Compatibility of Partitions with Trees, Hierarchies, and Split Systems

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Abstract

The question whether a partition $P$ and a hierarchy $H$ or a tree-like split system $S$ are compatible naturally arises in a wide range of classification problems. In the setting of phylogenetic trees, one asks whether the sets of $P$ coincide with leaf sets of connected components obtained by deleting some edges from the tree $T$ that represents $H$ or $S$, respectively. More generally, we ask whether a refinement $T'$ of $T$ exists such that $T'$ and $P$ are compatible in this sense. The latter is closely related to the question as to whether there exists a tree at all that is compatible with $P$. We report several characterizations for (refinements of) hierarchies and split systems that are compatible with (systems of) partitions. In addition, we provide a linear-time algorithm to check whether refinements of trees and a given partition are compatible. The latter problem becomes NP-complete but fixed-parameter tractable if a system of partitions is considered instead of a single partition. In this context, we also explore the close relationship of the concept of compatibility and so-called Fitch maps.

Keywords: hierarchy, split system, phylogenetic tree, partition, compatibility, recognition algorithm, Fitch map

1 Introduction

The selection of a partition $P$ from a hierarchy $H$ (or its equivalent rooted tree $T$) on a finite set $X$ is often the final step in applications of hierarchical clustering procedures [16, 21]. In this case, $P$, often called a “representative partition”, is composed of the pairwise disjoint leaf sets $L(T(u))$ of subtrees $T(u)$ rooted at some vertices $u$ of $T$. Equivalently, each set (class) of $P$ is a set in $H$, i.e., $P \subseteq H$. Cutting a hierarchy at different “levels” leads to partitions $P_i$ of $X$ that are ordered by refinement, i.e., every set $A \in P_i$ at the lower level is contained in a set $B \in P_j$ at the higher level. In the image processing literature, braids of partitions have been introduced as systems $\{P_i \mid i = 1, \ldots, k\}$ of partitions of $X$ that generalize such hierarchically ordered partitions. In a braid, all pairwise refinement suprema $P_i \lor P_j$ (i.e., the finest partition that is refined by both $P_i$ and $P_j$) must be hierarchically organized w.r.t. refinement, and moreover satisfy $\{X\} \neq P_i \lor P_j$ [15, 19]. Considering the distribution of attributes of species, biologists have been interested in systems of partitions $\{P_1, \ldots, P_k\}$ and the associated system of splits $A \mid (X \setminus A)$ with $A \in P_i$ for some $i$. In [14], the compatible split systems that are generated by partition systems are characterized.

Instead of considering systems of partitions, one can ask whether a single partition $P$, or – equivalently – its associated split system $\Sigma_P := \{A \mid (X \setminus A) : A \in P\}$ can be obtained from a rooted or unrooted tree $T$ by cutting a subset $H \subseteq E(T)$ of the tree edges and considering the leaf sets of the resulting connected components. For rooted trees, this question arises naturally in mathematical phylogenetics. The removal of those edges from the rooted gene tree that correspond
to horizontal gene transfer (HGT) then leaves subtrees of the gene phylogeny that can be analyzed independently [7, 8, 10]. If the tree $T$ and the partition $\mathcal{P}$ of the leaf set into HGT-free subsets are inferred independently, it is important to recognize whether the data are compatible with each other, i.e., whether $\mathcal{P}$ can be obtained from the tree $T$ by cutting some of its edges. If this is not possible for a tree that contains multifurcations, it may still be possible to achieve compatibility by refining some of the multifurcations in $T$. Here, we address these two main questions.

The split system $\mathcal{S}_\mathcal{P}$ introduced above suggests a different notion of compatibility with trees. Consider the partition $\mathcal{P} = \{\{a\}, \{b\}, \{c, d\}\}$. Clearly, $\mathcal{P}$ is compatible with the star tree $S_1$ on $X = \{a, b, c, d\}$. However, $S_1$ (more precisely, its unrooted version $S_1$) does not display the split $\{c, d\} \mid (X \setminus \{c, d\})$. In fact, the condition that $\mathcal{S}_\mathcal{P}$ is displayed by the unrooted tree $\overline{T}$ is closely related to the idea that $\mathcal{P}$ is a representative partition (of a suitably rooted version) of the tree $\overline{T}$. This example shows that the notion of compatibility considered here is more general than the concepts that have appeared in the literature so far.

In this contribution, we characterize compatibility of partitions with rooted and unrooted trees (or equivalently their hierarchies and split systems, respectively). After introducing the notation and some preliminary results, we give an overview of the main concepts and results in Section 3.

## 2 Preliminaries

### Basics

We denote the power set of a set $X$ by $2^X$. A set system $\mathcal{P} \subseteq 2^X$ is a partition of $X$ if (P0) $\emptyset \notin \mathcal{P}$, (P1) $\bigcup_{A \in \mathcal{P}} A = X$, and (P2) if $A, B \in \mathcal{P}$ and $A \cap B \neq \emptyset$ then $A = B$. We will interchangeably use the equivalent terms: set of partitions, collection of partitions and partition systems. Two sets $A$ and $B$ overlap if $A \cap B \neq \emptyset$, $A \setminus B \neq \emptyset$, and $B \setminus A \neq \emptyset$.

In this contribution, we consider both rooted and unrooted phylogenetic trees $T$ with vertex set $V(T)$, edge set $E(T)$, and leaf set $L(T) = X$. In this case, we also say that $T$ is a tree on $X$. A star tree $T$ is a tree for which $|V(T) \setminus L(T)| = 1$.

### Rooted Trees and Hierarchies

A rooted tree $T$ has a distinguished vertex $\rho_T$ called the root of $T$. For $u \in V(T)$, we write child$_T(u)$ for the set of its children, and parent$_T(u)$ for the parent of $u \neq \rho_T$. In both cases, we may omit the index $T$ whenever there is no risk of confusion. The subtree of $T$ rooted at $u$ is denoted by $T(u)$. Furthermore, we write $\preceq_T$ for the ancestor partial order on $T$, that is, $u \preceq_T v$ if $v$ lies on the path from $\rho_T$ to $u$. If $u \preceq_T v$ or $v \preceq_T u$, then $u$ and $v$ are comparable and, otherwise, incomparable. For a nonempty subset of $A \subseteq X$, we denote by $\text{lea}_T(A)$ the last common ancestor of $A$ in $T$. A rooted tree is phylogenetic if all its inner vertices $V(T) \setminus L(T)$ have at least two children. Hence, a rooted phylogenetic tree may contain one vertex with degree 2, namely the root $\rho_T$.

A set system $\mathcal{H} \subseteq 2^X$ is a hierarchy (on $X$) if (H0) $\emptyset \notin \mathcal{H}$, (H1) $X \in \mathcal{H}$, (H2) $A, B \in \mathcal{H}$ implies $A \cap B \in \mathcal{H} \cup \{A, B, \emptyset\}$, i.e., $A$ and $B$ do not overlap, and (H3) $\{x\} \in \mathcal{H}$ for all $x \in X$. For a given non-empty set $A \subseteq X$ and a hierarchy $\mathcal{H} \subseteq 2^X$, we define $A_\mathcal{H}$ as the inclusion-minimal element in $\mathcal{H}$ that contains $A$.

For a hierarchy $\mathcal{H} \subseteq 2^X$ we can define the closure as the function $\text{cl}_\mathcal{H} : 2^X \to 2^X$ satisfying

$$\text{cl}_\mathcal{H}(A) := \bigcap_{B \in \mathcal{H}, A \subseteq B} B$$

for all subsets $A \subseteq X$. Where there is no danger of confusion, we will drop the explicit reference to $\mathcal{H}$ and simply write $\text{cl}(A)$ instead of $\text{cl}_\mathcal{H}(A)$.

**Lemma 2.1.** Let $A \subseteq X$ be non-empty and $\mathcal{H}$ be a hierarchy on $X$. Then $\text{cl}(A) = A_\mathcal{H}$ for all $A \neq \emptyset$.

