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REPRESENTING PARTITIONS ON TREES*

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Abstract. In evolutionary biology, biologists often face the problem of constructing a phylogenetic tree on a set X of species from a multiset Π of partitions corresponding to various attributes of these species. One approach that is used to solve this problem is to try instead to associate a tree (or even a network) to the multiset Σ_Π consisting of all those bipartitions $\{A, X - A\}$ with A a part of some partition in Π. The rationale behind this approach is that a phylogenetic tree with leaf set X can be uniquely represented by the set of bipartitions of X induced by its edges. Motivated by these considerations, given a multiset Σ of bipartitions corresponding to a phylogenetic tree on X, in this paper we introduce and study the set $\mathbb{P}(\Sigma)$ consisting of those multisets of partitions Π of X with $\Sigma_\Pi = \Sigma$. More specifically, we characterize when $\mathbb{P}(\Sigma)$ is nonempty and also identify some partitions in $\mathbb{P}(\Sigma)$ that are of maximum and minimum size. We also show that it is NP-complete to decide when $\mathbb{P}(\Sigma)$ is nonempty in the case when Σ is an arbitrary multiset of bipartitions of X. Ultimately, we hope that by gaining a better understanding of the mapping that takes an arbitrary partition system Π to the multiset Σ_Π, we will obtain new insights into the use of median networks and, more generally, split networks, to visualize sets of partitions.

Key words. phylogenetics, partition systems, compatibility, split systems, X-trees

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1. Introduction.

In evolutionary biology, biologists are often faced with the task of constructing a phylogenetic tree (i.e., an unrooted, edge-weighted tree without degree-two vertices and leaf set X) that represents a multiset Π of partitions of a finite set X of species or taxa. Such multisets of partitions (or *partition systems*) usually arise from some collection of attributes or states of the species in question (e.g., "wings" versus "no wings" or the four possible nucleotides in the columns of some molecular sequence alignment). It is well known that a phylogenetic tree with leaf set X is determined by the bipartitions or *splits* of X that are induced by its edges [5]. Hence, when trying to derive such trees from multistate data, biologists sometimes consider instead the multiset Σ_Π of splits of X consisting of all those $\{A, X - A\}$ with $A \in \pi$ for some partition π contained in a partition system Π induced by the data [1, 13, 14]. The aim then becomes associating a tree (or possibly a network) to the multiset Σ_Π.

As an example of this process, for the set $X = \{1, 2, 3, 4, 5, 6\}$, consider the set of partitions $\Pi_1 = \{123|4|56, 1|2|3456, 3|12456, 5|6|1234\}$ on X (where, e.g., 123|4|56 denotes the partition $\{\{1, 2, 3\}, \{4\}, \{5, 6\}\}$). Then the multiset Σ_{Π_1} is represented (uniquely) by the phylogenetic tree in Figure 1. Intriguingly, Π_1 is not the only partition system that gives rise to the tree depicted in Figure 1. For example, the set $\Pi_2 = \{123|4|5|6, 1|2|3456, 3|12456, 56|1234\}$ gives rise to precisely the same tree (or,

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in other words, $\Sigma_{\Pi_1} = \Sigma_{\Pi_2}$). Thus, given a multiset Σ of splits of X that is *compatible* (i.e., corresponds to a phylogenetic tree), it is of interest to better understand the set $\mathbb{P}(\Sigma)$ that consists of all those partition systems Π on X such that $\Sigma_\Pi = \Sigma$ holds. As we shall see, the set $\mathbb{P}(\Sigma)$ can be quite complicated in general. For example, even for the simple tree in Figure 1 it can be shown that $\mathbb{P}(\Sigma_{\Pi_1})$ consists of Π_1 and Π_2 as well as the sets $\Pi_3 = \{12|3|4|56, 1|2|3|456, 5|6|1234\}$, $\Pi_4 = \{12|3|4|5|6, 1|2|3|456, 56|1234\}$, $\Pi_5 = \{1|2|3|4|56, 12|3|456, 5|6|1234\}$, and $\Pi_6 = \{1|2|3|4|5|6, 12|3|456, 56|1234\}$.

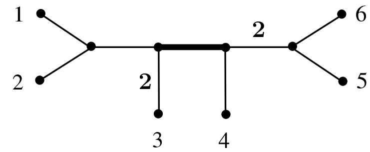

FIG. 1. *A tree that represents the multiset Σ_{Π_1} of splits on the set $X = \{1, 2, 3, 4, 5, 6\}$ given in the text. The removal of any edge of the tree gives a split of X, with multiplicity given by the weight in bold assigned to the edge (all unlabelled edges have weight* 1*). For example, the bold edge gives rise to the split* 123|456.

Although these considerations all appear rather abstract, our study of the set $\mathbb{P}(\Sigma)$ was motivated by its appearance in the construction of *median networks*. These networks generalize phylogenetic trees and are commonly used to visualize complex evolutionary relationships arising from mitochondrial sequences [2, 4, 16]. Median networks can be directly constructed from splits [6]. Moreover, given a multiple sequence alignment of a set X of sequences, one way to derive splits before constructing a median network is to convert each nonconstant column into a partition of X so as to give a multiset Π of partitions of X, and then construct the multiset Σ_Π (see, e.g., [1, 14]). Thus, we expect that by gaining a better understanding of the set $\mathbb{P}(\Sigma)$ (also for general split systems Σ) we will be able to obtain new insights into the use of median networks (and, more generally, *split networks*; cf. [15]) to represent partitions. In addition, through considerations such as those presented in [3], we hope that our results will help to further clarify the relationships between median and *quasi-median networks* given in [13].

We now present an overview of our main results. In the following two sections we present some notation and terminology as well as some preliminary results that will be used throughout the paper. Then, in section 4, we characterize those compatible multisets of splits Σ for which $\mathbb{P}(\Sigma)$ is nonempty (Theorem 4.2). In addition, for Σ a compatible multiset of splits of X, we show that if $\mathbb{P}(\Sigma)$ is nonempty, then there is always a unique partition system Π in $\mathbb{P}(\Sigma)$ which is *strongly compatible;* i.e., for all $\pi_1, \pi_2 \in \Pi$ either $\pi_1 = \pi_2$ or there are some $A \in \pi_1, B \in \pi_2$ such that $A \cup B = X$ [8]. For example, for the multiset Σ of splits giving rise to the tree depicted in Figure 1, the set Π_1 is the unique strongly compatible partition system in $\mathbb{P}(\Sigma)$.

As the example above illustrates, the size of the elements in $\mathbb{P}(\Sigma)$ can vary (e.g., the size of Π_1 is 4, whereas Π_6 has size 3). We are therefore interested in understanding the maximum- and minimum-sized elements in this set. In section 5, we show that the unique, strongly compatible partition system in $\mathbb{P}(\Sigma)$ is always of maximum size. In the subsequent section, we then focus on minimum-sized elements of $\mathbb{P}(\Sigma)$, giving a method to construct such a partition system. In general, it appears to be a difficult problem to characterize the maximum- and minimum-sized partition systems in $\mathbb{P}(\Sigma)$ for a compatible multiset Σ of splits. However, in section 6, we characterize the minimum-sized elements for a special type of multiset of splits that corresponds to a rooted tree in which the root is the same distance from all of the leaves in the tree.

In section 8, we investigate a related algorithmic question: Given an arbitrary split system Σ on X, can we decide in polynomial time in the size of X whether there exists a partition system Π of X such that $\Sigma_\Pi = \Sigma$? By reduction from the cubic edge coloring problem, we show that this problem is NP-complete, even if Σ is an arbitrary *set;* that is, the multiplicity of each split in Σ is equal to 1 (Theorem 8.1). This indicates that it might be difficult in general to extend our main results to arbitrary multisets of splits. In section 9, we discuss how the mapping from partition systems to split systems obtained by taking a partition system Π to the split system Σ_Π could be studied in a more general setting, and we mention some open problems that this leads to.

Before proceeding we note that the problem of representing partitions (or characters) by trees has also been studied in the context of the *perfect phylogeny problem*. This problem is concerned with representing partitions *convexly* on a phylogenetic tree, and a great deal of related theory has been developed (cf., e.g., [17, Chapter 4] and also [9, 11, 18] for more recent results). However, this approach differs from ours since, for example, there exist sets Π of partitions all of whose elements are convex on some phylogenetic tree for which Σ_Π is not compatible.

2. Preliminaries.

Multisets. If S is a finite nonempty set, a *multiset* chosen from S is a function m from S into the set of nonnegative integers $\mathbb{Z}^{\geq 0}$. The set S is sometimes called its *underlying set*. For an element t in S, the value $m(t)$ is the *multiplicity* of t. For example, let $S = \{1, 2, 3, 4\}$. Then the multiset $\{1, 1, 2, 2, 2, 3\}$ denotes the function m from S into $\mathbb{Z}^{\geq 0}$ with $m(1) = 2$, $m(2) = 3$, $m(3) = 1$, and $m(4) = 0$. The multiplicity of 2 is 3, while the multiplicity of 4 is 0. The size $|M|$ of a multiset M with underlying set S is the sum of the multiplicities over all elements in S. Let m_1 and m_2 be two functions from S into $\mathbb{Z}^{\geq 0}$, and let S_1 and S_2 denote the multisets corresponding to m_1 and m_2, respectively. We denote the *multiset union* of S_1 and S_2 by $S_1 \biguplus S_2$, where $S_1 \biguplus S_2$ is the function from S into $\mathbb{Z}^{\geq 0}$ defined by $m_1(t) + m_2(t)$ for all $t \in S$. Moreover, we denote the *multiset difference* of S_1 and S_2 by $S_1 - S_2$, where $S_1 - S_2$ is the function from S into $\mathbb{Z}^{\geq 0}$ defined by $\max\{0, m_1(t) - m_2(t)\}$ for all $t \in S$.

Weak *X*-trees. Throughout the paper, X will always denote a finite set of size at least 2. A *weak X-tree* $\mathcal{T}$ is an ordered pair $(T; \phi)$, where T is a tree with vertex set V and $\phi : X \to V$ is a map with the property that, for each vertex $v \in V$ of degree one, $v \in \phi(X)$. For convenience, we refer to the vertices and edges of T as the vertices and edges of $\mathcal{T}$, respectively, and write $V(\mathcal{T})$ for $V(T)$ and $E(\mathcal{T})$ for $E(T)$. A vertex v of $\mathcal{T}$ is *labelled* if $v \in \phi(X)$; otherwise, v is *unlabelled*. Given $u, v \in V$, we denote the length of the path joining u and v by $d_T(u, v)$. Sometimes we will also use $d_\mathcal{T}(u, v)$ rather than $d_T(u, v)$. A weak X-tree $\mathcal{T}$ is an *X-tree* if it additionally has the property that each degree-two vertex is labelled. Note that a phylogenetic X-tree $\mathcal{T}$ is an X-tree in which ϕ is a bijective map from X to the leaf set of $\mathcal{T}$. We say that two weak X-trees $\mathcal{T} = (T; \phi)$ and $\mathcal{T}' = (T'; \phi')$ are *isomorphic*, denoted by $\mathcal{T} \cong \mathcal{T}'$, if there exists a bijective map $\psi : V(T) \to V(T')$ that induces a graph isomorphism between T and T' for which $\phi'(x) = \psi(\phi(x))$ holds for all $x \in X$.

