoretic characterization for when there exists an X-tree with the desired properties. Corollary 1.3 is a consequence of Theorem 1.1. It does not seem to be explicitly stated anywhere, but, as shown below, it is easily deduced from results in [10].

Let  $\mathcal{T} = (T; \phi)$  be an X-tree and let e be an edge of T. Then e is the unique edge of T that displays the X-split  $\phi^{-1}(V_1)|\phi^{-1}(V_2)$ , where  $V_1$  and  $V_2$  are the vertex sets of the components of  $T \setminus e$ . We denote the collection of X-splits of T that are displayed by the edges of T by  $\Sigma(T)$ .

Corollary 1.3. For  $i \in \{1, 2, ..., n\}$ , let  $\mathcal{T}_i$  be an  $X_i$ -tree, where  $X_i \subseteq X$ . Let  $\Sigma = \bigcup_{i=1}^n \Sigma(\mathcal{T}_i)$ . Then there exists an X-tree  $\mathcal{T}$  such that, for all  $i, \mathcal{T}_i \leq \mathcal{T}$  if and only if there exists a restricted chordal completion of  $\operatorname{int}(\Sigma)$ .

*Proof.* It is shown in [10, Proposition 2(2)] that an X-tree  $\mathcal{T}'$  displays  $\Sigma$  if and only if  $\mathcal{T}_i \leq \mathcal{T}'$  for all i. Corollary 1.3 now readily follows from Theorem 1.1.  $\square$ 

Our second main result, Corollary 1.4, is the uniqueness analogue of Corollary 1.3 and is easily deduced using [10, Proposition 2(2)] in combination with Theorem 1.2.

Corollary 1.4. For  $i \in \{1, 2, ..., n\}$ , let  $\mathcal{T}_i$  be an  $X_i$ -tree, where  $X_i \subseteq X$ . Let  $\Sigma = \bigcup_{i=1}^n \Sigma(\mathcal{T}_i)$ . Then there is a unique X-tree that resolves  $\mathcal{T}_i$ , for all i, if and only if the following two conditions are satisfied:

- (i) there is a binary phylogenetic tree X-tree that displays  $\Sigma$  and is distinguished by  $\Sigma$ : and
- (ii) there is a unique minimal restricted chordal completion of  $int(\Sigma)$ .

Furthermore, if  $\mathcal{T}$  is the unique X-tree that resolves  $\mathcal{T}_i$  for all i, then  $\mathcal{T}$  is a binary phylogenetic X-tree that displays  $\Sigma$  and is distinguished by  $\Sigma$ , and  $G(\mathcal{T}, \Sigma)$  is the unique minimal restricted chordal completion of  $\operatorname{int}(\Sigma)$ .

#### 2. Some Useful Results

All of the results presented in this section are needed for the proof of Theorem 1.2. The first result is a characterization of chordal graphs published independently by Buneman [5], Gavril [6], and Walter [11]. The proof of Theorem 1.1 in [10] is based on this result.

**Theorem 2.1.** The following statements are equivalent for a graph G with vertex set V:

- (i) G is chordal;
- (ii) G is the intersection graph of a collection of subtrees of a tree; and
- (iii) There exists a tree T whose vertex set C is the set of maximal cliques of G such that, for each  $v \in V$ , the subgraph of T induced by the elements of C that contain v is a subtree of T.

Corollary 2.2 is an immediate consequence of the equivalence of Parts (i) and (ii) of Theorem 2.1.

Corollary 2.2. Let  $\Sigma$  be a set of partial partitions of X, and let T be an X-tree. Then  $G(\mathcal{T}, \Sigma)$  is chordal.

The next two lemmas are implicit in the proof of Theorem 1.1 given in [10]. However, because of their role in the proof of Theorem 1.2, we include their proofs. We freely use Lemma 2.3 in Section 3.

**Lemma 2.3.** Let  $\mathcal{T}$  be an X-tree, and let  $\Sigma$  be a set of partial partitions of X. Then  $G(\mathcal{T}, \Sigma)$  is a restricted chordal completion of  $\operatorname{int}(\Sigma)$  if and only if  $\mathcal{T}$  displays  $\Sigma$ .

*Proof.* If  $\mathcal{T}$  displays  $\Sigma$ , then, as the edge set of  $\operatorname{int}(\Sigma)$  is a subset of the edge set of  $G(\mathcal{T}, \Sigma)$ , it follows by Corollary 2.2 that  $G(\mathcal{T}, \Sigma)$  is a restricted chordal completion of  $\operatorname{int}(\Sigma)$ .

Conversely, suppose that  $\mathcal{T}$  does not display  $\Sigma$ . Then there is a pair of non-empty cells  $A_1$  and  $A_2$  of a partial partition of  $\Sigma$  such that  $\mathcal{T}(A_1) \cap \mathcal{T}(A_2)$  is non-empty. Therefore  $\{A_1, A_2\}$  is an edge of  $G(\mathcal{T}, \Sigma)$ , and so, although  $G(\mathcal{T}, \Sigma)$  is chordal, it is not a restricted chordal completion of  $\operatorname{int}(\Sigma)$ . This completes the proof.  $\square$ 

**Lemma 2.4.** Let  $\Sigma$  be a set of partial partitions of X. If G is a restricted chordal completion of  $\operatorname{int}(\Sigma)$ , then there exists an X-tree T such that  $E(G(T,\Sigma)) \subseteq E(G)$ .

*Proof.* If G is disconnected, then there is a partitioning of X based upon the components of G as an element x of X can only be an element of a vertex label of

exactly one component. With this in mind, it is easily seen that that, provided the result holds for when G is connected, it also holds for when G is disconnected.

Suppose G is connected with vertex set V. By Theorem 2.1, there exists a tree T'=(C,E) whose vertex set C is the set of maximal cliques of G such that, for each  $v \in V$ , the subgraph of T' induced by the elements of C that contain v is a subtree of T'. We complete the proof of Lemma 2.4 by defining an X-tree  $T=(T;\phi)$  via T' and showing that  $E(G(T,\Sigma)) \subseteq E(G)$ .

Let a be an element of X. Since  $\operatorname{int}(\Sigma)$  is a subgraph of G, the set  $V_a$  of vertices of G that contain a induce a clique of G, and so there is an element  $C_a$  of C in which  $V_a$  is a subset. Identify a with this vertex and set  $\phi(a) = C_a$ . Repeat this process for the remaining elements of X. Define T to be the tree obtained from  $T^*$  by suppressing all vertices of degree at most two that are not identified by an element of X. We claim that  $E(G(T, \Sigma)) \subset E(G)$ .