**Proof.** Since $A \subseteq X$, $X \in \mathcal{H}$, and no two elements in $\mathcal{H}$ overlap, there is a unique inclusion-minimal element $A_\mathcal{H}$ in $\mathcal{H}$ that contains $A$, i.e., every $A' \in \mathcal{H}$ that contains $A$ also contains $A_\mathcal{H}$. Thus $\text{cl}(A) = \bigcap\{B \in \mathcal{H} \mid A \subseteq B\} = \bigcap\{B \in \mathcal{H} \mid A_\mathcal{H} \subseteq B\} = A_\mathcal{H}$. \hfill $\square$

As an immediate consequence, we observe that for a hierarchy $\mathcal{H} \subseteq 2^X$, cl satisfies the classical properties of a closure operator: (C1) $A \subseteq \text{cl}(A)$ (enlarging); (C2) $\text{cl}(\text{cl}(A)) = \text{cl}(A)$ (idempotent); (C3) If $A \subseteq B$, then $\text{cl}(A) \subseteq \text{cl}(B)$ (isotone). For $|X| \geq 2$, $\mathcal{H}$ contains at least two distinct singletons $\{x\}$ and $\{y\}$ and thus $\text{cl}(\emptyset) \subseteq \{x\} \cap \{y\} = \emptyset$. Only in the special case $|X| = 1$, i.e., $\mathcal{H} = \{\{x\}\}$, we get $\text{cl}(\emptyset) = \{x\}$. This is the consequence of the usual practice of excluding $\emptyset$. 


from hierarchies to have the singleton as inclusion-minimal elements, which in turn is motivated by the 1-to-1 correspondence between rooted trees and hierarchies. We note that in the context of abstract convexities, on the other hand, it is customary to enforce $\emptyset \in \mathcal{H}$ so that $\mathcal{H}$ is closed under intersection \cite{20}, in which case $cl(\emptyset) = \emptyset$ also for $|X| \leq 1$. This subtlety is irrelevant for our discussion, however, since we are not interested in the trivial cases $|X| \leq 1$.

The following result shows that there is a 1-to-1 correspondence between hierarchies and rooted phylogenetic trees.

**Theorem 2.2** \cite{18}. Let $\mathcal{H}$ be a collection of non-empty subsets of $X$. Then, $\mathcal{H}$ is a hierarchy on $X$ if and only if there is a rooted phylogenetic tree $T$ on $X$ with $\mathcal{H} = \{ L(T(v)) \mid v \in V(T) \}$.

The sets $L(T(u))$ for $u \in V(T)$ or, equivalently, the sets of a hierarchy are commonly referred to as *clusters*. In view of Thm. 2.2, every set $A \in \mathcal{H}$ corresponds to a vertex $u_A \in V(T)$ such that $L(T(u_A)) = A$ and $u_A \leq_T u_B$ is equivalent to $A \subseteq B$. The hierarchy $\mathcal{H}(T)$ of a rooted phylogenetic tree $T$ is $\mathcal{H}(T) := \{ L(T(v)) \mid v \in V(T) \}$. Moreover, we say that a rooted tree $T$ corresponds to $\mathcal{H}$ if $\mathcal{H} = \mathcal{H}(T)$. In particular, Thm. 2.2 ensures that for all hierarchies there is a corresponding tree and, moreover, that all results established here for hierarchies do also hold for rooted phylogenetic trees and vice versa. As an immediate consequence, we can express the closure as

$$cl_{\mathcal{H}}(A) = L(T(lca_T(A))).$$

We therefore have $lca_T(A) \leq_T lca_T(B)$ if and only if $cl(A) \subseteq cl(B)$ for all $A, B \neq \emptyset$. Given a set $A \in \mathcal{H}$ with $|A| > 1$ (and corresponding vertex $u \in V(T)$ that satisfies $A = L(T(u)))$, we call $B \in \mathcal{H}$ a *child cluster* of $A$ if $B = L(T(v))$ for some $v \in child_T(u)$. Hence, the child clusters $B$ of $A$ are exactly the inclusion-maximal sets in $\mathcal{H}$ that satisfy $B \subseteq A$. For simplicity of notation, we will think of the leaves of $T$ in this case as the $x \in X$, i.e., $L(T) = X$. A phylogenetic tree $T$ is a modification of the phylogenetic tree $T'$ on the same set $X$ if the corresponding hierarchy $\mathcal{H}(T)$ is a modification of $\mathcal{H}(T')$, i.e., if $\mathcal{H}(T') \subseteq \mathcal{H}(T)$.

**Unrooted Trees and Split Systems** An unrooted tree is *phylogenetic* if all non-leaf vertices have degree at least three. A *split* $A_1/A_2 := \{A_1, A_2\}$ on $X$ is a partition of the set $X$ into two disjoint non-empty subsets $A_1$ and $A_2 = X \setminus A_1$. In every tree $T$ on $X$, we can associate with every edge $e \in E(T)$ the split $S_e = L(T_1) \sqcap L(T_2)$ where $L(T_1)$ and $L(T_2)$ are the leaf sets of the two (not necessarily phylogenetic) trees $T_1$ and $T_2$, respectively, obtained from $T$ by deletion of $e$. An unrooted phylogenetic tree $T$ is determined by its split system $\Sigma(T) = \{ S_e \mid e \in E(T) \}$. To be more precise, there is a 1-to-1 correspondence between unrooted phylogenetic trees $T$ with leaf set $X$ and split systems $\Sigma$ that (i) contain all “singleton splits” $\{x\} \sqcap (X \setminus \{x\})$ and (ii) are “compatible” in the sense that, for any two splits $A_1/A_2, B_1/B_2 \in \Sigma$, at least one of the four intersections $A_1 \cap B_1, A_1 \cap B_2, A_2 \cap B_1$, or $A_2 \cap B_2$ is empty \cite{4}. In this case, there is a unique (up to isomorphism) tree $T$ with $\Sigma(T) = \Sigma$. We call such split systems *tree-like*. An unrooted tree $T'$ is a refinement of $T$ if $\Sigma(T) \subseteq \Sigma(T')$.

We note that this is a special case of the analogous result for so-called X-trees, see e.g. \cite[Prop. 3.5.4]{18}. In an X-tree, a set of “taxa” $X$ is mapped (not necessarily injectively) to the vertex set $V(T)$ of a rooted or unrooted tree $T$ \cite{18}. The *phylogenetic* (rooted or unrooted) trees considered here are a slightly less general construction that identifies the taxa set $X$ with the leaf set $L(T)$ and insists that distinct taxa are represented by distinct vertices in the underlying trees. That is, they are equivalent to X-trees $T$ for which $X$ is bijectively mapped to $L(T)$.

**Remark.** Throughout this contribution, we assume that $X$ is finite and $|X| \geq 2$. Moreover, all rooted and unrooted trees are phylogenetic unless explicitly specified otherwise.

## 3 Main Ideas and Results

Let $T$ be a (rooted or unrooted) tree with leaf set $L(T) = X$ and $H \subseteq E(T)$ be a subset of edges. Removal of $H$ disconnects $T$ into a forest whose connected components induce the partition $\mathcal{F}(T, H)$ on the leaf set $X$. Of course, it may be possible that removal of the edges $H$ separates inner vertices, e.g., if all incident edges to an inner vertex are in $H$. This, however, does not change the fact that we still obtain a partition of $X$ after removal of the edges in $H$. We will refer to the edges $e \in H$ as *separating edges*. Fig. 1 shows two examples for sets of separating edges, $H_1$ and $H_2$ as indicated by the dashed lines, for a given tree $T$. The partition $P_1 = \mathcal{F}(T, H_1)$ is a “representative partition” for $T$, i.e., all sets in $P_1$ appear as clusters in $T$: $\{a, b, c\} = L(T(u)),$
Then any subset \( H \) of \( E(T) \) is a separating edge. In particular, since all edges in \( E(T) \) split system \( \{A, B\} \in X \), the edges in \( T \) are not compatible. In situations where the "ground truth" is a binary tree. In situations where hierarchies (and thus rooted trees).