Note that weak X-trees are closely related to weighted X-trees, where an X-tree is *weighted* if each edge is assigned a positive integer weight. For example, the phylogenetic tree depicted in Figure 1 is equivalent to a weak X-tree in which each edge with weight 2 is subdivided into two edges by inserting an extra vertex. Indeed, we can translate between weighted X-trees and weak X-trees in general by inserting or suppressing unlabelled degree-two vertices in a similar manner. However, in this paper we will use weak X-trees rather than weighted X-trees since they are more convenient for many of our proofs (e.g., their vertices and edges can be used to represent certain partition systems).

Compatible split systems and hierarchies. As mentioned in the introduction, a split of X, or, equivalently, an *X-split*, is a bipartition of X into two nonempty sets, that is, a partition $\pi = \{A_1, A_2, \dots, A_t\}$ of X with $t \geq 2$ in which each subset A_i, $i \in \{1, \dots, t\}$, is nonempty and $t = 2$ (rather than $t \geq 2$ as is the case for a general partition of X). We will refer to the subsets A_i as *parts* of π, and, to simplify notation, we write $\{A_1, A_2, \dots, A_t\}$ as $A_1|A_2|\cdots|A_t$, where the ordering of the parts of π is irrelevant. A multiset of X-splits is called a *split system on X*. Split systems on X naturally arise in the context of weak X-trees. In particular, let $\mathcal{T} = (T; \phi)$ be a weak X-tree, and let e be an edge of $\mathcal{T}$. We denote by σ_e the X-split $A|(X - A)$, where A is one of the two maximal subsets of X such that e is not traversed on the path from $\phi(x)$ to $\phi(y)$ for all $x, y \in A$. This X-split *corresponds* to, or, equivalently, is *displayed* by, e in $\mathcal{T}$. Note that, as $\mathcal{T}$ is a weak X-tree, it is possible that, for distinct edges e and f, we have $\sigma_e = \sigma_f$. We denote the split system on X corresponding to the edges of $\mathcal{T}$ by $\Sigma(\mathcal{T})$, that is,

$$\Sigma(\mathcal{T}) = \biguplus_{e \in E(\mathcal{T})} \{\sigma_e\}.$$

A pair of X-splits $A_1|B_1$ and $A_2|B_2$ is *compatible* if at least one of the sets $A_1 \cap A_2$, $A_1 \cap B_2$, $B_1 \cap A_2$, and $B_1 \cap B_2$ is the empty set. A split system Σ on X is *compatible* if the splits in Σ are pairwise compatible. The following theorem is a straightforward generalization of the splits-equivalence theorem [5] (also see [17, Theorem 3.1.4]).

THEOREM 2.1. *Let Σ be a split system on X. Then there is a weak X-tree $\mathcal{T}$ such that $\Sigma = \Sigma(\mathcal{T})$ if and only if Σ is compatible. Moreover, if such a weak X-tree exists, then, up to isomorphism, $\mathcal{T}$ is unique.*

In light of this last result, if Σ is a compatible split system on X, we denote the unique weak X-tree $\mathcal{T}$ for which $\Sigma(\mathcal{T}) = \Sigma$ holds by $\mathcal{T}_\Sigma$. Note that in the case when $\Sigma = \Sigma(\mathcal{T})$ for a weak X-tree $\mathcal{T}$, we will write $\mathbb{P}(\mathcal{T})$ rather than $\mathbb{P}(\Sigma(\mathcal{T}))$.

An analogue of Theorem 2.1 holds for trees having a root. To make this statement more precise, we introduce some further terminology. A *rooted weak X-tree* $\mathcal{T}_\rho$ is an ordered pair $(T_\rho; \phi)$, where T_ρ is a rooted tree with root ρ which has degree at least two and vertex set V, and $\phi : X \to V - \{\rho\}$ is a map with the property that, for each vertex $v \in V$ of degree one, $v \in \phi(X)$. Note that if we view $\mathcal{T}_\rho$ as an unrooted tree with ρ as ordinary interior vertex, we obtain a weak X-tree. We denote this weak X-tree by $\mathcal{T}_\rho^-$.

A *cluster* of X is a nonempty subset of X, and it is *proper* if it is distinct from X. Let $\mathcal{T}_\rho$ be a rooted weak X-tree, and let e be an edge of $\mathcal{T}_\rho$. The proper subset of X consisting of those elements that label a vertex in $\mathcal{T}_\rho$ whose path to the root traverses e is denoted by C_e. This cluster C_e *corresponds* to, or, equivalently, is *displayed* by, e in $\mathcal{T}_\rho$. We denote the multiset of clusters of X corresponding to the edges of $\mathcal{T}_\rho$ by $\mathcal{H}(\mathcal{T}_\rho)$, that is,

$$\mathcal{H}(\mathcal{T}_\rho) = \biguplus_{e \in E(\mathcal{T}_\rho)} \{C_e\}.$$

It is straightforward to show that this multiset of subsets of X is a *hierarchy;* that is, for all $A, B \in \mathcal{H}(\mathcal{T}_\rho)$, we have $A \cap B \in \{\emptyset, A, B\}$. The next result is the aforementioned analogue of Theorem 2.1. We omit the routine proof.

THEOREM 2.2. *Let $\mathcal{H}$ be a multiset of proper clusters of X whose union is X. Then there is a rooted weak X-tree $\mathcal{T}_\rho$ such that $\mathcal{H} = \mathcal{H}(\mathcal{T}_\rho)$ if and only if $\mathcal{H}$ is a hierarchy on X. Moreover, if such a rooted weak X-tree exists, then, up to isomorphism, $\mathcal{T}_\rho$ is unique.*

Partition systems. A partition system Π of X is *compatible* if Σ_Π is compatible. Again following Theorem 2.1, if Π is a compatible partition system on X, we denote by $\mathcal{T}_\Pi$ the weak X-tree $\mathcal{T}$ for which $\Sigma(\mathcal{T}) = \Sigma_\Pi$ holds. Similarly, a partition system Π on X is *hierarchical* if the set $\bigcup_{\pi \in \Pi} \pi$ of all subsets of X that appear as a part in some partition in Π is a hierarchy. Observe that, if Π is hierarchical, then every subset of Π is a hierarchical partition system on X. Furthermore, if $\pi_1, \pi_2 \in \Pi$ and Π is hierarchical, then, for each $A \in \pi_1$, either A is a subset of a part in π_2 or A is the disjoint union of parts in π_2.

Now, given a partition π of X, we let $\Sigma_\pi = \biguplus_{A \in \pi} \{A|(X - A)\}$, i.e., the multiset of bipartitions $A|(X - A)$ with $A \in \pi$. The proof of the next result follows immediately from the respective definitions.

LEMMA 2.3. *Let π be a partition of X, let Σ be a split system on X, and let $\Pi \in \mathbb{P}(\Sigma)$. Then the following hold.*

(i) $\Sigma_{\{\pi\} \uplus \Pi} = \Sigma \uplus \Sigma_\pi$.

(ii) *If $\pi \in \Pi$, then $\Sigma_{\Pi - \{\pi\}} = \Sigma - \Sigma_\pi$.*

3. Displaying partition systems.

In this section, we describe how weak X-trees can be used to represent partition systems. Let $\mathcal{T} = (T; \phi)$ be a weak X-tree, and let π be a partition of X. A subset $E_\pi \subseteq E(\mathcal{T})$ of edges of $\mathcal{T}$ *displays* π if there is a bijection $\xi_\pi : \pi \to E_\pi$ such that, for each $A \in \pi$, the X-split corresponding to the edge $\xi_\pi(A)$ is $A|(X - A)$. For convenience, if there exists such a subset E_π of edges of $\mathcal{T}$, then we say that $\mathcal{T}$ *displays* π. Note that such a subset E_π need not be unique.

For a compatible partition system Π on X, the following two lemmas that we use later describe how $\mathcal{T}_\Pi$ displays the partitions in Π. Suppose $\mathcal{T} = (T; \phi)$ is a weak X-tree, and let e denote an edge of T. Then we denote by $\mathcal{T} \backslash e$ the set of components of $\mathcal{T}$ obtained by deleting e from T. More generally, for E a nonempty subset of edges of T we denote by $\mathcal{T} \backslash E$ the set of components of $\mathcal{T}$ obtained by deleting all edges in E from T.

LEMMA 3.1. *Let Π be a compatible partition system on X, and let u be a vertex of $\mathcal{T}_\Pi = (T; \phi)$ such that $\phi^{-1}(u) \neq \emptyset$. Let e be an edge of $\mathcal{T}_\Pi$ incident with u, and let $B \in \sigma_e$ such that $\phi^{-1}(u) \subseteq B$. Then there exists some $\pi \in \Pi$ such that $B \in \pi$.*

Proof. Let $A|B$ be the X-split corresponding to e, where $\phi^{-1}(u) \subseteq B$. Since $\Sigma(\mathcal{T}_\Pi) = \Sigma_\Pi$, it follows that there is a partition π in Π such that either $A \in \pi$ or $B \in \pi$. Suppose that $A \in \pi$, but $B \notin \pi$. Then $|\pi| \geq 3$, and there exists a part $D \in \pi$ such that $\phi^{-1}(u) \subseteq D$. Hence, $A \cap D = \emptyset$ and $A \cup D \neq X$. Since π is displayed by $\mathcal{T}_\Pi$ and $D \in \pi$, there exists some edge e' of $\mathcal{T}_\Pi$ such that $\sigma_{e'} = D|X - D$. But then either e' is an edge in the connected component Z of $\mathcal{T}_\Pi \backslash e$ that contains u or e' is contained in the other component Z' of $\mathcal{T}_\Pi \backslash e$. In the former case it follows that $A \subsetneq D$ and so $A \cap D \neq \emptyset$, which is impossible. Thus, e' is an edge in Z'. But then the connected component of $\mathcal{T}_\Pi \backslash e'$ that contains u must contain Z. Since $\phi^{-1}(u) \subseteq B \cap D$, it follows that $B \subseteq D$ and thus $X = A \cup B \subseteq A \cup D \neq X$, which is also impossible. Thus $B \in \pi$. ∎

LEMMA 3.2. *Let Π be a compatible partition system on X, and let π be an element* *of* Π. *Let* E_π *be a subset of edges of* $\mathcal{T}_\Pi = (T;\phi)$ *that displays* π. *Then the following hold.*

(i) *Denoting by* $V_1, V_2, \ldots, V_k$, $k \geq 1$, *the vertex sets of the components of* $\mathcal{T}_\Pi \backslash E_\pi$, *we have that* $k = |\pi| + 1$ *and*

$$\{\phi^{-1}(V_1), \phi^{-1}(V_2), \ldots, \phi^{-1}(V_k)\} = \pi \cup \{\emptyset\}.$$

(ii) *For every pair of labelled vertices* u *and* v *of* $\mathcal{T}_\Pi$, *the path joining* u *to* v *contains exactly zero or two edges of* E_π.