Let  $A_1$  and  $A_2$  be elements of  $\mathcal{C}(\Sigma)$ , and suppose that  $A_1$  and  $A_2$  are non-adjacent in G. Then the subtrees  $T_1'$  and  $T_2'$  of T' induced by the elements of C that contain  $A_1$  and  $A_2$ , respectively, do not intersect. Since the elements of  $A_i$  can only be identified with vertices in  $T_i'$ , for each  $i \in \{1,2\}$ , it follows that  $\mathcal{T}(A_1) \cap \mathcal{T}(A_2)$  is empty. Therefore  $A_1$  and  $A_2$  are non-adjacent in  $G(\mathcal{T}, \Sigma)$ , and the claim follows.

If  $\Sigma$  is a set of partial partitions of X and G is a restricted chordal completion of  $\operatorname{int}(\Sigma)$ , then there no guarantee that there exists an X-tree T such that  $G(T,\Sigma)=G$ . For example, suppose that  $X=\{1,2,3,4,5,6\}$  and  $\Sigma=\{\{1,2\}|\{3,5\},\{2,3\}|\{4,5\},\{3,4\}|\{5,6\}\}$ . Let G be the graph obtained from  $\operatorname{int}(\Sigma)$  by adding the edge  $\{\{1,2\},\{3,4\}\}$ . Clearly, G is a restricted chordal completion of  $\operatorname{int}(\Sigma)$ . Furthermore, it is easily deduced that all of the X-trees that display  $\Sigma$  are resolutions of the X-tree that is a path consisting of four vertices labelled, in order,  $\{1,2\},\{3\},\{4\},$  and  $\{5,6\}$ . Since the subtrees of this X-tree induced by  $\{1,2\}$  and  $\{3,4\}$  do not intersect, it follows by Lemma 2.3 that there is no X-tree with the desired property.

An immediate consequence of Lemma 2.4 that becomes useful in the last part of the proof of Theorem 1.2 is Corollary 2.5.

Corollary 2.5. Let  $\Sigma$  be a set of partial partitions of X, and let G be a minimal restricted chordal completion of  $\operatorname{int}(\Sigma)$ . Then there exists an X-tree T such that  $G(\mathcal{T}, \Sigma) = G$ .

We noted earlier that if  $\Sigma$  is a set of partial partitions of X that defines an X-tree, then this X-tree must be a binary phylogenetic X-tree. Combining this note with [10, Proposition 6], we get Proposition 2.6.

**Proposition 2.6.** Let  $\Sigma$  be a set of partial partitions of X. If  $\Sigma$  defines an X-tree  $\mathcal{T}$ , then  $\mathcal{T}$  is a binary phylogenetic X-tree that displays  $\Sigma$  and is distinguished by  $\Sigma$ .

#### 3. Proof of Theorem 1.2

The proof of Theorem 1.2 is based on Lemma 3.1. Indeed, most of the work in proving this theorem goes into proving this lemma. Theorem 1.2 is formally proved after the proof of Lemma 3.1.

**Lemma 3.1.** Let  $\Sigma$  be a set of partial X-splits. Suppose that the following two conditions are satisfied:

- (i) there is a binary phylogenetic X-tree that displays  $\Sigma$  and is distinguished by  $\Sigma$ ; and
- (ii) there is a unique minimal restricted chordal completion of  $int(\Sigma)$ .

Then  $\Sigma$  defines an X-tree.

Before proving Lemma 3.1, we establish several results, the first of which may have independent interest, so we call it a theorem.

**Theorem 3.2.** Let  $\Sigma$  be a set of partial X-splits, and let T be a binary phylogenetic X-tree that displays  $\Sigma$  and is distinguished by  $\Sigma$ . Let T' be an X-tree that displays  $\Sigma$ . If the edge set of  $G(T', \Sigma)$  is a subset of the edge set of  $G(T, \Sigma)$ , then  $T' \cong T$ .

Proof. Let  $T=(T;\phi)$  and  $T'=(T';\phi')$ . We prove Theorem 3.2 by showing that the result holds if T' has the additional property that, for each edge e' of T', the edge set of  $G(T'/e',\Sigma)$  is not a subset of the edge set of  $G(T,\Sigma)$ . To see that this is sufficient, suppose that T' does not have this additional property. Then there is an X-tree  $T''=(T'';\phi'')$  that displays  $\Sigma$ , satisfies  $T''\leq T'$ , and has the property that, for each edge e'' of T'', the edge set of  $G(T''/e'',\Sigma)$  is not a subset of the edge set of  $G(T,\Sigma)$ . If  $T''\cong T$ , then, as T is a binary phylogenetic X-tree, T''=T'. Thus we may assume that T' does indeed have the additional property.

Let E and E' denote the edge sets of  $G(\mathcal{T}, \Sigma)$  and  $G(\mathcal{T}', \Sigma)$ , respectively. Since every edge of  $\mathcal{T}$  is distinguished by an element of  $\Sigma$  and since  $\mathcal{T}$  is phylogenetic, it follows that, for every element x of X, the set  $\{x\}$  is a vertex of  $\text{int}(\Sigma)$ . Therefore the map  $\phi'$  is one-to-one, for otherwise  $E' \not\subseteq E$ . We freely use this fact throughout the proof.

The proof is by induction on the cardinality of X. If  $|X| \in \{2,3\}$ , then the theorem clearly holds. Let |X| = n, where  $n \ge 4$ , and assume that the theorem holds for when |X| = n - 1.

Since T is a tree, there exists a pair of pendant vertices of T, u and v say, with the property that u and v are adjacent to the same vertex, w say, of T. As T is binary and  $|X| \geq 4$ , u and v are the only pendant vertices adjacent to w. Let a and b be the elements of X such that  $\phi(a) = u$  and  $\phi(b) = v$ . We make two observations. The first observation is that, as each edge of T is distinguished by an element of  $\Sigma$ ,  $\{a,b\}$  is a vertex of  $\operatorname{int}(\Sigma)$ . Furthermore, if C is a vertex of  $\operatorname{int}(\Sigma)$  and  $\{\{a,b\},C\}$  is an element of E, then either a or b is an element of C. The second observation is that, as T displays  $\Sigma$ , there is no element, A|B say, of  $\Sigma$  such that  $a \in A$ ,  $b \in B$ ,  $|A| \geq 2$ , and  $|B| \geq 2$ .

Let u' and v' be the vertices of T' such that  $\phi'(a) = u'$  and  $\phi'(b) = v'$ . The following result enables us to break the proof into two manageable cases.

**3.2.1.** In T', the path P' from u' to v' contains at most two edges and, moreover, the one possible intermediary vertex in P' is not an element of  $\phi'(X)$ .