\( \text{Definition 3.1. Let} \ P \ \text{be a partition of} \ X \ \text{and let} \ T \ \text{be a rooted or unrooted tree with leaf set} \ X. \ \text{Then} \ P \ \text{and} \ T \ \text{are compatible if there is a set of separating edges} \ H \subseteq E(T) \ \text{such that} \ P = F(T, H). \)

\( \text{in case} \ T \ \text{is rooted (or unrooted) and compatible with} \ P, \ \text{the corresponding hierarchy} \ H(T) \ (\text{or split system} \ \mathcal{S}(T), \ \text{resp.}) \ \text{are said to be compatible with} \ P. \)

As we shall see in Lemma 4.1, we can always find a tree on \( X \) that is compatible with \( P \) for a given partition \( P \) of \( X \). In particular, the tree corresponding to the hierarchy \( H_P := P \cup \{x \mid x \in X\} \cup \{X\} \) is always compatible with \( P \), see \( P \) and \( T_1 \) in Fig. 2 for an illustrative example. However, Fig. 2 also shows that there can be multiple different trees on \( X \) that are compatible with \( P \). The main result of Section 4, Thm. 4.5, is a characterization of compatibility of partitions and hierarchies (and thus rooted trees).

As it turns out, not all hierarchies are compatible with a given partition \( P \). In many applications, hierarchies (and their corresponding rooted trees) are not necessarily fully resolved, even though it is often assumed that the "ground truth" is a binary tree. In situations where \( H \) and \( P \) are not compatible, it is therefore of interest to ask whether it is possible to find a refinement of \( H \) that is compatible with \( P \). An example of a tree \( T \) that is not compatible with a partition \( P \) but that admits a compatible refinement \( T' \) is shown in Fig. 3. To see that \( P = \{A, B\} \) and \( T \) as in Fig. 3 are not compatible, the edges in \( T \) have been colored in orange and cyan if they lie on a path connecting two elements from \( A \) or \( B \), respectively. Clearly, none of these edges can be a separating edge. In particular, since all edges in \( T \) are colored, \( A \) and \( B \) cannot be separated by any subset \( H \subseteq E(T) \). For similar reasons the tree \( T' \) as in Fig. 3 is not compatible with \( P \). Since \( T' \) is already fully-resolved, it does not admit a compatible refinement.
Definition 3.2. A tree $T$ and a partition $\mathcal{P}$ are refinement-compatible (r-compatible for short) if there exists a refinement $T^*$ of $T$ that is compatible with $\mathcal{P}$.

In case $T$ is rooted (unrooted) and refinement-compatible with $\mathcal{P}$, the corresponding hierarchy $\mathcal{H}(T)$ (split system $\mathcal{G}(T)$, resp.) are said to be refinement-compatible with $\mathcal{P}$.

By definition, compatibility implies r-compatibility since every tree is a refinement of itself. In Section 5, we show that refining a hierarchy $\mathcal{H}$ or a rooted tree $T$ that is already compatible with a partition $\mathcal{P}$ never destroys compatibility. As a main result of Section 5, we obtain a characterization of r-compatibility in terms of the simple condition that no set $Y \in \mathcal{H}$ overlaps with two distinct sets $A, B \in \mathcal{P}$ (cf. Thm. 5.7). We later utilize these results to derive simple linear-time algorithms for both recognition of compatibility of a partition and a tree, as well as the construction of a compatible refinement if one exists in Section 7.

Even though compatibility of partitions and rooted trees is linear-time-decidable, the situation appears substantially more complicated when systems $\mathcal{Y} = \{\mathcal{P}_1, \mathcal{P}_2, \cdots, \mathcal{P}_k\}$ of partitions of $X$ are considered rather than single partitions. By definition, $T$ (or equivalently, the hierarchy, $\mathcal{H}(T)$) and each $\mathcal{P}_i$ are compatible if and only if $\mathcal{P}_i = \mathcal{F}(T, H_i)$ for some subset $H_i \subseteq E(T)$, $1 \leq i \leq k$. In this case, we say that $T$ (equiv. $\mathcal{H}(T)$) and $\mathcal{Y}$ are compatible. It is natural, then, to ask whether for a given system of partitions $\mathcal{Y}$, there exists a tree $T$ such that $\mathcal{Y}$ and $T$ are compatible:

**Problem (Existence of Tree compatible with Partition System (ExistTP)).**

Input: A partition system $\mathcal{Y}$ on $X$.

Question: Is there a tree $T$ on $X$ such that $T$ and $\mathcal{Y}$ are compatible?

Since every tree on $X$ is a refinement of the star tree on $X$, ExistTP is a special case of the following more general problem:

**Problem (Compatibility of Tree and Partition System (CompATP)).**

Input: A tree $T$ with leaf set $X$ and a partition system $\mathcal{Y}$ on $X$.

Question: Is there a refinement $T^*$ of $T$ such that $T^*$ and $\mathcal{Y}$ are compatible?

The difficulty of both ExistTP and CompATP stems from the fact that refinements of the underlying tree that are necessary to obtain compatibility with individual partitions in $\mathcal{Y}$ may
contradict one another. Consider the tree $T$ and three of its possible refinements $T^*_1, T^*_2$ and $T^*$ as shown in Fig. 4. In this example, $T$ is not compatible with $\mathcal{P} = \{P_1, P_2\}$, and the refinement $T^*_1$ is compatible with $P$, but not with $P_2$, $\{i, j\} = \{1, 2\}$. However, there is no common refinement of $T^*_1$ and $T^*_2$ that is compatible with $\mathcal{P}$. On the other hand, $T^*$ is compatible with both $P_1$ and $P_2$. Hence, $T$ admits a refinement $T^*$ that is compatible with $\mathcal{P}$. An example of a tree $T$ for which every partition $P \in \mathcal{P}$ is $r$-compatible with $T$ but there is no refinement of $T$ is compatible with $\mathcal{P}$ is provided in Fig. 7. Hence, EXISTTP and COMPTTP seem to be inherently difficult and indeed both are NP-complete decision problems, see Thm. 7.10.

In Section 6, compatibility of partitions with splits systems and their equivalent representations as unrooted phylogenetic trees is considered. As shown in Prop. 6.2, compatibility of partitions with unrooted and rooted trees are closely related. In fact, a partition is compatible with an unrooted tree if and only if it is compatible with any rooted version of this tree. Further characterization of (refinements of) split systems and unrooted trees being compatible with partitions will be established (cf. Thm. 6.4 as well as Lemma 6.7 and 6.8).

Section 7 is dedicated to algorithmic considerations and the complexity of deciding whether (systems of) partitions are compatible (with refinements) of hierarchies and split systems, represented by rooted and unrooted trees, respectively. As we have seen above, there are edges $e$ of a tree $T$ that can never be separating edges since their removal would break down some set $A \in \mathcal{P}$. In order to identify such edges, we provide an edge coloring that we have already used in an informal way to demonstrate incomparability in the example in Fig. 3:

**Definition 3.3.** Let $T$ be a tree on $X$ and $\mathcal{P}$ a partition of $X$. The $\mathcal{P}$-(edge-)coloring of $T$ is the map $\gamma_{T, \mathcal{P}}: E(T) \to 2^\mathcal{P}$ that is given by

$$A \in \gamma_{T, \mathcal{P}}(e) \iff e \text{ lies on the unique path connecting two } x, x' \in A.$$ 

The key property of this edge coloring $\gamma_{T, \mathcal{P}}$ is that any edge $e \in E(T)$ with $\gamma_{T, \mathcal{P}}(e) \neq \emptyset$ lies on some path between two vertices $a, a' \in X$ that are contained in the same set of $\mathcal{P}$, and thus, $e$ cannot be a separating edge. In contrast, all edges $e$ for which $\gamma_{T, \mathcal{P}}(e) = \emptyset$ do not separate any two leaves that are in the same set of $\mathcal{P}$, and thus can be safely added to the set of separating edges. A key result, proven in Section 7, is that $\mathcal{P}$ and $T$ are $r$-compatible if and only if $|\gamma_{T, \mathcal{P}}(e)| \leq 1$ for every $e \in E(T)$ (Prop. 7.3). In this case, the coloring $\gamma_{T, \mathcal{P}}$ can be computed in linear time and, based on this, deciding the existence of and finding a (refinement of) a tree that is compatible with a partition $\mathcal{P}$ can be done in linear time as well. To establish compatibility of $\mathcal{P}$ and $T$, it suffices to rule out the existence of a vertex $u \in V(T)$ that is incident with two differently colored edges (cf. Thm. 7.6). If $\mathcal{P}$ and $T$ are $r$-compatible but not compatible, the vertices $u \in V(T)$ that violate the latter condition coincide with $\text{lca}(A)$ for some $A \in \mathcal{P}$ and can be refined by collecting all children $v \in \text{child}(u)$ for which $L(T(v)) \cap A \neq \emptyset$ under a newly created vertex (cf. Thm. 7.5).