Proof. We first assume that $|\pi| = 2$, that is, $\pi = A|B$ for some split $A|B$ of X. Let E_π be a subset of edges of $\mathcal{T}_\Pi$ that displays π. Then E_π consists of two distinct edges $e_1 = \{u_1', u_1\}$ and $e_2 = \{u_2', u_2\}$ such that $\sigma_{e_1} = A|B = \sigma_{e_2}$. By swapping u_1' and u_1, and u_2' and u_2 if necessary, we may assume that u_1' and u_2' are not contained in the shortest path P between u_1 and u_2. Moreover, since $\sigma_{e_1} = \sigma_{e_2}$, each vertex of P, including u_1 and u_2, is unlabelled and has degree two. Hence the lemma holds for this case.

Next assume that $|\pi| \geq 3$. Suppose $e \in E_\pi$ and $B \in \sigma_e$ with $B \in \pi$. Let v_B denote the end-vertex of e that is contained in the connected component of $\mathcal{T}_\Pi \backslash e$ which contains some (and thus all) $u \in V(T)$ such that $\phi^{-1}(u) \subseteq B$. Since π is a partition of X, there is no edge in E_π on the path from v_B to a vertex w such that $\phi^{-1}(w) \subseteq B$. As π is a partition of X, part (i) of the Lemma 3.2 now follows.

For the proof of part (ii), let u and v be distinct labelled vertices of $\mathcal{T}_\Pi$. Suppose that the path from u to v contains (in order) three edges e_1, e_2, and e_3 of E_π. Since $|\pi| \geq 3$, the splits $A_1|B_1$, $A_2|B_2$, and $A_3|B_3$ corresponding to e_1, e_2, and e_3, respectively, are distinct. Without loss of generality, we may assume that $A_1 \subset A_2 \subset A_3$. But then $B_1 \cap A_2$ is nonempty, and $B_2 \cap A_3$ is nonempty. Since, for each $i \in \{1, 2, 3\}$, at least one of A_i and B_i must be contained in π, it follows that π is not a partition of X, a contradiction. Thus the path from u to v contains at most two edges of E_π.

Now suppose that the path from u to v contains exactly one edge e_1 of E_π. Let $A_1|B_1$ be the split corresponding to e_1. Without loss of generality, we may assume that $\phi^{-1}(u) \subseteq A_1$ and $A_1 \in \pi$. Then $\phi^{-1}(v) \cap A_1 = \emptyset$. Now $|E_\pi| \geq 3$, and no edge in $E_\pi - \{e_1\}$ is on the path from u to v. It follows that, for all edges $e' \in E_\pi - \{e_1\}$, the component of $\mathcal{T}_\Pi \backslash e'$ that contains v also contains u. In particular, there is a part in π that contains $\phi^{-1}(u) \cup \phi^{-1}(v)$, a contradiction as $\phi^{-1}(u) \subseteq A_1$ and $\phi^{-1}(v) \cap A_1 = \emptyset$. This completes the proof of (ii) and thus the proof of the lemma. ∎

For a tree T, the *diameter* of T, denoted $\Delta(T)$, is

$$\Delta(T) = \max\{d_T(u, v) : u \text{ and } v \text{ are leaves of } T\}.$$

The following corollary is an immediate consequence of Lemma 3.2(ii) and gives a lower bound on the size of a partition in $\mathbb{P}(\Sigma)$ for Σ compatible in terms of the tree corresponding to Σ.

COROLLARY 3.3. *Let* Σ *be a compatible split system on* X, *and let* $\Pi \in \mathbb{P}(\Sigma)$. *Then*

$$\Delta(\mathcal{T}_\Sigma) \leq 2|\Pi|.$$

4. A characterization of compatibility. In this section, for a given split system Σ on X, we characterize when there exists a partition system Π on X such that $\Sigma_\Pi = \Sigma$ (i.e., when $\mathbb{P}(\Sigma)$ is nonempty). We begin by presenting some definitions.

A 2-*coloring* of a graph G is a bipartition of the vertex set of G such that no two vertices in a part are joined by an edge. An *even X-tree* $\mathcal{T} = (T; \phi)$ is a weak X-tree with the additional property that $d_{\mathcal{T}}(\phi(x), \phi(y))$ is even for all $x, y \in X$. Let v be a vertex of an even X-tree $\mathcal{T} = (T, \phi)$. Then v is *even* if there is a leaf l in $\mathcal{T}$ such that $d_{\mathcal{T}}(v, l)$ is even; otherwise, v is *odd*. Note that all leaves of $\mathcal{T}$ are even and that we treat the number zero as an even number. We denote by $V_{\text{even}}(\mathcal{T})$ the subset of even vertices of $\mathcal{T}$ and by $V_{\text{odd}}(\mathcal{T})$ the subset of odd vertices of $\mathcal{T}$.

LEMMA 4.1. *Let $\mathcal{T}$ be an even X-tree. Then*

(i) *all labelled vertices of $\mathcal{T}$ are even, and*

(ii) *the even and odd vertices of $\mathcal{T}$ induce a* 2*-coloring of $\mathcal{T}$.*

Proof. Part (i) follows immediately from the definition of an even X-tree. For part (ii), it is easily checked that every edge is incident with exactly one even vertex and one odd vertex, and so the even and odd vertices induce a 2-coloring of $\mathcal{T}$. ∎

Let $\mathcal{T} = (T; \phi)$ be a weak X-tree, and let v be an unlabelled vertex of $\mathcal{T}$. Then the partition of X *displayed* by v is precisely the partition π in which two elements $x, y \in X$ are in the same part of π if and only if the path from $\phi(x)$ to $\phi(y)$ does not pass through v. We denote this partition by $\pi(v)$. Note that the degree of v equals $|\pi(v)|$. Moreover, for a graph G and a vertex $v \in V(G)$, we denote by $G \backslash v$ the graph obtained from G by deleting v and all its incident edges.

THEOREM 4.2. *Let Σ be a compatible split system on X. Then the following statements are equivalent:*

(i) *$\mathcal{T}_\Sigma$ is even.*

(ii) *There exists a partition system Π on X such that $\Sigma_\Pi = \Sigma$.*

(iii) *There exists a strongly compatible partition system Π_s on X such that $\Sigma_{\Pi_s} = \Sigma$.*

Furthermore, if (iii) *holds, then*

$$\Pi_s = \{\pi(v) : v \in V_{\text{odd}}(\mathcal{T}_\Sigma)\}$$

is the unique strongly compatible partition system with $\Sigma_{\Pi_s} = \Sigma$.

Proof. Evidently, (iii) implies (ii). To see that (ii) implies (i), suppose that Π is a partition system on X such that $\Sigma_\Pi = \Sigma$. Let $\mathcal{T}_\Sigma = (T, \phi)$, and let $x, y \in X$. Then $d_{\mathcal{T}_\Sigma}(\phi(x), \phi(y))$ is equal to the number of splits S in Σ_Π for which x and y are in different parts of S. By Lemma 3.2, each partition in Π contributes either zero or two such splits. Thus $d_{\mathcal{T}_\Sigma}(\phi(x), \phi(y))$ is even, and, hence, $\mathcal{T}_\Sigma$ is even.

We next show that (i) implies (iii). Suppose that $\mathcal{T}_\Sigma = (T, \phi)$ is even, and set $V_{\text{odd}} = V_{\text{odd}}(\mathcal{T}_\Sigma)$. By Lemma 4.1(i), V_{odd} contains no labelled vertex of $\mathcal{T}_\Sigma$. Let

$$\Pi_s = \{\pi(v) : v \in V_{\text{odd}}\}.$$

By Lemma 4.1(ii), every edge of $\mathcal{T}_\Sigma$ is incident with exactly one vertex in V_{odd}, and so it follows that $\Sigma_{\Pi_s} = \Sigma$. Furthermore, let v_1 and v_2 be distinct vertices in V_{odd}. Let V_2 (resp., V_1) be the vertex set of the component of $\mathcal{T}_\Sigma \backslash v_1$ (resp., $\mathcal{T}_\Sigma \backslash v_2$) that contains v_2 (resp., v_1). Then $\phi^{-1}(V_2) \in \pi(v_1)$ and $\phi^{-1}(V_1) \in \pi(v_2)$, and $\phi^{-1}(V_2) \cup \phi^{-1}(V_1) = X$. Thus Π_s is strongly compatible. This completes the proof that (i) implies (iii) and thus the proof of the equivalence of (i)–(iii).

To establish the uniqueness part of the theorem, let Π be a strongly compatible partition system on X such that $\Sigma_\Pi = \Sigma$. Let l be a leaf of $\mathcal{T}_\Sigma$, and let u be the unique vertex of $\mathcal{T}_\Sigma$ adjacent to l. Since $\mathcal{T}_\Sigma$ is even, it follows by Lemma 4.1(ii) that u is odd and so $\phi^{-1}(u) = \emptyset$. We next show that $\pi(u) \in \Pi$.

Suppose that $\pi(u) \notin \Pi$. Let $\pi(u) = \{A_1, A_2, \dots, A_t\}$, where $t \geq 2$, and, for all $i \in \{1, \dots, t\}$, denote by e_i the edge e of $\mathcal{T}_\Sigma$ incident with u such that $\sigma_e = A_i|X - A_i$ holds. Without loss of generality, we may assume that $A_1 = \phi^{-1}(l)$. By Lemma 3.1, there is a partition $\pi_1 \in \Pi$ such that $A_1 \in \pi_1$. Consider π_1. Since $A_1 \in \pi_1$, it follows by Lemma 3.2(ii) that each path joining l to another leaf of $\mathcal{T}_\Sigma$ contains exactly two edges of any subset E_{π_1} of edges of $\mathcal{T}_\Sigma$ displaying π_1. As no other part of π_1 contains A_1, it follows that π_1 is a refinement[1] of $\pi(u)$. Since $\pi(u) \notin \Pi$ and thus $\pi_1 \neq \pi(u)$, this implies that, for some $i \in \{2, 3, \dots, t\}$, the part A_i is the disjoint union of at least two parts in π_1. Without loss of generality, we may assume that $i = t$. Since A_t is the disjoint union of at least two parts in π_1, there is a partition, π_2 say, in Π with π_2 distinct from π_1 such that a subset E_{π_2} of edges of $\mathcal{T}$ that displays π_2 contains e_t. In particular, either $A_t \in \pi_2$ or $(X - A_t) \in \pi_2$.

We first show that $A_t \notin \pi_2$. Assume that $A_t \in \pi_2$ holds. Then independent of the size of π_2 we must have that the degree of u cannot be two as otherwise $\pi_2 = \pi(u)$ would follow, a contradiction. We next distinguish between $|\pi_2| \geq 3$ and $|\pi_2| = 2$. If $|\pi_2| \geq 3$, then there exists some $B \in \pi_2$ distinct from A_t such that $\phi^{-1}(l) \subseteq B$. Let e_B denote an edge of $\mathcal{T}$ that displays the split $B|(X - B)$ which must exist as $\pi_2 \in \Pi$. Note that $B \neq A_1$ as otherwise, since $A_1 \in \pi_1$, $B \in \pi_2$, and $\pi_1 \neq \pi_2$, the multiplicity of the split $B|X - B$ in Σ_Π is at least 2. But then the degree of u is two, which is impossible. Consequently, $e_B \neq e_1$. Moreover, since $|\pi_2| \geq 3$, it follows that $B = A_t$ or $B = X - A_t$ cannot hold either and so $e_B \neq e_t$. Thus the path from l to any vertex a of $\mathcal{T}_\Sigma$ with $\phi^{-1}(a) \subseteq A_t$ holding does not cross the edge e_B. Combining this with the fact that $A_1 = \phi^{-1}(l) \subseteq B$, it follows that $A_1 \cup A_t \subseteq B$, which is impossible as A_t and B are distinct parts of π_2. Thus, $|\pi_2| \geq 3$ cannot hold. If $|\pi_2| = 2$, then $\pi_2 = \{A_t, B\}$ and so π_1 is a refinement of π_2. But then π_1 and π_2 cannot be strongly compatible, a contradiction. Thus, $|\pi_2| = 2$ cannot hold either. Consequently, $A_t \notin \pi_2$, as required.