Proof. It follows from the first observation that there is no intermediary vertex on the path from u' to v' that is an element of  $\phi'(X)$ , for otherwise E' is not a subset of E. Now suppose, to the contrary, that P' contains at least three edges. Then there exists an edge, e' say, in P' that is incident with neither u' nor v'. Let  $w'_1$  and  $w'_2$  be the end-vertices of e' so that u' is in the same component of  $T' \setminus e'$  as  $w'_1$ . Since no intermediary vertex of P' is an element of  $\phi'(X)$  and since T' is an X-tree,  $w'_1$  and  $w'_2$  both have degree at least three. By our additional assumption on T',  $E(G(T'/e', \Sigma)) \not\subseteq E(G(T, \Sigma))$ . Therefore there are elements C and D of  $C(\Sigma)$  such that  $w'_1 \in T'(C)$ ,  $w'_2 \notin T'(C)$ ,  $w'_2 \in T'(D)$ ,  $w'_1 \notin T'(D)$ , and  $\{C, D\}$  is not an element of  $E(G(T, \Sigma))$ .

If  $a \notin C$ , then  $\{\{a,b\},C\}$  is an element of E'. However, as  $b \notin C$ ,  $\{\{a,b\},C\}$  is not an edge of E; a contradiction. Therefore  $a \in C$ . Similarly,  $b \in D$ . Since  $w'_1 \notin \phi'(X)$ , it follows that  $|C| \geq 2$ . Similarly,  $|D| \geq 2$ . But then, by considering  $\mathcal{T}$ , it is easily seen that  $\mathcal{T}(C) \cap \mathcal{T}(D)$  is non-empty, contradicting the fact that  $\{C,D\}$  is not an element of  $E(G(\mathcal{T},\Sigma))$ . This completes the proof of (3.2.1).

Let  $\Sigma_b$  be the set of partial  $(X - \{b\})$ -splits obtained from  $\Sigma$  by making the following replacements: (i) if  $\{a\}|B$  is an element of  $\Sigma$  such that  $b \in B$ , then replace  $\{a\}|B$  with  $\emptyset|B_b$ , where  $B_b$  is obtained from B by replacing b with a; (ii) if  $\{b\}|A$  is an element of  $\Sigma$  such that  $a \in A$ , then replace  $\{b\}|A$  with  $\emptyset|A$ ; and (iii), for each remaining element of  $\Sigma$ , replace b with a. The fact that  $\Sigma_b$  is a set of partial splits on  $X - \{b\}$  follows from the second observation.

By (3.2.1), there are two cases to consider depending upon whether the number of edges in P' is one or two.

Case (a). The number of edges in P' is two.

Let  $T_b$  be the tree obtained from T by contracting the edges  $\{u, w\}$  and  $\{v, w\}$ , and let  $w_b$  denote the vertex of  $T_b$  identifying u, v, and w. Let  $\phi_b$  be the map from  $X - \{b\}$  into the vertex set of  $T_b$  defined by  $\phi_b(a) = w_b$  and, for all  $x \in X - \{a, b\}$ ,  $\phi_b(x) = \phi(x)$ . Let  $T_b = (T_b; \phi_b)$ . Since T is a binary phylogenetic X-tree,  $T_b$  is a binary phylogenetic  $(X - \{b\})$ -tree. Denoting the vertex of T' adjacent to both u' and v' by w', let  $T'_b$  be the tree obtained from T' by contracting the edges  $\{u', w'\}$  and  $\{v', w'\}$ , and let  $w'_b$  denote the vertex of  $T'_b$  that identifies u', v', and w'. Let  $\phi'_b$  be the map from  $X - \{b\}$  into the vertex set of  $T'_b$  defined by  $\phi'_b(a) = w'_b$  and, for all  $x \in X - \{a, b\}$ ,  $\phi'_b(x) = \phi'(x)$ . Let  $T'_b = (T'_b; \phi'_b)$ .

Consider the assumptions made on  $\mathcal{T}$  and  $\mathcal{T}'$  in the statement of Theorem 3.2. We next show that the analogous assumptions hold for  $\mathcal{T}_b$  and  $\mathcal{T}_b'$ , respectively, with  $\Sigma_b$  replacing  $\Sigma$ .

It is easily checked that  $\mathcal{T}_b$  displays  $\Sigma_b$  and  $\mathcal{T}_b$  is distinguished by  $\Sigma_b$ . Suppose that  $\mathcal{T}_b'$  does not display  $\Sigma_b$ . Then, as  $\mathcal{T}'$  displays  $\Sigma$ , it is easily seen that there must be an element,  $A_1|B_1$  say, of  $\Sigma$  such that except for  $\{u', w'\}$  and  $\{v', w'\}$  no other edges of T' displays  $A_1|B_1$  in T', and so its counterpart in  $\Sigma_b$  is not displayed by  $T'_b$ . Clearly, this counterpart in  $\Sigma_b$  is not produced via a type (i) or (ii) replacement. Suppose that  $\{u', w'\}$  is distinguished by  $A_1|B_1$  in  $\mathcal{T}'$ . Without loss of generality, we may assume that  $\phi'(A_1)$  is a subset of the vertex set of the component of  $T'\setminus\{u',w'\}$ containing u', in which case,  $b \notin A_1$ . If a is not an element of  $A_1$ , then, by the first observation,  $\{\{a,b\},A_1\}$  is not an element of E, but  $\{\{a,b\},A_1\}$  is an element of E'; a contradiction. Thus  $a \in A_1$ . Since the counterpart of  $A_1|B_1$  in  $\Sigma_b$  is not produced via a type (i) or (ii) replacement,  $|A_1| \geq 2$ , and therefore, as  $w' \notin \phi'(X)$ , it follows by the second observation that  $b \notin B_1$ . This implies, by the first observation, that  $\{\{a,b\},B_1\}$  is not an element of E. However,  $\{\{a,b\},B_1\}$  is an element of E'; a contradiction. Hence  $\{u', w'\}$  is not distinguished by  $A_1|B_1$ . Similarly,  $\{v', w', \}$  is not distinguished by  $A_1|B_1$ . Therefore  $\{u',w'\}$  and  $\{v',w'\}$  are precisely the edges of T' that display  $A_1|B_1$  in T'. Without loss of generality, we may assume that  $\phi'(A_1)$  and  $\phi'(B_1)$  are subsets of the vertex sets of the components of  $T'\setminus\{u',w'\}$ and  $T'\setminus\{v',w'\}$  containing u' and v', respectively. Assuming a is not an element of  $A_1$  and arguing as above, we deduce that  $a \in A_1$ . Similarly,  $b \in B_1$ . Since the counterpart of  $A_1|B_1$  in  $\Sigma_b$  is not produced via a type (i) or (ii) replacement,  $|A_1| \geq 2$  and  $|B_1| \geq 2$ , contradicting the second observation. Thus  $\mathcal{T}_h'$  does indeed display  $\Sigma_b$ .