### 4 Compatibility of Partitions and Hierarchies

We first show that, for every partition, there is a compatible hierarchy.

**Lemma 4.1.** For every partition $\mathcal{P}$ of $X$, the set system $\mathcal{H}_\mathcal{P} := \mathcal{P} \cup \{\{x\} | x \in X\} \cup \{X\}$ is a hierarchy that is compatible with $\mathcal{P}$. In particular, every partition $\mathcal{P}$ of $X$ is compatible with a rooted tree on $X$.

**Proof.** Since $\mathcal{P}$ is a partition of $X$, no two sets overlap. This remains true for $\mathcal{H}_\mathcal{P}$ and thus $\mathcal{H}_\mathcal{P}$ is a hierarchy. Moreover, it is easy to see that if all edges incident to the root of the tree $T$ corresponding to $\mathcal{H}$ are added to $T$, then $\mathcal{P} = \mathcal{F}(T, H)$ whenever $\mathcal{P} \neq \{X\}$. In case $\mathcal{P} = \{X\}$, $T$ is a star tree and we have $\mathcal{P} = \mathcal{F}(T, \emptyset)$. □

The following result is a key step for the characterization of compatible partitions and hierarchies. In particular, it shows that, for any two elements $A, B \in \mathcal{P}$, the set $B$ can only intersect with at most one child of $\text{lca}(A)$.

**Lemma 4.2.** If a partition $\mathcal{P}$ of $X$ and a rooted tree $T$ on $X$ are compatible, then, for all $A, B \in \mathcal{P}$, there are no two distinct children $u, u' \in \text{child}(\text{lca}(A))$ such that $B \cap L(T(u)) \neq \emptyset$ and $B \cap L(T(u')) \neq \emptyset$.

**Proof.** Let $A \in \mathcal{P}$ and put $v_A := \text{lca}(A)$. Since $\mathcal{P}$ is compatible with $\mathcal{H}$, there is a set of separating edges $H \subseteq E(T)$ such that $\mathcal{P} = \mathcal{F}(T, H)$. Assume, for contradiction, that there are two children
Corollary 4.3. Suppose a partition $\mathcal{P}$ of $X$ and a hierarchy $\mathcal{H}$ on $X$ (with corresponding tree $T$) are compatible and $A, B \in \mathcal{P}$ are distinct. Then $\text{lca}_T(A) \neq \text{lca}_T(B)$ and $A_\mathcal{H} = \text{cl}(A) \neq \text{cl}(B) = B_\mathcal{H}$.

Lemma 4.4. Suppose a partition $\mathcal{P}$ of $X$ and a hierarchy $\mathcal{H}$ on $X$ are compatible, and $A \in \mathcal{P}$. The set $A_\mathcal{H}$ does not overlap with any $B \in \mathcal{P}$.

Proof. Assume, for contradiction, that $A_\mathcal{H}$ and $B$ overlap for some $A, B \in \mathcal{P}$. Since $A \subseteq A_\mathcal{H}$ and $B \subseteq B_\mathcal{H}$ we have $A \neq B$ and, by Lemma 4.2, $A_\mathcal{H} \neq B_\mathcal{H}$. Since $B$ overlaps with $A_\mathcal{H}$ and $\mathcal{H}$ is a hierarchy, we have $A_\mathcal{H} \subseteq B_\mathcal{H}$. Now let $T$ be the tree of $\mathcal{H}$ and set $v_A := \text{lca}_T(A)_\mathcal{H} \triangleleft_T \text{lca}_T(B)_\mathcal{H} =: v_B$.

Since $A_\mathcal{H}$ is the unique inclusion-minimal element in $\mathcal{H}$ that contains $A$, there are two distinct children $u, u' \in \text{child}(v_A)$ such that $A \cap L(T(u)) \neq \emptyset$ and $A \cap L(T(u')) \neq \emptyset$. Let $a \in A \cap L(T(u))$ and $a' \in A \cap L(T(u'))$. Since $\mathcal{P}$ and $\mathcal{H}$ are compatible, there is a set of separating edges $H \subseteq E(T)$ such that $\mathcal{P} = \mathcal{F}(T, H)$. Since $a, a' \in A$, the unique path $P_{a,a'}$ from $a$ to $a'$ in $T$, and in particular the path $P_{a,v_A}$ from $a$ to $v_A$, cannot contain any separating edge. Furthermore, since $A_\mathcal{H}$ and $B$ overlap, there is an element $b \in A_\mathcal{H} \cap B$. Since $A$ and $B$ are disjoint, we have $b \neq a, a'$. Hence, $b \not\preceq_T u''$ for some child $u'' \in \text{child}(v_A)$. Since $u$ and $u'$ are distinct children of $v_A$, we can assume w.l.o.g. that $u'' \neq u$. Moreover, $v_A \preceq_T v_B$ together with the fact that $B_\mathcal{H}$ is the unique inclusion-minimal element in $\mathcal{H}$ that contains $B$, implies that there are two distinct children $w, w' \in \text{child}(v_B)$ that satisfy $b \not\preceq_T u'' \preceq_T v_A \preceq_T w$ and $b' \in B \cap L(T(w'))$. Since $b, b' \in B$, the unique path $P_{b,b'}$ from $b$ to $b'$ in $T$, and in particular the path $P_{b,v_A}$ from $b$ to $v_A$, cannot contain a separating edge. Since $u \neq u''$ and both $u$ and $u''$ are children of $v_A$, the path from $a$ to $b$ is the concatenation of the paths $P_{a,v_A}$ and $P_{b,v_A}$, and thus, does not contain a separating edge. Therefore, there is a set $C \in \mathcal{F}(T, H)$ with $a, b \in C$. Now, $a \in A$ and $b \in B$ implies that $\mathcal{P} \neq \mathcal{F}(T, H)$; a contradiction.

\[\text{Figure 5: The tree } T \text{ (on } X = \{A \cup B \cup C_1 \cup C_2 \cup C_3 \cup D \cup \{\epsilon\}\}) \text{ and the partition } \mathcal{P} = \{A, B, C := C_1 \cup C_2 \cup C_3, D, E := \{\epsilon\}\} \text{ are compatible since removal of the separating edges (dashed-lined) that are chosen according to Eq. (3) induces } \mathcal{P}. \text{ To emphasize its connectedness after removal of the separating edges, the minimal subtree connecting all elements in } C \text{ is highlighted in cyan. Let } \mathcal{H} \text{ be the hierarchy corresponding to } T. \text{ For some } Y \in \mathcal{P}, \text{ we have } Y = Y_\mathcal{H}, \text{ that is, } L(T(v)) = A_\mathcal{H} \text{ (i.e. the vertex } v \text{ corresponds to } A_\mathcal{H} \in \mathcal{H}), L(T(u)) = C_\mathcal{H} \text{ and } L(T(\epsilon)) = \{\epsilon\} = E_\mathcal{H}. \text{ For } C \text{ it holds that } C \subseteq C_\mathcal{H} = L(T(u)). \text{ Moreover, some elements in } \mathcal{P} \text{ overlap with elements in } \mathcal{H}, \text{ e.g., } C \in \mathcal{P} \text{ overlaps with } D \cup C_3 \in \mathcal{H}. \text{ Note that it suffices to have only one of } \{\rho_T, u\} \text{ and } \{\rho_r, e\} \text{ as a separating edge.} \]
Figure 6: The tree \( T \) admits several possible choices for the set \( H \) of separating edges (dashed-lined) such that \( F(T, H) = \mathcal{P} = \{A, B, C\} \). The separating edges in Panel (a) are the ones specified in Eq. (3). The two sets of separating edges in Panel (b) and (c) are both of minimum size, while the set of separating edges in Panel (d) is of maximum size. The set of separating edges of minimum size thus is not unique in general. In contrast, Cor. 7.7 implies that the maximum-sized set of separating edges is always unique. The set \( H \) defined by Eq. (3) is neither of minimum nor of maximum size.