Now assume that $(X - A_t) \in \pi_2$. Since, as seen above, $A_t \notin \pi_2$, it follows that A_t is the disjoint union of at least two parts in π_2. By the choice of A_t as the union of at least two parts in π_1, it follows that π_1 and π_2 are not strongly compatible, a contradiction. Hence $\pi(u) \in \Pi$, as required.

We complete the uniqueness part of the proof using induction on $k = |\Sigma|$. If $k = 2$, then there is exactly one partition system Π such that $\Sigma_\Pi = \Sigma$, and the uniqueness result follows. Now suppose that $k \geq 3$ and the uniqueness result holds for all compatible split systems Σ' on X for which $\mathcal{T}_{\Sigma'}$ is an even X-tree and $|\Sigma'| \leq k-1$.

Let Π be a strongly compatible partition system on X such that $\Sigma_\Pi = \Sigma$. Let l be a leaf of $\mathcal{T}_\Sigma$, and let u be the vertex of $\mathcal{T}_\Sigma$ adjacent to l. By above, $\pi(u) \in \Pi$. Let $\Sigma' = \Sigma - \Sigma_{\pi(u)}$. Then Σ' is compatible, $|\Sigma'| \leq k - 1$, and $\mathcal{T}_{\Sigma'}$ is an even X-tree as it corresponds to the weak X-tree obtained from $\mathcal{T}_\Sigma$ by contracting all edges incident with u and labelling the resulting vertex with the union of the label sets of the vertices previously adjacent to u. Therefore, by the induction assumption,

$$\Pi'_s = \{\pi(v) : v \in V_{\text{odd}}(\mathcal{T}_{\Sigma'})\}$$

is the unique strongly compatible partition system on X for which $\Sigma_{\Pi'_s} = \Sigma'$. Therefore, as

$$V_{\text{odd}} - V_{\text{odd}}(\mathcal{T}_{\Sigma'}) = \{u\},$$

[1]A partition π' of X is called a *refinement* of a partition π on X if every part of π' is a subset of a part of π.

it follows that $\Pi = \Pi'_s \uplus \{\pi(u)\} = \Pi_s$. Thus the uniqueness property holds for Σ. This completes the proof of the theorem. ∎

Let $\mathcal{T}$ be a weak X-tree, and let e be an edge of $\mathcal{T}$. We denote by $\mathcal{T}/e$ the weak X-tree obtained from $\mathcal{T}$ by contracting e and labelling the new identified vertex with the union of the labels of the end vertices of e. If F is a subset of the edges of $\mathcal{T}$, then $\mathcal{T}/F$ denotes the weak X-tree obtained from $\mathcal{T}$ by contracting each of the edges in F in this way, where, of course, the order of contraction is of no relevance.

The next result sheds light on the structure of weak X-trees obtained from even X-trees by contracting edges. Its proof follows from Lemma 3.2(ii) and is omitted.

Lemma 4.3. *Let $\mathcal{T}$ be an even X-tree, and let π be a partition of X displayed by $\mathcal{T}$. Let F be a subset of edges of $\mathcal{T}$ that displays π. Then $\mathcal{T}/F$ is an even X-tree.*

The following corollary may be viewed as the converse of Lemma 3.2(ii).

Corollary 4.4. *Let $\mathcal{T}$ be an even X-tree, and let F be a nonempty subset of edges of $\mathcal{T}$ with the property that, for every pair of labelled vertices u and v, the path joining u and v contains exactly zero or two edges of F. Then there are a partition system $\Pi \in \mathbb{P}(\mathcal{T})$ and a partition $\pi \in \Pi$ such that F displays π.*

Proof. Let $F = \{f_1, f_2, \dots, f_t\}$, $t \geq 2$, and let $i \in \{1, 2, \dots, t\}$. Let $\mathcal{T} = (T, \phi)$, and consider $\mathcal{T}\backslash f_i$. Since there are exactly two edges in F on the path between a leaf in one component of $\mathcal{T}\backslash f_i$ and a leaf in the other component, one of the components contains no edges in F. For each i, let V_i denote the vertex set of the component of $\mathcal{T}\backslash f_i$ containing no edges in F.

We now show that

$$\pi = \{\phi^{-1}(V_1), \phi^{-1}(V_2), \dots, \phi^{-1}(V_t)\}$$

is a partition of X. If not, then there is a labelled vertex, w say, such that the component of $\mathcal{T}\backslash F$ that contains w in its vertex set is not contained in $\{V_1, V_2, \dots, V_t\}$. But then, in the path from w to a leaf in any one of the components $V_1, V_2, \dots, V_t$, there is exactly one edge in F, a contradiction. Thus π is a partition of X.

To see that there is a partition system in $\mathbb{P}(\mathcal{T})$ containing π, observe that, by Lemma 4.3, $\mathcal{T}/F$ is an even X-tree, and so, by Theorem 4.2, there is a partition system Π' on X such that $\Sigma_{\Pi'} = \Sigma(\mathcal{T}/F)$, that is, $\Pi' \in \mathbb{P}(\mathcal{T}/F)$. By Lemma 2.3(i), it now follows that $\Pi' \uplus \{\pi\}$ is a partition system in $\mathbb{P}(\mathcal{T})$. ∎

5. Maximum-sized partition systems.

In this section, for a compatible split system Σ on X, we show that the unique strongly compatible partition system in $\mathbb{P}(\Sigma)$ is a partition system in $\mathbb{P}(\Sigma)$ of maximum size.

We begin by proving a lemma for which we require some additional notation. Let T be a tree with at least two leaves. We denote by $V_{\text{int}}(T)$ the set of interior vertices of T. Suppose "odd" and "even" are the colors of a 2-coloring of T. Extending our notation for even X-trees, we denote the sets of vertices of T colored "odd" and "even" by $V_{\text{odd}}(T)$ and $V_{\text{even}}(T)$, respectively. Furthermore, we denote the sets of interior vertices of T colored "odd" and "even" by $(V_{\text{int}})_{\text{odd}}(T)$ and $(V_{\text{int}})_{\text{even}}(T)$, respectively.

Lemma 5.1. *Let T be a tree with at least two leaves, and suppose that we have a 2-coloring of the vertex set of T using the set* {odd, even}. *Then*

$$|V_{\text{odd}}(T)| \geq |(V_{\text{int}})_{\text{even}}(T)| + 1.$$

Proof. The proof is by induction on the size m of the vertex set of T. If $m = 2$, then a routine check shows that the lemma holds. Now suppose that $m \geq 3$ and the result holds for all trees with fewer than m vertices. Let v be a leaf of T, and let T'

be the tree obtained from T by deleting v and the edge incident with it. For ease of presentation, set $V_{\rm odd} = V_{\rm odd}(T)$, $V'_{\rm odd} = V'_{\rm odd}(T)$, $(V_{\rm int})_{\rm even} = (V_{\rm int})_{\rm even}(T)$, and $(V'_{\rm int})_{\rm even} = (V_{\rm int})_{\rm even}(T')$. Since $|V(T')| < m$ and the given 2-coloring of T induces a 2-coloring of T', it follows by the induction assumption that

$$|V'_{\rm odd}| \geq |(V'_{\rm int})_{\rm even}| + 1. \tag{5.1}$$

Let t and t' denote the size of the leaf sets of T and T', respectively, and let u denote the unique vertex adjacent to v in T. We divide the rest of the proof into two cases depending upon whether $t' = t - 1$, in which case the degree of u in T is at least three, or $t' = t$, in which case the degree of u in T is two. If $t' = t - 1$, then $V_{\rm int}(T) = V_{\rm int}(T')$. Therefore, by (5.1),

$$|V_{\rm odd}| \geq |V'_{\rm odd}| \geq |(V'_{\rm int})_{\rm even}| + 1 = |(V_{\rm int})_{\rm even}| + 1,$$

and the lemma holds.

Now suppose that $t' = t$. If v is colored even, then $(V_{\rm int})_{\rm even} = (V'_{\rm int})_{\rm even}$ and so, by (5.1),

$$|V_{\rm odd}| \geq |V'_{\rm odd}| \geq |(V'_{\rm int})_{\rm even}| + 1 = |(V_{\rm int})_{\rm even}| + 1.$$

So we may assume that v is colored odd. Then $|(V_{\rm int})_{\rm even}| = |(V'_{\rm int})_{\rm even}| + 1$ and $|V_{\rm odd}| = |V'_{\rm odd}| + 1$. Combining these two equations with (5.1), it follows that

$$|V_{\rm odd}| = |V'_{\rm odd}| + 1 \geq |(V'_{\rm int})_{\rm even}| + 2 = |(V_{\rm int})_{\rm even}| + 1.$$

This completes the proof of the lemma. $\square$

Denoting for a vertex v of a graph the degree of v by $\deg(v)$, we are now ready to give the aforementioned characterization.

THEOREM 5.2. *Let Π be a compatible partition system on X, and let Π_s be the unique strongly compatible partition system in $\mathbb{P}(\Sigma_\Pi)$. Then $|\Pi'| \leq |\Pi_s|$ for all $\Pi' \in \mathbb{P}(\Sigma_\Pi)$.*

Proof. Let $\Pi' \in \mathbb{P}(\Sigma_\Pi)$ and $\pi_1 \in \Pi'$. Let Π'_1 denote $\Pi' - \{\pi_1\}$. Since $\mathcal{T}_\Pi \cong \mathcal{T}_{\Pi'}$ and, by Lemma 2.3(ii), $\Sigma_{\Pi'} = \Sigma_{\Pi - \{\pi_1\}} = \Sigma_\Pi - \Sigma_{\pi_1}$ holds, it follows that $\mathcal{T}_{\Pi'_1} \cong \mathcal{T}_\Pi / E_{\pi_1}$, where E_{π_1} is a subset of edges of $\mathcal{T}_\Pi$ that displays π_1. Since, by Theorem 4.2, $\mathcal{T}_\Pi$ is even, Lemma 4.3 implies that $\mathcal{T}_{\Pi'_1}$ is even. Set $V_{\rm odd} = V_{\rm odd}(\mathcal{T}_\Pi)$ and $(V'_1)_{\rm odd} = V_{\rm odd}(\mathcal{T}_{\Pi'_1})$. We next show that

$$|V_{\rm odd}| \geq |(V'_1)_{\rm odd}| + 1 \tag{5.2}$$

holds, which will be crucial for an inductive argument on the edge set of $\mathcal{T}_\Pi$ which will allow us to establish the theorem.