Let  $E_b$  and  $E'_b$  denote the edge sets of the graphs  $G(\mathcal{T}_b, \Sigma_b)$  and  $G(\mathcal{T}_b', \Sigma_b)$ , respectively. We now show that  $E'_b \subseteq E_b$ . Let  $C_b$  and  $D_b$  be elements of  $\mathcal{C}(\Sigma_b)$ , and suppose that  $\{C_b, D_b\}$  is an element of  $E'_b$ . Let C and D be the counterparts of  $C_b$  and  $D_b$  in  $\mathcal{C}(\Sigma)$ , respectively. If a is an element of both  $C_b$  and  $D_b$ , then  $\{C_b, D_b\}$  is an element of  $E_b$ . Therefore we may assume that a is not an element of both  $C_b$  and  $D_b$ . We next show that  $\{C, D\}$  is an element of E'. The only plausible case where this may not happen is when  $\mathcal{T}'_b(C_b) \cap \mathcal{T}'_b(D_b) = \{w'_b\}$  and  $\mathcal{T}'(C) \cap \mathcal{T}'(D) = \emptyset$ , in which case,  $\{\{a,b\},C\}$  and  $\{\{a,b\},D\}$  are both elements of E'. Since  $E' \subseteq E$ , it follows by the first observation that either a or b is an element of C and either  $C_b$  or  $C_b$  is an element of  $C_b$ . But then  $C_b$  is an element of  $C_b$  and  $C_b$ , contradicting our assumption earlier in the paragraph. Thus  $\{C_b, D_b\} \in E'$ . So, as  $C' \subseteq E$ ,  $\{C_b, D_b\} \in E$ , which in turn implies that  $\{C_b, D_b\} \in E_b$ . Hence  $E'_b \subseteq E_b$  as claimed.

At last, we can invoke the induction assumption which implies that  $T_b'$  is isomorphic to  $T_b$ . Using the facts that  $T_b'$  is obtained by contracting  $\{u', w'\}$  and  $\{v', w'\}$  in T', and that each of  $\{u, w\}$  and  $\{v, w\}$  of T is distinguished by an element of  $\Sigma$ , it is easily deduced that T' is isomorphic to T. This completes the proof of Case (a).

#### Case (b). The number of edges in P' is one.

In this case, we argue, as in Case (a), to deduce that  $T_b'$  is isomorphic to  $T_b$ . However, in this case, as each of  $\{u, w\}$  and  $\{v, w\}$  of T is distinguished by an element of  $\Sigma$  in T, we deduce a contradiction. This completes the proof of Theorem 3.2.  $\square$ 

The next lemma, [9, Rule 2], is needed for the proof of Lemma 3.4.

**Lemma 3.3.** Let  $A_1|B_1$  and  $A_2|B_2$  be partial X-splits. Let  $\mathcal{T}$  be a phylogenetic X-tree that displays  $A_1|B_1$  and  $A_2|B_2$ . If  $\mathcal{T}(A_1) \cap \mathcal{T}(A_2)$ ,  $\mathcal{T}(A_2) \cap \mathcal{T}(B_1)$ , and  $\mathcal{T}(B_1) \cap \mathcal{T}(B_2)$  are all non-empty, then  $\mathcal{T}$  displays  $(A_1 \cup A_2)|B_2$ .

Let  $\mathcal{T} = (T; \phi)$  be a phylogenetic X-tree, and let  $e = \{u, v\}$  be an internal edge of T that displays the partial X-split A|B so that A is a subset of the vertex set of the component of  $T \setminus e$  containing u. Then e is strongly distinguished by A|B if the vertex set of each component of  $T \setminus u$ , except for the one containing v, contains an element of A and the vertex set of each component of  $T \setminus v$ , except for the one containing u, contains an element of B. Observe that if e is strongly distinguished by A|B, then e is distinguished by A|B. Moreover, if T is a binary phylogenetic X-tree, then the notions of distinguished and strongly distinguished are equivalent.

**Lemma 3.4.** Let  $\Sigma$  be a set of partial X-splits. Let  $\mathcal{T}_1 = (T_1; \phi_1)$  and  $\mathcal{T}_2 = (T_2; \phi_2)$  be phylogenetic X-trees that display  $\Sigma$ . Suppose that every internal edge of  $T_1$  is strongly distinguished by an element of  $\Sigma$  and, moreover,  $|\Sigma|$  is equal to the number of internal edges of  $T_1$ . If the edge set of  $G(\mathcal{T}_1, \Sigma)$  is a subset of the edge set of  $G(\mathcal{T}_2, \Sigma)$ , then  $\mathcal{T}_1 \leq \mathcal{T}_2$ .

*Proof.* The proof of Lemma 3.4 is by induction on the number of internal edges of  $T_1$ . If  $T_1$  has exactly one internal edge, then, as  $\mathcal{T}_2$  displays  $\Sigma$ , it is clear that  $\mathcal{T}_1 \leq \mathcal{T}_2$ . Suppose that  $T_1$  has n internal edges, where  $n \geq 2$ , and assume that the result holds for all phylogenetic X-trees with a smaller number of internal edges. Throughout the proof, we denote the edge sets of  $G(\mathcal{T}_1, \Sigma)$  and  $G(\mathcal{T}_2, \Sigma)$  by  $E_1$  and  $E_2$ , respectively.

Let e be an internal edge of  $T_1$  with the property that every vertex adjacent to one of its end-vertices is a pendant vertex. Note that  $T_1$  must have such an edge. Denote the end-vertex of e with this property by  $w_1$  and denote the other end-vertex of e by  $w_2$ . Let  $f_1, f_2, \ldots, f_r$  and  $g_1, g_2, \ldots, g_s$  denote the pendant edges of  $T_1$  that are incident with  $w_1$  and  $w_2$ , respectively. Let  $h_1, h_2, \ldots, h_t$  denote the internal edges of  $T_1$ , other than e, that are incident with  $w_2$ . Note that  $r \geq 2$  and  $s+t \geq 2$  since  $T_1$  is a phylogenetic X-tree. Let A|B be the (unique) partial X-split of  $\Sigma$  that strongly distinguishes e. Without loss of generality, we may assume that  $A = \{a_1, a_2, \ldots, a_r\}$ , where  $a_1, a_2, \ldots, a_r$  are the pendant vertices of  $T_1$  corresponding to the end-vertices of  $f_1, f_2, \ldots, f_r$ , respectively. Let  $b_1, b_2, \ldots, b_{s+t}$  be elements of B such that, for each distinct  $j, k \in \{1, 2, \ldots, s+t\}$ ,  $b_j$  and  $b_k$  are in different components of  $T_1 \setminus w_2$ . Thus e is strongly distinguished by  $A|\{b_1, b_2, \ldots, b_{s+t}\}$  in  $T_1$ .