**Theorem 4.5.** Let \( \mathcal{H} \) be a hierarchy on \( X \) and \( \mathcal{P} \) be a partition of \( X \). Then, \( \mathcal{P} \) and \( \mathcal{H} \) are compatible if and only if the following two conditions are satisfied for all \( A, B \in \mathcal{P} \):

(i) \( A_{\mathcal{H}} \) is a union of sets of \( \mathcal{P} \).
(ii) If \( A_{\mathcal{H}} = B_{\mathcal{H}} \), then \( A = B \).

**Proof.** Let \( T \) be the tree with \( \mathcal{H}(T) = \mathcal{H} \).

Assume that \( \mathcal{P} \) is compatible with \( \mathcal{H} \). First observe that, for all \( A \in \mathcal{P} \), \( A \subseteq A_{\mathcal{H}} \) implies that \( A_{\mathcal{H}} \) is the union of sets of \( \mathcal{P} \) if and only if \( A_{\mathcal{H}} \) does not overlap with any \( B \in \mathcal{P} \). Hence, Condition (i) follows immediately from Lemma 4.4. Condition (ii) follows immediately from the fact that \( A_{\mathcal{H}} = B_{\mathcal{H}} \) implies \( \text{lca}_T(A) = \text{lca}_T(B) \) and Cor. 4.3.

Now suppose (i) and (ii) holds. Consider the tree \( T \) and the following set of separating edges

\[
H := \{ \{\text{par}(\text{lca}_T(A)), \text{lca}_T(A)\} \mid A \in \mathcal{P}, \text{lca}_T(A) \neq \rho_T \},
\]

Thus, an edge \( e = \{u, v\} \in E(T) \) is a separating edge if and only if \( L(T(v)) = A_{\mathcal{H}} \) and thus \( v = \text{lca}_T(A) \) for some \( A \in \mathcal{P} \).

We first show that any two distinct \( A, B \in \mathcal{P} \) are separated by at least one separating edge in \( H \), i.e., there is no path in \( T \setminus H \) connecting any vertex \( a \in A \) with any vertex \( b \in B \). To this end, let \( A, B \in \mathcal{P} \) be chosen arbitrarily but distinct. By contraposition of Condition (ii), we have \( A_{\mathcal{H}} \neq B_{\mathcal{H}} \). Therefore and since \( \mathcal{H} \) is a hierarchy, we have to consider the two cases (a) \( A_{\mathcal{H}} \cap B_{\mathcal{H}} = \emptyset \), and (b) \( A_{\mathcal{H}} \subseteq B_{\mathcal{H}} \) or \( B_{\mathcal{H}} \subseteq A_{\mathcal{H}} \). Case (a) corresponds to the situation in which \( v_A := \text{lca}_T(A) \) and \( v_B := \text{lca}_T(B) \) are incomparable in \( T \), which is, moreover, only possible if neither \( v_A \) nor \( v_B \) are the root. Hence, the edges \( \{\text{par}(v_A), v_A\} \) and \( \{\text{par}(v_B), v_B\} \) are contained in \( H \) and every path from some \( a \in A \) to some \( b \in B \) contains these two edges. Thus, the two sets \( A \) and \( B \) are separated by separating edges in \( T \). In case (b), we assume w.l.o.g. that \( A_{\mathcal{H}} \subseteq B_{\mathcal{H}} \) which corresponds to the situation in which \( v_A := \text{lca}_T(A) \prec_T \text{lca}_T(B) = v_B \). Hence, \( v_A \) is not the root of \( T \), and we have \( \{\text{par}(v_A), v_A\} \in H \). Since \( L(T(v_A)) = A_{\mathcal{H}} \) contains all elements in \( A \), the two sets \( A \) and \( B \) are completely separated by this separating edge if \( A_{\mathcal{H}} \) does not contain any element of \( B \). Thus, assume for contradiction that \( A_{\mathcal{H}} \cap B \neq \emptyset \). This together with the facts that \( A \subseteq A_{\mathcal{H}} \subseteq B_{\mathcal{H}} \), \( A \cap B = \emptyset \) and \( B_{\mathcal{H}} \) is inclusion-minimal for \( B \) implies that \( A_{\mathcal{H}} \) and \( B \) overlap. Therefore, \( A_{\mathcal{H}} \) is not the union of sets of \( \mathcal{P} \); a contradiction to Condition (i).

It remains to show that no set \( A \in \mathcal{P} \) contains two elements \( a, a' \in A \) which are separated by a separating edge in \( T \). Thus, assume for contradiction that there is such an edge \( e = \{u, v\} \in H \) lying on the path that connects two \( a, a' \in A \) for some \( A \in \mathcal{P} \). We can assume w.l.o.g. that \( a \in L(T(v)) \) and \( a' \in L(T) \setminus L(T(v)) \). Since \( e \in H \), we have that \( v = \text{lca}_T(B) \) corresponds to \( B_{\mathcal{H}} \) for some \( B \in \mathcal{P} \). Since \( a \in B_{\mathcal{H}} = L(T(v)) \) but \( a' \notin B_{\mathcal{H}} \) and by similar arguments as above, the sets \( A \) and \( B_{\mathcal{H}} \) overlap which is again a contradiction to Condition (i).

In summary, we have \( A \in F(T, H) = \mathcal{P} \) for all \( A \in \mathcal{P} \) and thus \( \mathcal{P} = F(T, H) \). Therefore, \( \mathcal{P} \) is compatible with \( \mathcal{H} \).

The second part of the proof of Theorem 4.5 implies a simple algorithm to determine whether \( \mathcal{P} \) and \( \mathcal{H} \) are compatible and to construct a (minimal) set \( H \) of separating edges that realizes the partition \( \mathcal{P} \) on \( T \): In Section 7, we derive a linear-time compatibility test algorithm. The set \( H \)
of separating edges in Eq. (3) can also be constructed in polynomial time. Moreover, if there is an element \( A \in \mathcal{P} \) with \( A_H = X \), then the set \( H \) as in Eq. (3) is minimal because it contains, by construction, \( |\mathcal{P}| - 1 \) separating edges, i.e., the minimal number of splits required to decompose a tree into \( |\mathcal{P}| \) connected components. If there is no \( A \in \mathcal{P} \) with \( A_H = X \), however, then there is one edge too many. A minimal set of separating edges can easily obtained in this case by omitting the separating edge \( \{\text{par}(\text{lca}_T(A)), \text{lca}_T(A)\} \) for one of the sets that are inclusion-maximal among the inclusion-minimal sets \( A_H \), i.e., those which correspond to vertices that are closest to the root (see Fig. 5 and 6 for further examples). We summarize the latter discussion in the following

**Lemma 4.6.** Suppose that a partition \( \mathcal{P} \) of \( X \) and a rooted tree \( T \) on \( X \) are compatible. Then, there always exists a minimum-sized set of separating edges \( H^* \) such that \( \mathcal{P} = \mathcal{F}(T, H^*) \) and \( |H^*| = |\mathcal{P}| - 1 \). In particular, if \( H \) is chosen as in Eq. (3), then \( |H| \in \{|\mathcal{P}| - 1, |\mathcal{P}|\} \) and \( |H| = |\mathcal{P}| - 1 \) if and only if there is no \( A \in \mathcal{P} \) with \( A_H = X \).

The following result is a simple consequence of Thm. 4.5 and the discussion above.