To observe (5.2), let $V_1, V_2, \ldots, V_t$ denote the vertex sets of the components of $\mathcal{T}_\Pi \backslash E_{\pi_1}$. By Lemma 3.2(i), precisely one of these vertex sets has the property that no vertex is labelled. Without loss of generality, we may assume that this vertex set is V_t. We consider two cases depending on the size of V_t. Suppose first that $|V_t| = 1$, and let $V_t = \{u\}$. If u is odd, then each of the $\deg(u)$ vertices adjacent to u is even, and it follows that $(V'_1)_{\rm odd}$ has exactly one less vertex than $V_{\rm odd}$. In particular, (5.2) holds. If u is even, then each of the $\deg(u)$ vertices adjacent to u is odd. Therefore

$$|V_{\rm odd}| = |(V'_1)_{\rm odd}| + \deg(u) - 1.$$

But $\deg(u) - 1 \geq 1$ as $\deg(u) \geq 2$, and so (5.2) holds.

Now suppose that $|V_t| \geq 2$. Let $\mathcal{T}_t$ be the subtree of $\mathcal{T}_\Pi$ induced by V_t, and let $\mathcal{T}_t^+$ be the subtree of $\mathcal{T}_\Pi$ whose edge set is precisely $E(\mathcal{T}_t) \cup E_{\pi_1}$. Let $(V_t)_{\text{even}} = V_{\text{even}}(\mathcal{T}_t)$ and $(V_t^+)_{\text{odd}} = V_{\text{odd}}(\mathcal{T}_t^+)$. Then

$$|(V_1')_{\text{odd}}| = |(V_t)_{\text{even}}| + \big(|V_{\text{odd}}| - |(V_t^+)_{\text{odd}}|\big),$$

and therefore

$$|V_{\text{odd}}| - |(V_1')_{\text{odd}}| = |(V_t^+)_{\text{odd}}| - |(V_t)_{\text{even}}|.$$

Since $(V_{\text{int}})_{\text{even}}(\mathcal{T}_t^+) = (V_t)_{\text{even}}$, we have $|(V_t^+)_{\text{odd}}| - |(V_t)_{\text{even}}| \geq 1$ by Lemma 5.1, and so (5.2) follows.

Having established (5.2), we complete the proof of the theorem by induction on the size of the edge set E_Π of $\mathcal{T}_\Pi$. If $|E_\Pi| = 2$, then Π is the unique partition system in $\mathbb{P}(\Sigma_\Pi)$. In particular, Π is the unique strongly compatible partition system in $\mathbb{P}(\Sigma_\Pi)$, and so the theorem holds. Now assume that the theorem holds for all compatible partition systems whose corresponding even X-tree has fewer edges than $\mathcal{T}_\Pi$. Let Π', π_1, and Π_1' be as defined at the beginning of the proof. Then, as observed there, $\mathcal{T}_{\Pi_1'}$ must be even. By Theorem 4.2, $\mathbb{P}(\Sigma_{\Pi_1'})$ must contain a unique strongly compatible partition system $(\Pi_1')_s$ on X. But then $|\Pi_1'| \leq |(\Pi_1')_s|$, by the induction assumption. Combining this with (5.2) and Theorem 4.2, which implies that $|V_{\text{odd}}| = |\Pi_s|$ and $|(V_1')_{\text{odd}}| = |(\Pi_1')_s|$ hold, we obtain

$$|\Pi'| = |\Pi_1'| + 1 \leq |(\Pi_1')_s| + 1 = |(V_1')_{\text{odd}}| + 1 \leq |V_{\text{odd}}| = |\Pi_s|.$$

This completes the proof of the theorem. ∎

As we have seen in the example presented in the introduction, for a compatible split system Σ with $\mathbb{P}(\Sigma) \neq \emptyset$, the strongly compatible partition system in $\mathbb{P}(\Sigma)$ is not necessarily the only partition system in $\mathbb{P}(\Sigma)$ of maximum size. For such Σ, it could therefore be of interest to try to characterize the set of partition systems in $\mathbb{P}(\Sigma)$ of maximum size. In regard to this, it is worth noting that, in the case when Σ is a compatible set of splits corresponding to a phylogenetic X-tree with all interior vertices of degree three, it is not difficult to show that there is a unique partition system in $\mathbb{P}(\Sigma)$ of maximum size, namely the strongly compatible partition system.

6. Constructing minimum-sized partition systems. We now turn our attention to the problem of understanding minimum elements in the set $\mathbb{P}(\Sigma)$ for a compatible split system Σ. More specifically, we construct, for an even X-tree $\mathcal{T}$, a $\mathbb{P}(\mathcal{T})$-*minimum* partition system on X, that is, a partition system Π on X such that $\Sigma(\mathcal{T}) = \Sigma_\Pi$ and Π is of minimum size with respect to this property. The construction is presented in the form of the MinSizePartition algorithm in Figure 2. It will make use of the following decomposition of a weak X-tree.

Let $\mathcal{T} = (T; \phi)$ be a weak X-tree with edge set E, and let v be a labelled interior vertex of $\mathcal{T}$. Suppose that v has degree $k \geq 2$. Now partition E so that, for all edges e and f, we have e and f in the same part if and only if the path from e to f in $\mathcal{T}$ avoids v. Let $\{E_1, E_2, \ldots, E_k\}$ denote the resulting partition on E. For each $i \in [k] = \{1, \ldots, k\}$, $k \geq 2$, let e_i denote the unique edge in E_i incident with v in $\mathcal{T}$, and let $A_i|B_i$ denote the X-split corresponding to e_i, where $\phi^{-1}(v) \subseteq B_i$. For each $i \in [k]$, let $\mathcal{T}_i$ denote the weak X-tree induced by E_i, where the label of every vertex of $\mathcal{T}$ is retained except for v, whose label changes to B_i. The collection $\{\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_k\}$

MinSizePartition($\mathcal{T}$)

Input: An even X-tree $\mathcal{T}$.
Output: A partition system $\Pi_{\min}(\mathcal{T})$ on X that is $\mathbb{P}(\mathcal{T})$-minimum.

If there exists an interior vertex v in $\mathcal{T}$ that is labelled
    Construct the decomposition $\mathcal{D}(\mathcal{T}, v)$, say $\{\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_k\}$, of $\mathcal{T}$
    For each $i \in [k]$, call MinSizePartition($\mathcal{T}_i$)
    Return $\Pi_{\min}(\mathcal{T}) \leftarrow \Pi_{\min}(\mathcal{T}_1) \biguplus \Pi_{\min}(\mathcal{T}_2) \biguplus \cdots \biguplus \Pi_{\min}(\mathcal{T}_k)$
Else, set $\pi_{\min} = \pi_{\min}(\mathcal{T})$ and set $\Sigma' = \Sigma(\mathcal{T}) - \Sigma_{\pi_{\min}}$
    If Σ' is nonempty
        Construct the even X-tree $\mathcal{T}'$ for which $\Sigma(\mathcal{T}') = \Sigma'$
        Call MinSizePartition($\mathcal{T}'$)
        Return $\Pi_{\min}(\mathcal{T}) \leftarrow \{\pi_{\min}\} \biguplus \Pi_{\min}(\mathcal{T}')$
    Else
        Return $\Pi_{\min}(\mathcal{T}) \leftarrow \{\pi_{\min}\}$
    Endif
Endif

Fig. 2. *Pseudocode for* MinSizePartition.

is called the *decomposition of $\mathcal{T}$ with respect to v* and is denoted by $\mathcal{D}(\mathcal{T}, v)$. To illustrate the decomposition, consider the even X-tree $\mathcal{T}$ shown in Figure 3, where $X = \{1, 2, 3, 4, 5, 6, 7\}$. The decomposition of $\mathcal{T}$ with respect to the vertex labelled 3 is shown in the right-hand side of the figure.

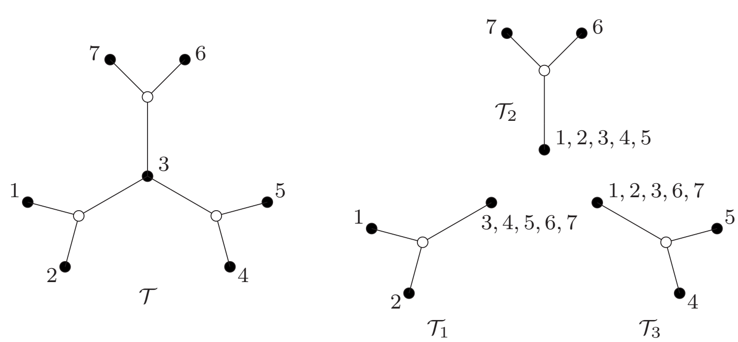

Fig. 3. *A weak X-tree $\mathcal{T}$ with $X = \{1, 2, \ldots, 7\}$ (left) and the decomposition $\{\mathcal{T}_1, \mathcal{T}_2, \mathcal{T}_3\}$ of $\mathcal{T}$ with respect to the vertex labelled 3 (right). Filled vertices denote labelled vertices.*

Two observations that we freely use in the rest of this section are the following. First,

$$\Sigma(\mathcal{T}) = \Sigma(\mathcal{T}_1) \uplus \Sigma(\mathcal{T}_2) \uplus \cdots \uplus \Sigma(\mathcal{T}_k),$$

and, for all distinct $i, j \in [k]$, we have $\Sigma(\mathcal{T}_i) \cap \Sigma(\mathcal{T}_j) = \emptyset$. Second, if $\mathcal{T}$ is an even X-tree, then each of the weak X-trees $\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_k$ is even.

The next lemma will be used later in this section.

Lemma 6.1. *Let $\mathcal{T}$ be a weak X-tree, and let v be a labelled interior vertex of $\mathcal{T}$. Let $\mathcal{D}(\mathcal{T}, v) = \{\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_k\}$, and let Π be a partition system on X. Then $\Pi \in \mathbb{P}(\mathcal{T})$*

if and only if there is a partition $\{\Pi_1, \Pi_2, \ldots, \Pi_k\}$ *of* Π *such that, for all* $i \in [k]$*, we have* $\Pi_i \in \mathbb{P}(\mathcal{T}_i)$*. Moreover, if* $\Pi \in \mathbb{P}(\mathcal{T})$*, then such a partition of* Π *is unique.*

Proof. Suppose first that there is a partition $\{\Pi_1, \Pi_2, \ldots, \Pi_k\}$ of Π such that, for all $i \in [k]$, we have $\Pi_i \in \mathbb{P}(\mathcal{T}_i)$. Then, as

$$\Sigma(\mathcal{T}) = \Sigma(\mathcal{T}_1) \uplus \Sigma(\mathcal{T}_2) \uplus \cdots \uplus \Sigma(\mathcal{T}_k)$$

and $\Sigma_{\Pi_i} = \Sigma(\mathcal{T}_i)$ holds for all $i \in [k]$, Lemma 2.3 implies

$$\Pi = \Pi_1 \uplus \Pi_2 \uplus \cdots \uplus \Pi_k \in \mathbb{P}(\mathcal{T}).$$

Conversely, suppose that $\Pi \in \mathbb{P}(\mathcal{T})$. For each $i \in [k]$, let E_i denote the edge set of $\mathcal{T}_i$. Let $\pi \in \Pi$, and let E_π be a subset of edges of $\mathcal{T}$ that displays π. If E_π contains distinct edges e and f, then with $x \in e$ and $y \in f$ such that x and y lie on the path from $a \in e - \{x\}$ to $b \in f - \{y\}$, it is easily seen that the path from x to y avoids the labelled vertex v. In particular, $E_\pi \subseteq E_i$ for some $i \in [k]$. Furthermore, as $\Sigma(\mathcal{T}_i) \cap \Sigma(\mathcal{T}_j) = \emptyset$ for all distinct $i, j \in [k]$, there is a unique $i^* \in [k]$ for which $E_\pi \subseteq E_{i^*}$. Now let $\{\Pi_1, \Pi_2, \ldots, \Pi_k\}$ denote the unique partition of Π such that, for all $i \in [k]$, we have $\Sigma_{\Pi_i} \subseteq \Sigma(\mathcal{T}_i)$. But $\Sigma_\Pi = \Sigma(\mathcal{T})$, and so, for all $i \in [k]$, we have $\Sigma_{\Pi_i} = \Sigma(\mathcal{T}_i)$, that is, $\Pi_i \in \mathbb{P}(\mathcal{T}_i)$. This completes the proof of the lemma. ∎

For an even X-tree $\mathcal{T}$, we next present our construction MinSizePartition in the form of pseudocode and establish its correctness in Theorem 6.3. For example, for the even X-tree $\mathcal{T}$ depicted in Figure 1, the $\mathbb{P}(\mathcal{T})$-minimum partition system that we construct is the partition system Π_6 given in the introduction.