Let  $\Sigma_e$  be the set of partial X-splits obtained from  $\Sigma$  by removing A|B and, for each  $i \in \{1, 2, ..., t\}$ , replacing the element  $A_i|B_i$  of  $\Sigma$  that strongly distinguishes  $h_i$  by  $(A_i \cup A)|B_i$ , where  $A_i \cap A$  is non-empty.

Consider  $\mathcal{T}_1/e$ . Evidently,  $\mathcal{T}_1/e$  is a phylogenetic X-tree that displays  $\Sigma_e$  and  $|\Sigma_e|$  is equal to the number of internal edges of  $T_1/e$ . Furthermore, as every internal edge of  $T_1$  is strongly distinguished by an element of  $\Sigma$  in  $\mathcal{T}_1$ , it is easily seen that every internal edge of  $T_1/e$  is strongly distinguished by an element of  $\Sigma_e$  in  $\mathcal{T}_1$ . Now

consider  $\mathcal{T}_2$ . We next show that  $\mathcal{T}_2$  displays  $\Sigma_e$ . Since  $\mathcal{T}_2$  displays  $\Sigma$ , it suffices to show that, for each  $i \in \{1, 2, \ldots, t\}$ ,  $\mathcal{T}_2$  displays  $(A_i \cup A)|B_i$ . It is straightforward to deduce that each of  $\mathcal{T}_1(A) \cap \mathcal{T}_1(A_i)$ ,  $\mathcal{T}_1(A_i) \cap \mathcal{T}_1(B)$ , and  $\mathcal{T}_1(B) \cap \mathcal{T}_1(B_i)$  is non-empty. Therefore, as  $E_1 \subseteq E_2$ , each of  $\mathcal{T}_2(A) \cap \mathcal{T}_2(A_i)$ ,  $\mathcal{T}_2(A_i) \cap \mathcal{T}_2(B)$ , and  $\mathcal{T}_2(B) \cap \mathcal{T}_2(B_i)$  is non-empty. Hence, by Lemma 3.3,  $\mathcal{T}_2$  displays  $(A_i \cup A)|B_i$ .

To invoke the induction assumption, we lastly show that the edge set  $E_{1e}$  of  $G(\mathcal{T}_1/e, \Sigma_e)$  is a subset of the edge set  $E_{2e}$  of  $G(\mathcal{T}_2, \Sigma_e)$ . Let  $\{C, D\}$  be an element of  $E_{1e}$ . Then  $\mathcal{T}_1/e(C) \cap \mathcal{T}_1/e(D)$  is non-empty. There are three possibilities to consider depending upon whether C or D is of the form  $A_i \cup A$  for some  $i \in \{1, 2, \ldots, t\}$ .

Evidently, if C and D are of the forms  $A_i \cup A$  and  $A_j \cup A$ , for some  $i, j \in \{1, 2_{\bar{1}}, \ldots, t\}$ , then  $\mathcal{T}_2(C) \cap \mathcal{T}_2(D)$  is non-empty. Suppose that exactly one of C and D is of the form  $A_i \cup A$  for some i. Without loss of generality, we may assume that C has this property. If  $D \cap A$  is non-empty, then  $\mathcal{T}_2(C) \cap \mathcal{T}_2(D)$  is non-empty. Therefore assume that  $D \cap A$  is empty. Then, as every element of A is adjacent to  $w_1$  in  $\mathcal{T}_1$  and  $\mathcal{T}_1/e(C) \cap \mathcal{T}_1/e(D)$  is non-empty, it follows that  $\mathcal{T}_1(A_i) \cap \mathcal{T}_1(D)$  is non-empty. This in turn implies that  $\mathcal{T}_2(A_i) \cap \mathcal{T}_2(D)$  is non-empty as  $E_1 \subseteq E_2$ , and therefore  $\mathcal{T}_2(C) \cap \mathcal{T}_2(D)$  is non-empty.

Now suppose that neither C nor D is of the form  $A_i \cup A$ . For this possibility, we show that  $\mathcal{T}_1(C) \cap \mathcal{T}_1(D)$  is non-empty, thus showing that  $\mathcal{T}_2(C) \cap \mathcal{T}_2(D)$  is non-empty as  $E_1 \subseteq E_2$ . Assume that  $\mathcal{T}_1(C) \cap \mathcal{T}_1(D)$  is empty. Then, as  $\mathcal{T}_1/e(C) \cap \mathcal{T}_1/e(D)$  is non-empty,  $w_1 \in \mathcal{T}_1(C)$  and  $w_2 \notin \mathcal{T}_1(C)$ . Therefore, by the assumptions on  $\Sigma$  in the statement of the theorem, C must equal A. However, A is not an element of  $\mathcal{C}(\Sigma_e)$ . This contradiction completes the proof of the last possibility, and so  $E_{1e} \subseteq E_{2e}$ .

It now follows by the induction assumption that  $\mathcal{T}_1/e \leq \mathcal{T}_2$ . Suppose that  $\mathcal{T}_2$  is not a resolution of  $\mathcal{T}_1$ . Then  $\mathcal{T}_2$  must resolve  $\mathcal{T}_1/e$  so that, for every internal edge e' of  $\mathcal{T}_2$  with the property that A is a subset of the vertex set V' of one component of  $\mathcal{T}_2 \setminus e'$ ,  $B \cap V'$  is non-empty. But this implies that  $\mathcal{T}_2$  does not display A|B. This contradiction completes the proof of Lemma 3.4.

The next corollary generalizes Lemma 3.4.

Corollary 3.5. Let  $\Sigma$  be a set of partial X-splits. Let  $\mathcal{T}_1$  and  $\mathcal{T}_2$  be phylogenetic X-trees that display  $\Sigma$ . Suppose that every internal edge of  $\mathcal{T}_1$  is strongly distinguished by an element of  $\Sigma$ . If the edge set of  $G(\mathcal{T}_1, \Sigma)$  is a subset of  $G(\mathcal{T}_2, \Sigma)$ , then  $\mathcal{T}_1 \leq \mathcal{T}_2$ .