**Corollary 4.7.** Let \( \mathcal{P} \) be a partition of \( X \), \( \mathcal{H} \) a hierarchy on \( X \) with corresponding tree \( T \), and let \( H \) be the edge set defined in Eq. (3). Then \( \mathcal{P} \) and \( \mathcal{H} \) are compatible if and only if \( \mathcal{P} = \mathcal{F}(T, H) \).

**Lemma 4.8.** If the partition \( \mathcal{P} \) and the hierarchy \( \mathcal{H} \) on \( X \) are compatible, then the following conditions hold for all \( A, B \in \mathcal{P} \): If \( B \subseteq A_H \) and \( B \neq A \), then \( B_H \cap A = \emptyset \).

**Proof.** By Property (i) of Thm. 4.5, \( B_H \) is a union of sets of \( \mathcal{P} \), and thus either (a) \( A \subseteq B_H \) or (b) \( A \cap B_H = \emptyset \). In case (a), we have \( A_H = \text{cl}(A) \subseteq \text{cl}(B_H) = B_H \) by isotony and idempotence of the closure. Similarly, we obtain \( B_H \subseteq A_H \) from the assumption \( B \subseteq A_H \). Therefore, \( A_H = B_H \). By Property (ii) of Thm. 4.5 this is a contradiction to \( A \neq B \). Thus, case (a) is impossible and we always have \( A \cap B_H = \emptyset \).

Thm. 4.5 and Lemma 4.8 together can be rephrased as

**Corollary 4.9.** The partition \( \mathcal{P} \) and the hierarchy \( \mathcal{H} \) are compatible if and only if

\[
A = A_H \setminus \bigcup_{B \in \mathcal{P}, B_H \subseteq A_H} B_H
\]

(4)

holds for all \( A \in \mathcal{P} \).

5 Compatibility of (Systems of) Partitions and Refinements of Hierarchies

In many applications hierarchies (and their associated trees) are not necessarily fully resolved, even though it is often assumed that the “ground truth” is a binary tree. We show first that refining a hierarchy \( \mathcal{H} \) or a tree \( T \) that is already compatible with a partition \( \mathcal{P} \) never destroys compatibility.

**Proposition 5.1.** A hierarchy \( \mathcal{H} \) on \( X \) and a partition \( \mathcal{P} \) of \( X \) are compatible if and only if \( \mathcal{P} \) is compatible with every refinement \( \mathcal{H}^* \) of \( \mathcal{H} \).

**Proof.** The if-direction immediately follows from the fact that \( \mathcal{H}^* = \mathcal{H} \) is a refinement of \( \mathcal{H} \). For the only-if-direction, let \( T \) be the tree corresponding to \( \mathcal{H} \), denote by \( H \subseteq E(T) \) the set of separating edges as defined in Eq. (3). Thus, we have \( e = \{\text{par}_T(v), v\} \in E(T) \cap H \) if and only if \( v = \text{lca}_T(A) \neq \rho_T \). Since \( \mathcal{H} \) and \( \mathcal{P} \) are compatible, we can apply Cor. 4.7 to conclude that \( \mathcal{P} = \mathcal{F}(T, H) \). Therefore, the path connecting any two vertices \( a \in A \) and \( b \in B \) from distinct \( A, B \in \mathcal{P} \) contains at least one edge in \( H \). Let \( \mathcal{Y} \) be the set of all \( Y \in \mathcal{H} \) with \( v = \text{lca}_T(Y) \) and \( \{\text{par}_T(v), v\} \in H \). For all \( Y \in \mathcal{Y} \subseteq \mathcal{H} \setminus \{X\} \), therefore, there is an \( A \in \mathcal{P} \) such that \( Y = A_H \).

Now consider an arbitrary refinement \( \mathcal{H}^* \) of \( \mathcal{H} \) and the corresponding refinement \( T^* \) of \( T \). By construction, we have \( \mathcal{Y} \subset \mathcal{Y} \subseteq \mathcal{H}^* \). For each \( Y \in \mathcal{Y} \), we set \( v_Y := \text{lca}_T(Y) \) and set

\[
H^* := \{\{\text{par}_{T^*}(v_Y), v_Y\} \mid Y \in \mathcal{Y}\}
\]

Since \( X \notin \mathcal{Y} \) by construction, we have \( v_Y \neq \rho_{T^*} \) and thus \( \text{par}_{T^*}(v_Y) \) and, in particular, \( H^* \) is well-defined.

Now consider two arbitrary two vertices \( a \in A \) and \( b \in B \) in distinct \( A, B \in \mathcal{P} \). As argued above, the path connecting them in \( T \) contains an edge \( \{\text{par}_T(v), v\} \in H \). By construction, we
have \( Y := L(T(v)) \in \mathcal{Y} \). We can assume w.l.o.g. that \( a \in Y \) and \( b \in X \setminus Y \). This together with \( Y \in H^* \) implies that the path connecting \( a \) and \( b \) in \( T^* \) contains the edge \( \{ \text{par}_T(v_Y), v_Y \} \). By construction of \( H^* \) and since \( Y \in \mathcal{Y} \), we have \( \{ \text{par}_T(v_Y), v_Y \} \in H^* \).

It remains to show that the path in \( T^* \) connecting any two \( a, a' \in A \) for some \( A \in P \) never contains an edge that is in \( H^* \). Assume, for contradiction, that this is the case, i.e., there is an edge \( \{ \text{par}_T(v), v \} \in H^* \) such that w.l.o.g. \( a \in L(T(v)) = Y^* \) and \( a' \in X \setminus Y^* \). By construction of \( H^*, Y^* \in \mathcal{Y} \) and \( Y^* = B^H \) for some \( B \in P \). Since \( H^* \) and \( P \) are compatible, Thm. 4.5(i) implies that \( Y^* = B^H \) is the union of sets of \( P \); a contradiction to the fact that \( a \in Y^* \) and \( a' \notin Y^* \).

In summary, we conclude that \( \mathcal{P} = F(T^*, H^*) \), and, therefore, \( \mathcal{P} \) is compatible with \( H^* \). □

We next provide a necessary condition for \( r \)-compatibility. We will show later that this condition is also sufficient.

**Lemma 5.2.** Let \( H \) be a hierarchy on \( X \) and \( P \) a partition of \( X \). If \( P \) is compatible with a refinement \( H^* \) of \( H \), then there is no set \( Y \in \mathcal{H} \) that overlaps with two distinct sets \( A, B \in P \).

**Proof.** Let \( P \) and \( H^* \) with \( \mathcal{H} \subseteq H^* \) be compatible. Assume, for contradiction, that some \( Y \in \mathcal{H} \) overlaps with two distinct \( A, B \in P \). First observe that \( Y \in H^* \). Now consider \( A_H^* \) and \( B_H^* \).

Since \( A \neq B \) and \( P \) is compatible with \( H^* \), we have \( A_H^* \neq B_H^* \) by contraposition of Thm. 4.5(ii).

Since \( Y \) overlaps with \( A \) and \( B \), both \( A \) and \( B \), and thus \( A_H^* \) and \( B_H^* \), contain elements that are in \( Y \) as well as elements that are not in \( Y \). This together with the fact that \( Y \), \( A_H^* \), and \( B_H^* \), are all sets in \( H^* \) implies that \( Y \subseteq A_H^* \) and \( Y \subseteq B_H^* \). Therefore, we have \( Y \subseteq A_H^* \cap B_H^* \). Since \( Y \neq \emptyset \), \( H^* \) is a hierarchy, and \( A_H^* \neq B_H^* \), this implies that either \( A_H^* \subseteq B_H^* \) or \( B_H^* \subseteq A_H^* \). Assume w.l.o.g. that \( A_H^* \subseteq B_H^* \). Since \( Y \) overlaps with \( B \) and \( Y \subseteq A_H^* \), we have \( A_H^* \cap B \neq \emptyset \). However, since \( A_H^* \subseteq B_H^* \) and \( B_H^* \) is inclusion-minimal for \( B \) in the hierarchy \( H^* \), we conclude that \( B \) and \( A_H^* \) overlap. Hence, \( A_H^* \) is not the union of sets of \( P \). This violates Condition (i) for compatible partitions in Thm. 4.5; a contradiction. □

To show that the converse of Lemma 5.2 is satisfied as well, we will explicitly construct a compatible refinement of \( H \). To this end, we introduce the following subset of a partition \( P \):

\[
\mathcal{Y}(H, P) := \{ A \in P \mid \exists B \in P \setminus \{ A \} \text{ with } B \cap A_H^* \neq \emptyset \text{ and } A_H^* \subseteq B_H^* \}
\]

(5)

The set \( \mathcal{Y}(H, P) \) contains the sets \( A \in P \) for which \( A_H^* \in \mathcal{H} \) or, equivalently, the vertex \( u = \text{lca}_T(A) \) is “not resolved enough”:

**Proposition 5.3.** A hierarchy \( H \) on \( X \) and a partition \( P \) of \( X \) are compatible if and only if \( \mathcal{Y}(H, P) \) is empty.