For a weak X-tree $\mathcal{T} = (T; \phi)$ in which all interior vertices are unlabelled, set $\pi_{\min}(\mathcal{T})$ to be the partition

$$\pi_{\min}(\mathcal{T}) = \{\phi^{-1}(v) : v \text{ is a leaf of } \mathcal{T}\}$$

of X. Note that $\Sigma_{\pi_{\min}(\mathcal{T})} \subseteq \Sigma(\mathcal{T})$ and that, for the even X-tree $\mathcal{T}$ depicted in Figure 1, we have $\pi_{\min}(\mathcal{T}) = \{1|2|3|4|5|6\}$.

To establish the correctness of MinSizePartition, we make use of the next lemma.

Lemma 6.2. *Let* $\mathcal{T}$ *be an even* X*-tree with no labelled interior vertices. Then there exists a* $\mathbb{P}(\mathcal{T})$*-minimum partition system that contains* $\pi_{\min}(\mathcal{T})$*.*

Proof. For convenience, set $\pi_{\min} = \pi_{\min}(\mathcal{T})$. If $A \in \pi_{\min}$, then, by Lemma 3.1, each partition system in $\mathbb{P}(\mathcal{T})$ contains a partition π with $A \in \pi$. Suppose that Π is a $\mathbb{P}(\mathcal{T})$-minimum partition system. We may assume that $\pi_{\min} \notin \Pi$. Let Π' be a minimum-sized subset of Π such that, for each $A \in \pi_{\min}$, there is a partition π' in Π' with $A \in \pi'$. Note that $\Sigma_{\Pi'} = \Sigma(\mathcal{T})$ need not hold. Without loss of generality, we may assume that Π' is a minimum-sized partition system contained in a $\mathbb{P}(\mathcal{T})$-minimum partition system with this property. We break the proof into two cases depending on whether or not Π' is a strongly compatible partition system on X.

First suppose that Π' is strongly compatible. Then $\Sigma_{\Pi'}$ is compatible, and so Theorem 4.2 implies that $\mathcal{T}_{\Sigma_{\Pi'}}$ is even. Let F denote the subset of edges of $\mathcal{T}_{\Sigma_{\Pi'}}$ that are incident with some leaf of $\mathcal{T}_{\Sigma_{\Pi'}}$. Then, for any two leaves u and v of $\mathcal{T}_{\Sigma_{\Pi'}}$, the path between u and v contains either zero or precisely two edges in F. Hence, by Corollary 4.4, there exists a partition system Π'' in $\mathbb{P}(\Sigma_{\Pi'})$ and a partition $\pi \in \Pi''$ that displays F. But now the definition of $\pi_{\min}$ implies that $\pi = \pi_{\min}$, and so $\pi_{\min} \in \Pi''$. Consider the partition system

$$\hat{\Pi} = (\Pi - \Pi') \uplus \Pi''.$$

Since $\Sigma_{\Pi'} = \Sigma_{\Pi''}$, it follows that $\hat{\Pi}$ is in $\mathbb{P}(\mathcal{T})$. As Π' is strongly compatible, it follows by Theorem 5.2 that $|\Pi''| \leq |\Pi'|$. Since $\Pi' \subseteq \Pi$ and Π is a $\mathbb{P}(\mathcal{T})$-minimum partition system, it follows that $|\Pi| = |\hat{\Pi}|$ and so $\hat{\Pi}$ is also a $\mathbb{P}(\mathcal{T})$-minimum partition system. Observing that $\pi_{\min} \in \hat{\Pi}$ completes the proof of the case when Π' is strongly compatible.

Now suppose that Π' is not strongly compatible. Then there exist distinct partitions π and π' in Π' that are not strongly compatible. This implies that $\pi \cup \pi'$ is a hierarchy. To see this, suppose that $\pi \cup \pi'$ is not a hierarchy. Then there exist $A \in \pi$ and $A' \in \pi'$ such that each of the sets $A \cap A'$, $A \cap (X - A')$, $(X - A) \cap A'$ is nonempty. Furthermore, $(X - A) \cap (X - A')$ is also nonempty as $A \cup A' \neq X$. But $\pi, \pi' \in \Pi$ and Π is compatible, so at least one of these intersections is empty, a contradiction.

Since $\pi \cup \pi'$ is a hierarchy, it follows that, for each $A \in \pi$, either A is a subset of a part in π' or A is the disjoint union of parts in π'. Similarly, for each $A' \in \pi'$, either A' is a subset of a part in π or A' is the disjoint union of parts in π. It now follows that there is a partition system $\{\pi_1, \pi_2\}$ on X such that $\Sigma_{\{\pi_1,\pi_2\}} = \Sigma_{\{\pi,\pi'\}}$, and, for all $B \in \pi_1$, we have that B is a subset of a part in π_2. Let

$$\Pi'' = (\Pi' - \{\pi, \pi'\}) \uplus \{\pi_1\}.$$

Clearly, $|\Pi''| = |\Pi'| - 1$. Furthermore, for each $A \in \pi_{\min}$, there exists, by assumption, a partition in Π' containing A, and so, for each $A \in \pi_{\min}$, there is a partition in Π'' containing A. Now consider the partition system

$$\hat{\Pi} = (\Pi - \Pi') \uplus \Pi'' \uplus \{\pi_2\} = (\Pi - \{\pi, \pi'\}) \uplus \{\pi_1, \pi_2\}.$$

Since $\Sigma_{\Pi} = \Sigma_{\hat{\Pi}}$, it follows that $\hat{\Pi}$ is in $\mathbb{P}(\mathcal{T})$. Therefore, as Π is $\mathbb{P}(\mathcal{T})$-minimum, $\hat{\Pi}$ is $\mathbb{P}(\mathcal{T})$-minimum. But $|\Pi''| < |\Pi'|$ and Π'' is a subset of $\hat{\Pi}$ with the property that, for each $A \in \pi_{\min}$, there is a partition in Π'' containing A, a contradiction. This completes the proof of the case that Π' is not strongly compatible. ∎

THEOREM 6.3. *Let $\mathcal{T}$ be an even X-tree. Then the partition system $\Pi_{\min}(\mathcal{T})$ returned by* MINSIZEPARTITION *applied to $\mathcal{T}$ is a $\mathbb{P}(\mathcal{T})$-minimum partition system.*

Proof. We prove the theorem by induction on the number m of interior vertices of $\mathcal{T}$. Since $\mathcal{T}$ is even, $m \geq 1$. If $m = 1$, then the unique interior vertex is adjacent to each leaf of $\mathcal{T}$. It now follows by Lemma 3.1 combined with the definition of $\pi_{\min}(\mathcal{T})$ that $\{\pi_{\min}(\mathcal{T})\}$ is the unique partition system in $\mathbb{P}(\mathcal{T})$, and so MINSIZEPARTITION correctly returns $\{\pi_{\min}(\mathcal{T})\}$.

Let $m \geq 2$, and assume that MINSIZEPARTITION correctly returns a $\mathbb{P}(\mathcal{T}')$-minimum partition system whenever it is applied to an even X-tree $\mathcal{T}'$ with fewer than m interior vertices. We distinguish two cases depending on whether or not $\mathcal{T}$ has a labelled interior vertex.

First suppose that $\mathcal{T}$ has a labelled interior vertex v. Without loss of generality, we may assume that, at the first iteration of MINSIZEPARTITION applied to $\mathcal{T}$, the algorithm constructs the decomposition

$$\mathcal{D}(\mathcal{T}, v) = \{\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_k\}$$

of $\mathcal{T}$ with respect to v, where k is the degree of v. Thus, to complete the proof of this case, it suffices to show that

$$\hat{\Pi} = \Pi_{\min}(\mathcal{T}_1) \uplus \Pi_{\min}(\mathcal{T}_2) \uplus \cdots \uplus \Pi_{\min}(\mathcal{T}_k)$$

is $\mathbb{P}(\mathcal{T})$-minimum, where, for all $i \in [k]$, $\Pi_{\min}(\mathcal{T}_i)$ is the partition system on X returned by MinSizePartition applied to the even X-tree $\mathcal{T}_i$.

Let $i \in [k]$. Then, as $\mathcal{T}_i$ has fewer interior vertices than $\mathcal{T}$, it follows by the induction assumption that $\Pi_{\min}(\mathcal{T}_i)$ is $\mathbb{P}(\mathcal{T}_i)$-minimum. One consequence of this fact is that $\Pi_{\min}(\mathcal{T}_i)$ is a partition system in $\mathbb{P}(\mathcal{T}_i)$. Combined with the definition of Π, Lemma 6.1 implies that $\hat{\Pi}$ is a partition system in $\mathbb{P}(\mathcal{T})$. Now if $\hat{\Pi}$ is not $\mathbb{P}(\mathcal{T})$-minimum, then there exists a partition system $\Pi \in \mathbb{P}(\mathcal{T})$ such that $|\Pi| < |\hat{\Pi}|$. By Lemma 6.1, there is a partition $\{\Pi_1, \Pi_2, \ldots, \Pi_k\}$ of Π such that, for all $i \in [k]$, we have $\Pi_i \in \mathbb{P}(\mathcal{T}_i)$. But $|\Pi| < |\hat{\Pi}|$, and so there exists some $j \in [k]$ such that $|\Pi_j| < |\Pi_{\min}(\mathcal{T}_i)|$ for some $i \in [k]$, a contradiction. Thus $\hat{\Pi}$ is $\mathbb{P}(\mathcal{T})$-minimum, as required.

Now suppose that $\mathcal{T}$ has no labelled interior vertex, and set $\pi_{\min} = \pi_{\min}(\mathcal{T})$ and $\Sigma' = \Sigma(\mathcal{T}) - \Sigma_{\pi_{\min}}$. Then if $\Sigma' \neq \emptyset$, the algorithm constructs the weak X-tree $\mathcal{T}'$ for which $\Sigma(\mathcal{T}') = \Sigma'$. Note that $\mathcal{T}' \cong \mathcal{T}/E$, where E is a set of edges of $\mathcal{T}$ that displays $\pi_{\min}$, and so, since $\mathcal{T}$ is an even X-tree, it follows by Lemma 4.3 that $\mathcal{T}'$ is in fact an even X-tree. For this case, it now suffices to show that

$$\hat{\Pi} = \{\pi_{\min}\} \uplus \Pi_{\min}(\mathcal{T}')$$

is $\mathbb{P}(\mathcal{T})$-minimum, where $\Pi_{\min}(\mathcal{T}')$ is the partition system on X returned by MinSizePartition applied to $\mathcal{T}'$.