*Proof.* Let  $\mathcal{T}_1 = (T_1; \phi_1)$ , and choose  $\Sigma'$  to be a subset of  $\Sigma$  so that  $|\Sigma'|$  is equal to the number of internal edges of  $T_1$  and every internal edge of  $T_1$  is strongly distinguished by an element of  $\Sigma'$ . Since  $E(G(\mathcal{T}_1, \Sigma)) \subseteq E(G(\mathcal{T}_2, \Sigma))$ , it follows that  $E(G(\mathcal{T}_1, \Sigma')) \subseteq E(G(\mathcal{T}_2, \Sigma'))$ . Therefore, by Lemma 3.4,  $\mathcal{T}_1 \leq \mathcal{T}_2$  as required.  $\square$ 

We now combine Theorem 3.2 and Corollary 3.5 to formally prove Lemma 3.1.

Proof of Lemma 3.1. Let  $\mathcal{T}$  be a binary phylogenetic X-tree that displays  $\Sigma$  and is distinguished by  $\Sigma$ , and let G be the unique minimal restricted chordal completion of int( $\Sigma$ ). Combining Corollary 2.5 and Theorem 3.2, we deduce that  $G(\mathcal{T}, \Sigma) = G$ .

Suppose that  $\mathcal{T}'$  is an X-tree that displays  $\Sigma$ . Then there is a phylogenetic X-tree  $\mathcal{T}''$  that displays  $\Sigma$  such that  $\mathcal{T}' \leq \mathcal{T}''$ . Since  $\mathcal{T}$  is binary and is distinguished by  $\Sigma$ , every internal edge of T is strongly distinguished by an element of  $\Sigma$ . Therefore, by Corollary 3.5,  $\mathcal{T} \leq \mathcal{T}''$ . But  $\mathcal{T}$  is a binary phylogenetic X-tree, and so  $\mathcal{T}'' \cong \mathcal{T}$ . As  $\mathcal{T}$  is distinguished by  $\Sigma$ , it follows that  $\mathcal{T}' = \mathcal{T}''$ . We conclude that  $\Sigma$  defines  $\mathcal{T}$ .

Proof of Theorem 1.2. Suppose that  $\Sigma$  defines an X-tree  $\mathcal{T}$ . Then, by Proposition 2.6,  $\mathcal{T}$  satisfies the properties of (i). Let G be a restricted chordal completion of  $\operatorname{int}(\Sigma)$ . We next show that there is a unique minimal restricted chordal completion of  $\operatorname{int}(\Sigma)$ , namely,  $G(\mathcal{T}, \Sigma)$ .

Let G' be a minimal restricted chordal completion of  $\operatorname{int}(\Sigma)$  so that E(G') is a subset of E(G). Then, by Corollary 2.5, there exists an X-tree  $\mathcal{T}'$  such that  $E(G(\mathcal{T}',\Sigma))=E(G')$ . By Lemma 2.3,  $\mathcal{T}'$  displays  $\Sigma$  and so, as  $\Sigma$  defines  $\mathcal{T}$ , we must have  $\mathcal{T}'\cong \mathcal{T}$ . Since  $E(G(\mathcal{T}',\Sigma))\subseteq E(G)$ , it follows that  $E(G(\mathcal{T},\Sigma))\subseteq E(G)$ . Hence there is a unique minimal restricted chordal completion of  $\operatorname{int}(\Sigma)$ , namely,  $G(\mathcal{T},\Sigma)$ .

It now follows that the proof of Theorem 1.2 is completed by showing that if (i) and (ii) hold, then  $\Sigma$  defines an X-tree. We begin with three lemmas. For  $n \geq 2$ , let  $A_1|A_2|\cdots|A_n$  be an element of  $\Sigma$ , and consider the set  $\bigcup_{1\leq i< j\leq n} \{A_i|A_j\}$ . Let  $\Sigma'$  denote the collection of all such sets that are obtained in this way from the elements of  $\Sigma$ .

Lemma 3.6. An X-tree T' displays  $\Sigma$  if and only if T' displays  $\Sigma'$ .

Proof. Let  $A_1|A_2|\cdots|A_n$  be an element of  $\Sigma$ , where  $n\geq 2$ . To prove Lemma 3.6, we simply need to show that  $\mathcal{T}'$  displays  $A_1|A_2|\cdots|A_n$  if and only if  $\mathcal{T}'$  displays  $\bigcup_{1\leq i< j\leq n}\{A_i|A_j\}$ . The "only if" part of this last statement clearly holds. To prove the converse, suppose that  $\mathcal{T}'$  does not display  $A_1|A_2|\cdots|A_n$ . Then, for some distinct i and j of  $\{1,2,\ldots,n\}$ , the set  $\mathcal{T}'(A_i)\cap\mathcal{T}'(A_j)$  is non-empty. But then  $\mathcal{T}'$  does not display  $A_i|A_j$ , and so  $\mathcal{T}'$  does not display  $\bigcup_{1\leq i< j\leq n}\{A_i|A_j\}$ . This completes the proof of Lemma 3.6.

The first of the next two lemmas is a useful observation which is repeatedly use in the rest of the proof.

**Lemma 3.7.** Let T' be an X-tree that displays  $\Sigma$  (or, equivalently, displays  $\Sigma'$ ). Let A and B be elements of  $C(\Sigma)$  such that  $A \cap B$  is empty. Then  $\{A, B\}$  is an edge of  $G(T', \Sigma')$  if and only if  $\{A, B\}$  is an edge of  $G(T', \Sigma')$ .

Lemma 3.8. Let T' be an X-tree that displays  $\Sigma$  (or, equivalently, displays  $\Sigma'$ ). If  $G(T', \Sigma')$  is a minimal restricted chordal completion of  $\operatorname{int}(\Sigma')$ , then  $G(T', \Sigma)$  is a minimal restricted chordal completion of  $\operatorname{int}(\Sigma)$ .

Proof. Suppose that  $G(\mathcal{T}', \Sigma')$  is a minimal restricted chordal completion of  $\operatorname{int}(\Sigma')$ , but  $G(\mathcal{T}', \Sigma)$  is not a minimal restricted chordal completion of  $\operatorname{int}(\Sigma)$ . Then, by Corollary 2.5, there is an X-tree  $\mathcal{T}''$  that displays  $\Sigma$  such that  $E(G(\mathcal{T}'', \Sigma))$  is a proper subset of  $E(G(\mathcal{T}', \Sigma))$ . By Lemma 3.6,  $\mathcal{T}''$  displays  $\Sigma'$ , and so, by

Lemma 2.3,  $G(\mathcal{T}'', \Sigma')$  is a restricted chordal completion of  $\operatorname{int}(\Sigma')$ . We obtain a contradiction by showing that  $E(G(\mathcal{T}'', \Sigma'))$  is a proper subset of  $E(G(\mathcal{T}', \Sigma'))$ .