**Proof.** By Thm. 4.5, \( H \) and \( P \) are compatible if and only if, for all \( A, B \in P \), the following two conditions are satisfied: (i) \( A_H^* \) is a union of sets of \( P \), and (ii) \( A_H^* = B_H^* \) implies \( A = B \). Hence, it suffices to show that \( \mathcal{Y}(H, P) = \emptyset \) is equivalent to these two conditions.

First assume, for contraposition, that \( \mathcal{Y}(H, P) \) is not empty. Hence, there are distinct \( A, B \in P \) such that \( B \cap A_H^* \neq \emptyset \) and \( A_H^* \subseteq B_H^* \). If \( A_H^* = B_H^* \), then Condition (i) is violated. If on the other hand \( A_H^* \subseteq B_H^* \), then the fact that \( B_H^* \) is inclusion-minimal for \( B \) implies that \( B \setminus A_H^* \neq \emptyset \). This together with \( B \cap A_H^* \neq \emptyset \) in turn implies that \( A_H^* \) is not a union of sets of \( P \); a violation of Condition (i).

The converse can be shown by very similar arguments starting with the assumption that Condition (i) or (ii) is not satisfied. If Condition (i) does not hold, then \( A_H^* \neq X \) and, in particular, there is a \( B \in P \) such that \( A_H^* \setminus B \) and \( B \) overlap. Since \( H \) is a hierarchy, it holds that \( A_H^* \subseteq B_H^* \subseteq X \). The latter two arguments imply \( \mathcal{Y}(H, P) \neq \emptyset \) since it contains \( A \). If Condition (ii) does not hold, then there are two distinct elements \( A, B \in P \) with \( A_H^* = B_H^* \). Hence, \( B \subseteq B_H^* \) implies \( B \cap A_H^* \neq \emptyset \). Thus, \( A \in \mathcal{Y}(H, P) \). □

In particular, the set \( \mathcal{Y}(H, P) \) can be used to characterize the cases in which a compatible refinement of \( H \) exists and, if this is the case, to construct such a refinement.

**Definition 5.4.** Let \( H \) be a hierarchy on \( X \) and \( P \) a partition of \( X \) such that no set \( Y \in \mathcal{H} \) overlaps with two distinct sets \( A, B \in P \). We define, for \( A \in \mathcal{Y}(H, P) \), the subset \( Y_A \) of \( A_H^* \) as

\[
Y_A := W_1 \cup W_2 \cup \ldots \cup W_k
\]

where \( W_1, W_2, \ldots, W_k \in \mathcal{H} \) are the child clusters of \( A_H^* \) for which \( W_i \cap A \neq \emptyset \). Moreover, the subset \( H_{\mathcal{Y}} \) of \( 2^X \) is given by

\[
H_{\mathcal{Y}} := \mathcal{H} \cup \{ Y_A \mid A \in \mathcal{Y}(H, P) \}.
\]
Note that, by Eq. (5), for every $A \in \mathcal{Y}(\mathcal{H}, \mathcal{P})$, the set $A_{\mathcal{H}}$ cannot be a singleton. Since $A_{\mathcal{H}}$ is inclusion-minimal w.r.t. $A$, by definition, we immediately conclude that $k \geq 2$ and thus the $W_i$ are proper subsets of $Y_A$. In terms of the tree $T$ corresponding to $\mathcal{H}$, the vertices $w_i \coloneqq \text{lca}_T(W_i)$ are the children of $y \coloneqq \text{lca}_T(A_{\mathcal{H}})$ with $A \cap \bigcup_i L(T(w_i)) \neq \emptyset$.

**Lemma 5.5.** Let $\mathcal{H}$ be a hierarchy on $X$ and $\mathcal{P}$ a partition of $X$ such that no set $Y \in \mathcal{H}$ overlaps with two distinct sets $A, B \in \mathcal{P}$. Then the following two statements are satisfied:

1. For each $A \in \mathcal{Y}(\mathcal{H}, \mathcal{P})$, it holds $Y_A \notin \mathcal{H}$ and, in particular, $Y_A \subseteq A_{\mathcal{H}}$.

2. The set $\mathcal{H}_P$ is a hierarchy.

**Proof.** To show (1), set $A \in \mathcal{Y} \coloneqq \mathcal{Y}(\mathcal{H}, \mathcal{P})$. By construction, we have $Y_A \subseteq A_{\mathcal{H}}$. Assume for contradiction that $Y_A = A_{\mathcal{H}}$, i.e., all child clusters of $A_{\mathcal{H}}$ in $\mathcal{H}$ have a non-empty intersection with $A$. By definition of $\mathcal{Y}$, we must have $|A_{\mathcal{H}}| > 1$ and, in particular, $A_{\mathcal{H}}$ has a child cluster $Y' \subseteq A_{\mathcal{H}}$ satisfying $B \cap Y' \neq \emptyset$ for some $B \in \mathcal{P} \setminus \{A\}$ such that $A_{\mathcal{H}} \subseteq B_{\mathcal{H}}$. Thus $Y' \setminus A \neq \emptyset$ and $A \setminus Y' \neq \emptyset$, i.e., $A$ and $Y'$ overlap. Since $Y' \subseteq A_{\mathcal{H}} \subseteq B_{\mathcal{H}}$ and $B_{\mathcal{H}}$ is inclusion-minimal w.r.t. $B$, we conclude that $B \setminus Y' \neq \emptyset$. On the other hand, since $Y' \cap A \neq \emptyset$ and $A, B \in \mathcal{P}$ are disjoint, we have $Y' \setminus B \neq \emptyset$. Thus $B$ and $Y'$ overlap. Thus there are two distinct sets $A, B \in \mathcal{P}$ that overlap with $Y' \in \mathcal{H}$. This contradicts the assumption that no such pair of sets exists, hence $Y_A \neq A_{\mathcal{H}}$. Since $Y_A \subseteq Y$ by construction, $Y_A$ is a proper subset of $A_{\mathcal{H}}$. This together with the fact that $\mathcal{H}$ is a hierarchy and $Y_A$ is the union of at least two child clusters of $A_{\mathcal{H}}$ in $\mathcal{H}$ implies that $Y_A \notin \mathcal{H}$.