Since $\mathcal{T}'$ has fewer interior vertices than $\mathcal{T}$, it follows by the induction assumption that $\Pi_{\min}(\mathcal{T}')$ is $\mathbb{P}(\mathcal{T}')$-minimum. This immediately implies that $\Pi_{\min}(\mathcal{T}')$ is a partition system in $\mathbb{P}(\mathcal{T}')$, and so $\hat{\Pi} \in \mathbb{P}(\mathcal{T})$. Now, by Lemma 6.2, there is a $\mathbb{P}(\mathcal{T})$-minimum partition system Π containing $\pi_{\min}$. Let $\Pi' = \Pi - \{\pi_{\min}\}$. By Lemma 2.3, $\Pi' \in \mathbb{P}(\mathcal{T}')$, and so $|\Pi_{\min}(\mathcal{T}')| \leq |\Pi'|$. Hence

$$|\hat{\Pi}| = |\Pi_{\min}(\mathcal{T}')| + 1 \leq |\Pi'| + 1 = |\Pi|.$$

Thus, as Π is $\mathbb{P}(\mathcal{T})$-minimum, we deduce that $|\Pi| = |\hat{\Pi}|$ and so $\hat{\Pi}$ must also be $\mathbb{P}(\mathcal{T})$-minimum, as required. This completes the proof of the second case and the theorem. ∎

7. Hierarchical partition systems. In the previous section we showed how to construct, for an even X-tree $\mathcal{T}$, a $\mathbb{P}(\mathcal{T})$-minimum partition system Π on X. It appears to be a difficult problem to characterize the set of $\mathbb{P}(\mathcal{T})$-minimum partition systems for arbitrary $\mathcal{T}$. However, in this section we shall show that in the case when $\mathcal{T}$ contains a vertex ρ that is the same distance from every leaf in $\mathcal{T}$, then we can characterize the $\mathbb{P}(\mathcal{T})$-minimum partition systems (Theorem 7.4). Note that such trees are sometimes called *equidistant* trees [17, p. 150].

The first result in this section shows that hierarchical partition systems are compatible.

Proposition 7.1. *Let Π be a hierarchical partition system on X. Then Π is compatible. Moreover, $\mathcal{T}_\Pi$ is isomorphic to $\mathcal{T}_\rho^-$, where $\mathcal{T}_\rho$ is the rooted weak X-tree with $\mathcal{H}(\mathcal{T}_\rho) = \biguplus_{\pi \in \Pi} \pi$.*

Proof. By Theorem 2.2, there is a unique rooted weak X-tree, $\mathcal{T}_\rho$ say, with $\mathcal{H}(\mathcal{T}_\rho) = \biguplus_{\pi \in \Pi} \pi$. This implies that $\Sigma(\mathcal{T}_\rho^-) = \Sigma_\Pi$. In particular, Π is compatible and $\mathcal{T}_\Pi$ is isomorphic to $\mathcal{T}_\rho^-$. ∎

The next result gives some properties of $\mathcal{T}_\Pi$ in the case when Π is a hierarchical partition system.

Corollary 7.2. *Let Π be a hierarchical partition system on X.*

(i) *If u is an interior vertex of $\mathcal{T}_\Pi$, then u is unlabelled.*

(ii) *There is a vertex ρ of $\mathcal{T}_\Pi$ such that, for all leaves u and v,*

$$d_{\mathcal{T}_\Pi}(\rho, u) = d_{\mathcal{T}_\Pi}(\rho, v) = |\Pi|.$$

Proof. To prove (i), let $\mathcal{T}_\Pi = (T_\Pi; \phi)$, and suppose that there is a labelled interior vertex u of $\mathcal{T}_\Pi$. Let $A = \phi^{-1}(u)$. By Lemma 3.1, for each edge incident with u, there is a distinct partition in Π with a part that properly contains A. Since u is an interior vertex, it has degree at least two, so there are at least two such partitions, π_1 and π_2 say. Let A_1 and A_2 be the parts of π_1 and π_2, respectively, that properly contain A. It is easily seen that neither $A_1 \subseteq A_2$ nor $A_2 \subseteq A_1$. But then, as $A \subseteq A_1 \cap A_2$ and A is nonempty, it follows that Π is not hierarchical, a contradiction. This completes the proof of (i).

For the proof of (ii), let $\mathcal{T}_\rho = (T_\rho; \phi)$ be the rooted weak X-tree with root ρ for which $\mathcal{H}(\mathcal{T}_\rho) = \biguplus_{\pi \in \Pi} \pi$. Let u be a leaf of $\mathcal{T}_\rho$. Now, the clusters displayed by the edges on the path from ρ to u are precisely the sets in $\biguplus_{\pi \in \Pi} \pi$ containing $\phi^{-1}(u)$. Since each partition in Π contains exactly one such set as a part, it follows that $d_{\mathcal{T}_\rho}(\rho, u) = |\Pi|$. By Proposition 7.1, this in turn implies that

$$d_{\mathcal{T}_\Pi}(\rho, u) = d_{\mathcal{T}_\Pi}(\rho, v)$$

for all leaves u and v of $\mathcal{T}_\Pi$, thereby completing the proof of (ii). ∎

We now characterize the compatible split systems Σ for which there exists some hierarchical partition system Π with $\Sigma_\Pi = \Sigma$.

THEOREM 7.3. *Let Σ be a compatible split system on X. Then there exists a hierarchical partition system $\Pi \in \mathbb{P}(\Sigma)$ if and only if $\mathcal{T}_\Sigma$ has a vertex ρ such that, for all labelled vertices u and v of $\mathcal{T}_\Sigma$,*

$$d_{\mathcal{T}_\Sigma}(\rho, u) = d_{\mathcal{T}_\Sigma}(\rho, v). \tag{7.1}$$

Proof. If there exists a hierarchical partition system $\Pi \in \mathbb{P}(\Sigma)$, then it follows by Corollary 7.2 that $\mathcal{T}_\Sigma$ has a vertex ρ such that, for all labelled vertices u and v of $\mathcal{T}_\Sigma$, we have

$$d_{\mathcal{T}_\Sigma}(\rho, u) = d_{\mathcal{T}_\Sigma}(\rho, v).$$

To prove the converse, suppose that $\mathcal{T}_\Sigma$ has such a vertex ρ. Then no interior vertex of $\mathcal{T}_\Sigma$ is labelled. Let d denote the distance from ρ to a leaf of $\mathcal{T}_\Sigma$. For each $i \in \{1, \ldots, d\}$, let E_i denote the subset of edges whose end-vertex farthest from ρ is at distance i to ρ. Note that $\{E_1, E_2, \ldots, E_d\}$ is a partition of $E(\mathcal{T}_\Sigma)$. Viewing $\mathcal{T}_\Sigma$ as a rooted weak X-tree with root ρ, let

$$\pi_i = \{C_e : e \in E_i\}$$

for each i. Since the leaves of $\mathcal{T}_\Sigma$ all have the same distance to ρ, it follows that π_i is a partition of X for all i. In particular,

$$\Pi_h = \biguplus_{i \in \{1,\ldots,d\}} \pi_i$$

is a partition system on X with $\Sigma_{\Pi_h} = \Sigma$. To see that Π_h is hierarchical, let $A_i \in \pi_i$ and $A_j \in \pi_j$, where $\pi_i, \pi_j \in \Pi_h$. If $i = j$, then either $A_i \cap A_j = \emptyset$ or $A_i = A_j$. Thus we may assume that $i \neq j$. Without loss of generality, we may further assume that

$i < j$. But then, again viewing $\mathcal{T}_\Sigma$ as a rooted weak X-tree with root ρ, it is easily seen that either $A_i \cap A_j = \emptyset$ or $A_i \cap A_j = A_j$ as $A_i = C_{e_i}$ and $A_j = C_{e_j}$ for some $e_i \in E_i$ and some $e_j \in E_j$, and $\mathcal{H}(\mathcal{T}_\Sigma) = \biguplus_{\pi \in \Pi_h} \pi$. Consequently, Π_h is hierarchical. This completes the proof of the converse and thereby the proof of the theorem. □

We conclude this section by characterizing, for a compatible split system Σ for which $\mathbb{P}(\Sigma)$ contains a hierarchical partition system, the $\mathbb{P}(\mathcal{T}_\Sigma)$-minimum partition systems.

THEOREM 7.4. *Let Σ be a compatible split system on X such that $\mathbb{P}(\Sigma)$ contains a hierarchical partition system, and let $\Pi \in \mathbb{P}(\Sigma)$. Then Π is hierarchical if and only if Π is $\mathbb{P}(\mathcal{T}_\Sigma)$-minimum.*

Proof. Note that, since $\mathbb{P}(\Sigma)$ contains a hierarchical partition system, it follows by Theorem 7.3 that $\mathcal{T}_\Sigma$ has a vertex ρ such that, for all leaves u and v in $\mathcal{T}_\Sigma$,

$$d_{\mathcal{T}_\Sigma}(\rho, u) = d_{\mathcal{T}_\Sigma}(\rho, v).$$

First suppose that Π is hierarchical. Then, since $\Pi \in \mathbb{P}(\Sigma)$ and thus $\mathcal{T}_\Sigma \cong \mathcal{T}_\Pi$, Corollary 7.2(ii) implies

$$\Delta(\mathcal{T}_\Sigma) = 2d_{\mathcal{T}_\Sigma}(\rho, u) = 2|\Pi|,$$

where u is a leaf of $\mathcal{T}_\Sigma$. But, by Corollary 3.3,

$$\Delta(\mathcal{T}_\Sigma) \leq 2|\Pi'|$$

for all partition systems $\Pi' \in \mathbb{P}(\Sigma)$. Thus $|\Pi| \leq |\Pi'|$ for all partition systems $\Pi' \in \mathbb{P}(\Sigma)$, and so Π is $\mathbb{P}(\mathcal{T}_\Sigma)$-minimum.