Let  $\{A', B'\}$  be an edge of  $G(T'', \Sigma')$ . If  $A' \cap B' \neq \emptyset$ , then  $\{A', B'\}$  is an edge of  $G(T', \Sigma')$ . Therefore assume that  $A' \cap B' = \emptyset$ . Then, by Lemma 3.7,  $\{A', B'\}$  is an edge of  $G(T'', \Sigma)$ , and so, as  $E(G(T'', \Sigma)) \subset E(G(T', \Sigma))$ ,  $\{A', B'\}$  is an edge of  $G(T', \Sigma)$ . By Lemma 3.7,  $\{A', B'\}$  is an edge of  $G(T', \Sigma')$ . Thus  $E(G(T'', \Sigma'))$  is a subset of  $E(G(T', \Sigma'))$ . To see that this inclusion is proper, let  $\{A, B\}$  be an element of  $E(G(T', \Sigma)) - E(G(T'', \Sigma))$ . Clearly,  $A \cap B$  is empty, and so using Lemma 3.7 twice, we get that  $\{A, B\}$  is an edge of  $G(T', \Sigma')$ , but is not an edge of  $G(T'', \Sigma')$ . Hence  $E(G(T'', \Sigma'))$  is a proper subset of  $E(G(T', \Sigma'))$ , thus completing the proof of Lemma 3.8.

We now combine Lemmas 3.6 and 3.8 with Lemma 3.1 to complete the proof of Theorem 1.2.

Suppose that (i) and (ii) hold. We first show that (i) and (ii) of Lemma 3.1 hold with  $\Sigma'$  replacing " $\Sigma$ ". Using Lemma 3.6, it is easily seen that an X-tree that satisfies (i) of Theorem 1.2 satisfies (i) of Lemma 3.1. Now suppose, to the contrary, that there is not a unique minimal restricted chordal completion of  $\operatorname{int}(\Sigma')$ . Let  $G'_1$  and  $G'_2$  be two distinct minimal restricted chordal completions of  $\operatorname{int}(\Sigma')$ . By Corollary 2.5, there exists two distinct X-trees,  $T'_1$  and  $T'_2$  say, such that  $G(T'_1, \Sigma') = G'_1$  and  $G(T'_2, \Sigma') = G'_2$ . By Lemma 3.8,  $G(T'_1, \Sigma)$  and  $G(T'_2, \Sigma)$  are both minimal restricted chordal completions of  $\operatorname{int}(\Sigma)$ . We show that the last two graphs are distinct, thus getting our desired contradiction.

Since  $G_1'$  and  $G_2'$  are distinct, there is an edge  $\{C', D'\}$  of  $G_1'$  that is not an edge of  $G_2'$ . Clearly,  $C' \cap D' = \emptyset$ . Therefore, by Lemma 3.7,  $\{C', D'\}$  is an edge of  $G(T_1', \Sigma)$ , but is not an edge of  $G(T_2', \Sigma)$ . Thus  $G(T_1, \Sigma)$  and  $G(T_2, \Sigma)$  are distinct; a contradiction. Hence there is a unique minimal restricted chordal completion of  $\operatorname{int}(\Sigma')$ .

With (i) and (ii) of Lemma 3.1 satisfied it now follows that  $\Sigma'$  defines an X-tree, which in turn implies by Lemma 3.6 that  $\Sigma$  defines an X-tree, completing the proof of Theorem 1.2.

#### 4. Examples and Further Results

We begin this section with two examples highlighting the fact that conditions (i) and (ii) in the statement of Theorem 1.2 cannot be weakened.

The first example shows that if (i) holds, the uniqueness part of (ii) in the statement of Theorem 1.2 is necessary. Let  $X = \{1, 2, ..., 6\}$  and let  $\Sigma$  be the set

$$\{\{1,2\}|\{3,5\},\{3,4\}|\{2,6\},\{5,6\}|\{1,4\}\}\cup\{\{i\}|X-\{i\}:i\in\{1,2,\ldots,6\}\}$$

of partial partitions of X. The two binary phylogenetic X-trees in Figure 3 display  $\Sigma$ , and thus  $\Sigma$  does not define an X-tree. However, as shown in [2], the first of these binary phylogenetic X-trees (as well as the second) also distinguishes  $\Sigma$ , and

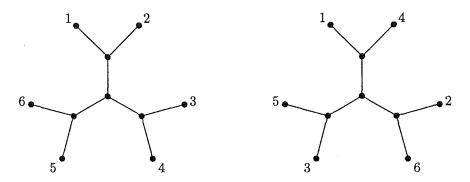


Figure 3. Two binary phylogenetic X-trees with  $X = \{1, 2, \dots, 6\}$ .

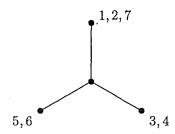


FIGURE 4. An X-tree that is distinguished by  $\{\{1,2\}|\{3,5\},\{3,4\}|\{2,6,7\},\{5,6\}|\{1,4,7\}\}\}$ .

so, by Theorem 1.2, there are at least two minimal restricted chordal completions of  $int(\Sigma)$ .

The next example shows that even deleting "minimal" in the second condition in the statement of Theorem 1.2 is no guarantee that the theorem holds without the full strength of (i). Let  $X = \{1, 2, ..., 7\}$  and let  $\Sigma$  be the set

$$\{\{1,2\}|\{3,5\},\{3,4\}|\{2,6,7\},\{5,6\}|\{1,4,7\}\}$$

of partial partitions of X. The graph in Figure 2(ii) is the unique restricted chordal completion of  $\operatorname{int}(\Sigma)$ . However, every resolution of the X-tree in Figure 4 displays  $\Sigma$ . The tree in Figure 2(i) is one such X-tree. Hence, by Theorem 1.2, no X-tree displaying  $\Sigma$  can be a binary phylogenetic X-tree that is distinguished by  $\Sigma$ .

We finish this section with some minor results relating to Theorems 1.1 and 1.2.

**Proposition 4.1.** Let  $\Sigma$  be a set of partial partitions of X, where  $|X| \geq 3$ . If  $\Sigma$  defines a binary phylogenetic tree, then  $\operatorname{int}(\Sigma)$  is connected.

*Proof.* Suppose, to the contrary, that  $\operatorname{int}(\Sigma)$  is disconnected. We prove the case for when  $\operatorname{int}(\Sigma)$  has two components,  $G_1$  and  $G_2$  say. This argument extends straightforwardly to cover the case when  $\operatorname{int}(\Sigma)$  has at least three components.