We prove the converse by establishing that if Π is not hierarchical, then Π is not $\mathbb{P}(\mathcal{T}_\Sigma)$-minimum. Suppose that Π is not hierarchical. Then there exist distinct $\pi_1, \pi_2 \in \Pi$ with $A_1 \in \pi_1$ and $A_2 \in \pi_2$ such that $A_1 \cap A_2 \notin \{\emptyset, A_1, A_2\}$. Let $\mathcal{T}_\Sigma^\rho$ denote the rooted weak X-tree obtained by viewing $\mathcal{T}_\Sigma$ rooted at ρ. Since $A_1 \cap A_2 \notin \{\emptyset, A_1, A_2\}$, either A_1 or A_2 is not a cluster of $\mathcal{T}_\Sigma^\rho$. Without loss of generality, we may assume that A_2 is not a cluster of $\mathcal{T}_\Sigma^\rho$. Let E_{π_2} denote a subset of edges of $\mathcal{T}_\Sigma$ that displays π_2, and let e denote the edge in E_{π_2} displaying $A_2|(X - A_2)$. Observe that, as A_2 is not a cluster of $\mathcal{T}_\Sigma^\rho$, it is easily seen that, for each edge $e' \in E_{\pi_2} - \{e\}$, the unique path in $\mathcal{T}_\Sigma$ from ρ to the vertex of e' closer to ρ traverses e. Now, by Theorem 4.2, $\mathcal{T}_\Sigma$ is an even X-tree, and so, by Lemma 4.3, $\mathcal{T}_\Sigma/E_{\pi_2}$ is an even X-tree. We show next that

$$\Delta(\mathcal{T}_\Sigma) = \Delta(\mathcal{T}_\Sigma/E_{\pi_2}). \tag{7.2}$$

If the degree of ρ is at least three, then, by the previous observation on the unique path in $\mathcal{T}_\Sigma$ starting at ρ, there must exist leaves x and y in $\mathcal{T}_\Sigma$ such that the path from ρ to either of them does not traverse an edge in E_{π_2}. Thus,

$$\Delta(\mathcal{T}_\Sigma) \geq \Delta(\mathcal{T}_\Sigma/E_{\pi_2}) \geq d_{\mathcal{T}_\Sigma/E_{\pi_2}}(x, y) = d_{\mathcal{T}_\Sigma}(x, y) = \Delta(\mathcal{T}_\Sigma),$$

by Theorem 7.3. Consequently, (7.2) must hold in this case.

Now assume that the degree of ρ equals two. Since, by assumption, $\mathbb{P}(\Sigma)$ contains as hierarchical partition system Π_h and $\mathcal{T}_\Sigma \cong \mathcal{T}_{\Pi_h}$, it follows by Corollary 7.2 that $\mathcal{T}_\Sigma$ does not contain an interior vertex that is labelled. Since A_2 is not a cluster of $\mathcal{T}_\Sigma^\rho$, it follows that $\mathcal{T}_\Sigma^\rho$ must contain a vertex of degree at least three on the path from ρ to the closer one of the two vertices of e. By the observation above on the unique path in $\mathcal{T}_\Sigma$ starting at ρ, the same arguments as in the case that ρ is of degree at least three imply that (7.2) must hold in this case too.

To complete the proof of the converse, let Π_h denote again a hierarchical partition system in $\mathbb{P}(\Sigma)$. Then, combining Corollary 7.2, (7.2), and Corollary 3.3,

$$2|\Pi_h| = \Delta(\mathcal{T}_\Sigma) = \Delta(\mathcal{T}_\Sigma/E_{\pi_2}) \leq 2(|\Pi| - 1) < 2|\Pi|.$$

In particular, $|\Pi_h| < |\Pi|$, so Π is not $\mathbb{P}(\mathcal{T}_\Sigma)$-minimum. This completes the proof of the converse and the theorem. □

8. A decision problem. It could be of interest to try to extend the main results in this paper to other types of multisets of splits (e.g., weakly compatible or k-compatible sets [10]). For example, by Theorem 4.2, if we are given a compatible multiset Σ of splits of a set X, it is easy to decide whether or not there exists some partition system Π on X with $\Sigma_\Pi = \Sigma$, but what if Σ is not compatible? We now prove a result that indicates that extending our results could be quite challenging. In particular, we show that the following decision problem is NP-complete.

Partition System
Instance: A split system Σ on X.
Question: Is there a partition system Π on X such that $\Sigma_\Pi = \Sigma$?

To prove this result we first recall some useful facts. Suppose that G is a graph. Then G is called *simple* if it does not contain a loop and *cubic* if every vertex has degree three. A *matching* M of G is a subset of edges of G such that no two edges in M share a vertex. A matching M of G is called *perfect* if every vertex of G is incident with some edge in M. A *k-edge coloring* of G is an assignment of at most $k \geq 2$ colors to the edges of G so that no two edges incident with the same vertex have the same color. The *edge chromatic number* of G is the smallest k for which G is k-edge colorable. A consequence of a theorem due to Vizing [19] is that the edge chromatic number of a simple cubic graph G is either 3 or 4, where it is 3 if and only if the edges of G can be partitioned into three perfect matchings. To show that Partition System is NP-complete, we use the following NP-complete problem [12].

Cubic Edge Coloring
Instance: A simple cubic graph G.
Question: Is the edge chromatic number of G 3?

Theorem 8.1. *The decision problem* Partition System *is NP-complete even if the split system Σ is a* set *of splits.*

Proof. Clearly, Partition System is in NP. Now, let G be an instance of Cubic Edge Coloring with vertex and edge sets V and E, respectively. We may assume that $|V| \geq 5$. We construct an instance of Partition System as follows. Let $X = V$, and let

$$\Sigma = \biguplus_{\{u,v\}\in E} \{\{u, v\}|(X - \{u, v\})\}.$$

Note that the time taken for this construction and the size of the constructed instance are polynomial in the size of G. Moreover, since G is simple, the multiplicity of each split in Σ is 1; that is, Σ is a set. We next show that there exists a partition system Π on X with $\Sigma_\Pi = \Sigma$ if and only if E can be partitioned into three perfect matchings of G.

First suppose that G has three pairwise-disjoint perfect matchings M_1, M_2, and M_3. Since M_i is a partition of X for all i and since each edge $\{u, v\}$ of G is in precisely one of M_1, M_2, and M_3, it follows that the partition system $\Pi' = \{M_1, M_2, M_3\}$ on X has the property that $\Sigma_{\Pi'} = \Sigma$.

Now suppose that there is a partition system Π on X such that $\Sigma_\Pi = \Sigma$. Let $\pi \in \Pi$, and let $A \in \pi$. Since $A|(X - A) \in \Sigma$, either A or $X - A$ is an edge of G. If $X - A$ is an edge of G, then, as $|X| \geq 5$, we have $\pi = \{A, X - A\}$. But then the multiplicity of $A|(X - A)$ in Σ_Π is at least 2, which is a contradiction as Σ is a set and not a multiset. Therefore A is an edge of G. As each vertex is incident with exactly three edges, it now follows that Π consists of three partitions of X with each partition being a perfect matching of G. Since these matchings are pairwise disjoint, E can be partitioned into three perfect matchings. This completes the proof of the theorem. □

9. Discussion. In this section, we shall consider the mapping that takes a partition system Π to the split system Σ_Π in a more general setting. The study of similar mappings between combinatorial objects relevant to phylogenetic analysis, such as split systems and distances, has proved to be a fruitful approach to various problems in the area of phylogenetic combinatorics (cf., e.g., [7]).

We begin with some additional terminology and notation. Given a finite set X, let $\underline{\Pi}(X)$ and $\underline{\Sigma}(X)$ be the *set* of partitions and splits of X, respectively. In addition, for a subset A of X, let $\underline{\Pi}(X; A)$ be the set of partitions π in $\underline{\Pi}(X)$ with $A \in \pi$. A *real partition family* on X is a map μ from $\underline{\Pi}(X)$ into $\mathbb{R}_{\geq 0}$, and a *real split family* on X is a map ν from $\underline{\Sigma}(X)$ into $\mathbb{R}_{\geq 0}$. Moreover, μ is called an *integral partition family* if $\mu(\pi)$ is a nonnegative integer for every $\pi \in \underline{\Pi}(X)$, and *integral split families* are defined in a similar manner. Note that each partition system Π on X gives rise to a real partition family μ_Π on X in which μ_Π maps each partition π in $\underline{\Pi}(X)$ to the multiplicity of π in Π if $\pi \in \Pi$, and 0 otherwise.

Now consider the map $\kappa : \mathbb{R}_{\geq 0}^{\underline{\Pi}(X)} \longrightarrow \mathbb{R}_{\geq 0}^{\underline{\Sigma}(X)}$ that takes a real partition family μ on X to the real split family $\kappa(\mu)$ on X defined by

$$\kappa(\mu)(A|B) = \sum_{\pi \in \underline{\Pi}(X;A)} \mu(\pi) + \sum_{\pi \in \underline{\Pi}(X;B)} \mu(\pi)$$

for each split $A|B$ in $\underline{\Sigma}(X)$. Then, for a given partition system Π on X and each split $A|B$ in $\underline{\Sigma}(X)$, the value $\kappa(\mu_\Pi)(A|B)$ is equal to the multiplicity of $A|B$ in the split system Σ_Π if $A|B \in \Sigma_\Pi$, and 0 otherwise. Therefore, the map κ can be regarded as a generalization of the mapping that takes a partition system Π on X to the split system Σ_Π.

In this framework, the results of the previous sections are mainly concerned with understanding the *kernel* of the map κ, that is, the set $\kappa^{-1}(\nu)$ for a real split family ν on X. In this context, we are especially interested in the case when ν is an integral split family and the *support* of ν, defined as the set $\{S \in \underline{\Sigma}(X) : \nu(S) > 0\}$, is compatible. In particular, Theorem 4.2 presents a criterion for deciding whether or not the kernel $\kappa^{-1}(\nu)$ contains an integral partition family. Moreover, if such an integral partition family exists, then Theorem 5.2 provides a canonical construction for a maximum-sized integral partition family in that kernel, and algorithm MIN-SIZEPARTITION obtains an integral partition family in the kernel with the minimum size (see also Theorem 6.3). Finally, as shown in Theorem 8.1, if the support of ν is not compatible, then it is NP-complete to determine whether the kernel $\kappa^{-1}(\nu)$ contains an integral partition family.

In light of these facts, it would be interesting to characterize the set of real split families ν for which the kernel $\kappa^{-1}(\nu)$ contains an integral partition family. Note that,

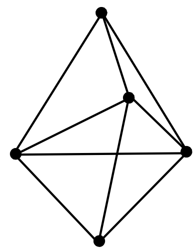

FIG. 4. *The* 1*-skeleton of the polytope* $\kappa^{-1}(\nu_0)$ *for the integral partition family* ν_0 *given in section* 9*.*

given a real split family ν, the kernel $\kappa^{-1}(\nu)$ may not contain an integral partition family, even if ν itself is integral. For example, consider the set $X = \{1, 2, 3, 4\}$, the splits $S_i = \{\{i\}, X - \{i\}\}$ for $1 \leq i \leq 4$ and $S_5 = \{\{1, 2\}, \{3, 4\}\}$, and let ν_0 be the integral split family on X defined by setting $\nu_0(S_i) = 1$ for $1 \leq i \leq 5$. Then it is straightforward to check that $\kappa^{-1}(\nu_0)$ does not contain an integral partition family. However, it is not difficult to see that $\kappa^{-1}(\nu_0)$ is not empty and that it is in fact a three-dimensional polytope with five vertices (see Figure 4 for the 1-skeleton of $\kappa^{-1}(\nu_0)$ and [20] for definitions related to polytopes).

More generally, it can be shown that the kernel $\kappa^{-1}(\nu)$ is always a polytope for each real split family ν on X. The proof of this fact is beyond the scope of this paper and will be presented elsewhere. Note that the polytope $\kappa^{-1}(\nu)$ can be much more complicated in general and there are several interesting questions that can be asked concerning its structure. For example, it could be of interest to find formulas for its dimension and the number of its faces and vertices, or to find interesting characterizations for its faces and vertices. A better understanding of these questions should, we hope, shed further light on mappings from partition systems to split systems and, ultimately, their application to phylogenetics.

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