For each  $i \in \{1,2\}$ , let  $\mathcal{C}_i$  denote the vertex set of  $G_i$ , and let  $X_i$  denote the union of the elements of  $\mathcal{C}_i$ . As  $\operatorname{int}(\Sigma)$  is disconnected, X is the disjoint union of  $X_1$  and  $X_2$ . Let  $\mathcal{T}$  be the binary phylogenetic tree defined by  $\Sigma$ . Since  $|X| \geq 3$ ,

either  $|X_1| \geq 2$  or  $|X_2| \geq 2$ . Without loss of generality, we may assume that  $|X_1| \geq 2$ : Since both  $X_1$  and  $X_2$  are non-empty, and since  $|X| \geq 3$ , there exists a binary phylogenetic tree on X, different from  $\mathcal{T}$ , that can be constructed by adding a vertex to an edge of  $\mathcal{T}|X_1$  and either (i) adding a vertex to an edge of  $\mathcal{T}|X_2$ , and then joining the two new vertices with an edge if  $|X_2| \geq 2$ , or (ii) joining the new vertex with the vertex of  $\mathcal{T}|X_2$  with an edge if  $|X_2| = 1$ . In either case, denote the resulting binary phylogenetic tree on X by  $\mathcal{T}'$ .

We now show that  $G(T', \Sigma)$  is a restricted chordal completion of  $\operatorname{int}(\Sigma)$ . By Corollary 2.2,  $G(T', \Sigma)$  is chordal. Let A and A' be non-empty cells of an element of  $\Sigma$ . We need to show that A and A' are non-adjacent in  $G(T', \Sigma)$ . If A and A' are in different components of  $\operatorname{int}(\Sigma)$ , then A and A' are non-adjacent in  $G(T', \Sigma)$ . Suppose that A and A' are in the same component of  $\operatorname{int}(\Sigma)$ . Without loss of generality, we may assume that both A and A' are vertices of  $G_1$ . Then both A and A' are subsets of  $X_1$ . Since T displays  $\Sigma$ , T displays every partial partition of  $\Sigma$  containing A and A'. Therefore A|A' is a partial split of T. By our construction of T', this means that A|A' is a partial split of T'. Therefore A and A' are non-adjacent in  $G(T', \Sigma)$ . Thus  $G(T', \Sigma)$  is a restricted chordal completion of  $\operatorname{int}(\Sigma)$ , and so, by Lemma 2.3, T' displays  $\Sigma$ . This contradiction to the fact that  $\Sigma$  defines T completes the proof of Proposition 4.1.

Let  $\Sigma$  be a collection of partial partitions of X, and let x be an element of X. For any subset A of X, let  $A_x$  denote the set  $A - \{x\}$  and, for any  $\sigma$  in  $\Sigma$ , let  $\sigma_x$  denote the partial partition of X obtained from  $\sigma$  by deleting x from every cell. Provided  $\{x\}$  is not an element of  $\mathcal{C}(\Sigma)$ , let  $\Sigma_x = \{\sigma_x : \sigma \in \Sigma\}$  We say x is redundant (relative to  $\Sigma$ ) if the x-deletion map  $\psi$  from  $\Sigma$  into  $\Sigma_x$  defined by  $\psi(\sigma) = \sigma_x$  induces a graph isomorphism between  $\operatorname{int}(\Sigma)$  and  $\operatorname{int}(\Sigma_x)$ .

**Lemma 4.2.** Let x be an element of X, and let  $\Sigma$  be a set of partial partitions of X. If x is redundant, and  $T_x$  is an  $X_x$ -tree that displays  $\Sigma_x$ , then there exists an X-tree T that displays  $\Sigma$  and satisfies  $T|X_x = T_x$ .

*Proof.* Let V denote the subset of  $\mathcal{C}(\Sigma)$  in which each element contains x. Thus every two elements of V is adjacent in  $\operatorname{int}(\Sigma)$ . Let  $V_x = \{A_x : A \in V\}$ .

Since  $\operatorname{int}(\Sigma) \cong \operatorname{int}(\Sigma_x)$  under the x-deletion map, every two elements of  $V_x$  are adjacent in  $\operatorname{int}(\Sigma_x)$ . Consequently, for all pairs  $A_x$  and  $A'_x$  in  $V_x$ , we have  $\mathcal{T}_x(A_x) \cap \mathcal{T}_x(A'_x) \neq \emptyset$ . By the Helly property for subtrees of a tree (see [7, p. 92]), it follows that

$$\bigcap_{A_x \in V_x} \mathcal{T}_x(A_x) \neq \emptyset.$$

Select a vertex  $v \in \bigcap_{A_x \in V_x} \mathcal{T}_x(A_x)$ , and let  $\mathcal{T}$  be the X-tree obtained from  $\mathcal{T}_x$  by mapping x to v. Clearly  $\mathcal{T}|X_x = \mathcal{T}_x$ , so provided  $\mathcal{T}$  displays  $\Sigma$  the proof is complete.

Let B and B' be elements of  $C(\Sigma)$ . If  $T_x(B_x) \cap T_x(B'_x) \neq \emptyset$ , then  $T(B) \cap T(B') \neq \emptyset$ . Conversely, if  $T_x(B_x) \cap T_x(B'_x) = \emptyset$ , then  $T(B) \cap T(B') = \emptyset$  as x labels a vertex in  $\bigcap_{A_x \in V_x} T_x(A_x)$ . Therefore the x-deletion map from  $\Sigma$  to  $\Sigma_x$  induces, not only the isomorphism between  $\operatorname{int}(\Sigma)$  and  $\operatorname{int}(\Sigma_x)$ , but also an isomorphism between

int( $\{\mathcal{T}(B): B \in \mathcal{C}(\Sigma)\}$ ) and int( $\{\mathcal{T}_x(B_x): B \in \mathcal{C}(\Sigma)\}$ ). Hence int( $\{\mathcal{T}(B): B \in \mathcal{C}(\Sigma)\}$ ) is a restricted chordal completion for int( $\Sigma$ ), and so, by Lemma 2.3,  $\mathcal{T}$  displays  $\Sigma$  as required.

The proof of Corollary 4.3 is omitted. It is a straightforward consequence of Lemma 4.2.

Corollary 4.3. Let  $\Sigma$  be a set of partial partitions of X. Suppose that  $x \in X$  is redundant. Then

- (i) there exists an X-tree that displays  $\Sigma$  if and only if there exists an X-tree that displays  $\Sigma_x$ ; and
- (ii)  $\Sigma$  defines an X-tree if and only if  $\Sigma_x$  defines an X-tree.

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