We proceed by showing that the set system $\mathcal{H}_P = \mathcal{H} \cup \{Y_A \mid A \in \mathcal{Y}\}$ is again a hierarchy and thus, that (2) is satisfied. To this end, consider first one of the newly-created sets $Y_A = W_1 \cup W_2 \cup \ldots \cup W_k$ and an arbitrary set $Y' \in \mathcal{H}$. If $W_i \cap Y' = \emptyset$ for all $1 \leq i \leq k$, then $Y_A \subseteq Y' = \emptyset$. Otherwise, there is some $W_i$ such that $W_i \cap Y' \neq \emptyset$. Since both $W_i$ and $Y'$ are sets of the hierarchy $\mathcal{H}$, this implies that $Y' \subseteq W_i \subseteq Y_A$, or $W_i \subseteq Y'$. In the latter case, we have $A_{\mathcal{H}} \subseteq Y'$ by the hierarchy property of $\mathcal{H}$ and the fact that $W_i$ is a child cluster of $A_{\mathcal{H}}(\in \mathcal{H})$. Hence, we have $Y_A \cap Y' \subseteq \{\emptyset, Y_A, Y'\}$ for all $Y' \in \mathcal{H}$. Now consider two newly-created sets $Y_A$ and $Y_B$ for distinct $A, B \in \mathcal{Y}$, and assume first that $A_{\mathcal{H}} \neq B_{\mathcal{H}}$. If $A_{\mathcal{H}} \cap B_{\mathcal{H}} = \emptyset$, then $Y_A \subseteq Y_B$ and $Y_B \subseteq Y_A$ immediately imply that $Y_A \cap Y_B = \emptyset$. Otherwise, we can assume w.l.o.g. that $B_{\mathcal{H}} \subseteq A_{\mathcal{H}}$ since $A_{\mathcal{H}}$ and $B_{\mathcal{H}}$ are both sets in the hierarchy $\mathcal{H}$. This together with the fact that $Y_A$ is the union of child clusters $W_1, W_2, \ldots, W_k \in \mathcal{H}$ of $A_{\mathcal{H}}$ implies that either $B_{\mathcal{H}} \subseteq W_i$ for some $1 \leq i \leq k$, and thus $Y_B \subseteq W_i \subseteq Y_A$, or, if no such $W_i$ exists, $Y_B \cap Y_A = \emptyset$. It remains to consider two distinct sets $A, B \in \mathcal{Y}$ with $A_{\mathcal{H}} = B_{\mathcal{H}}$. If $Y_A$ and $Y_B$ overlap, then there is by construction a child cluster $W' \subseteq A_{\mathcal{H}} = B_{\mathcal{H}}$ in $\mathcal{H}$ such that $W' \cap A \neq \emptyset$ and $W' \cap B \neq \emptyset$. Since, moreover, $A_{\mathcal{H}} = B_{\mathcal{H}}$ is inclusion-minimal w.r.t. $A$ and $B$, this implies that $W' \in \mathcal{H}$ overlaps with both $A$ and $B$: a contradiction to the assumption. Thus $Y_A$ and $Y_B$ are disjoint. In summary, no two sets in $\mathcal{H}_P$ overlap. Since $\mathcal{H} \subseteq \mathcal{H}_P$, $X \in \mathcal{H}$ and $\{x\} \in \mathcal{H}$ for all $x \in X$, we conclude that $\mathcal{H}_P$ is a hierarchy that refines $\mathcal{H}$. \[\square\]

The final step towards characterizing $r$-compatibility is a sufficient condition for $\mathcal{H}_P$ to be compatible with $\mathcal{P}$.

**Lemma 5.6.** Let $\mathcal{H}$ be a hierarchy on $X$ and $\mathcal{P}$ a partition of $X$. If no set $Y \in \mathcal{H}$ that overlaps with two distinct sets $A, B \in \mathcal{P}$, then the hierarchy $\mathcal{H}_P$ is compatible with $\mathcal{P}$.

**Proof.** Recall that $\mathcal{H}_P$ is a hierarchy by Lemma 5.5(2). To prove that $\mathcal{H}_P$ is compatible with $\mathcal{P}$, we show that the Condition (i) and (ii) in Thm. 4.5 are satisfied for $\mathcal{H}_P$ and $\mathcal{P}$.

To show Condition (i) in Thm. 4.5, we assume, for contradiction, that there is a set $A \in \mathcal{P}$ for which $A_{\mathcal{H}_P}$ is not the union of sets of $\mathcal{P}$. Thus there is a set $B \in \mathcal{P} \setminus \{A\}$ such that $A_{\mathcal{H}_P} \cap B \neq \emptyset$ and $B \setminus A_{\mathcal{H}_P} \neq \emptyset$. We distinguish the two cases (1) $A_{\mathcal{H}_P} \notin \mathcal{H}$ and (2) $A_{\mathcal{H}_P} \in \mathcal{H}$.

In case (1), we have $A_{\mathcal{H}_P} = Y_A$ for some $A \in \mathcal{Y}$. Thus $A_{\mathcal{H}_P}$ is the union $W_1 \cup W_2 \cup \ldots \cup W_k$ of $k \geq 2$ sets $W_1, W_2, \ldots, W_k \in \mathcal{H}$ all satisfying $W_i \cap A' \neq \emptyset$. Since $B \setminus A_{\mathcal{H}_P} \neq \emptyset$ and by construction $A' \subseteq Y_A = A_{\mathcal{H}_P}$, we have $A' \neq B$. Since $A_{\mathcal{H}_P} \cap B \neq \emptyset$, there must be some $W' \subseteq \{W_1, W_2, \ldots, W_k\} \in \mathcal{H}$ such that $B \cap W' \neq \emptyset$. Since $W' \subseteq A_{\mathcal{H}_P}$ and $B \setminus A_{\mathcal{H}_P} \neq \emptyset$, we have $B \setminus W' \neq \emptyset$. On the other hand, we also have $A' \setminus W' \neq \emptyset$ because $k \geq 2$ and $W_i \cap A' \neq \emptyset$ for all $1 \leq i \leq k$. Since $A'$ and $B$ are disjoint and both have a non-empty intersection with $W'$, we also obtain $W' \setminus A' \neq \emptyset$ and $W' \setminus B \neq \emptyset$. In summary, the set $W' \in \mathcal{H}$ overlaps with the two distinct sets $A', B \in \mathcal{P}$; a contradiction to the assumption.

In case (2), we have $A_{\mathcal{H}_P} \in \mathcal{H}$. Since $A_{\mathcal{H}_P}$ is inclusion-minimal for $A$ in $\mathcal{H}_P$ and $\mathcal{H} \subseteq \mathcal{H}_P$, we conclude that $A_{\mathcal{H}_P}$ is also inclusion-minimal for $A$ in $\mathcal{H}$, and thus $A_{\mathcal{H}} = A_{\mathcal{H}_P}$. Since $A_{\mathcal{H}} \cap B \neq \emptyset$, $B \setminus A_{\mathcal{H}_P} \neq \emptyset$, and $\mathcal{H}$ is a hierarchy, we conclude that $A_{\mathcal{H}} \subseteq B_{\mathcal{H}}$. In summary, we obtain $A \in \mathcal{Y}$.
Hence, we have added a set $Y_A$ that satisfies $A \subseteq Y_A$ and, by the arguments above, $Y_A \subseteq A_H$. Therefore, $A_{Y_A}$ is not inclusion-minimal for $A$ in $H^*_P$; a contradiction.

To show Condition (ii) in Thm. 4.5, we assume, for contradiction, that $Y^* := A_{Y_A}$ for two distinct $A, B \in \mathcal{P}$. As above, we distinguish the two cases (1') $Y^* \notin H$ and (2') $Y^* \in H$.

In case (1'), we have $Y^* = Y_A$ for some $A \in \mathcal{P}$, Thus $Y^*$ is the union $W_1 \cup W_2 \cup \ldots \cup W_k$ of $k \geq 2$ sets $W_1, W_2, \ldots, W_k \in H$ all satisfying $W_i \cap A' \neq \emptyset$. Since $A$ and $B$ are distinct, we can assume w.l.o.g. that $A' \neq B$. Since $Y^* \cap B \neq \emptyset$, there must be some $W' \in \{W_1, W_2, \ldots, W_k\}$ such that $B \cap W' \neq \emptyset$. Since $W' \subseteq Y^*$ and $Y^*$ is inclusion-minimal for $B$ in $H^*_P$, we have $B \cap W' \neq \emptyset$. On the other hand, we also have $A' \cap W' \neq \emptyset$ since $k \geq 2$ and $W_i \cap A' \neq \emptyset$ for all $1 \leq i \leq k$. Since $A'$ and $B$ are disjoint and both have a non-empty intersection with $W'$, we also obtain $W' \cap A' \neq \emptyset$ and $W' \cap B \neq \emptyset$. In summary, the set $W' \in H$ overlaps with the two distinct sets $A', B \in \mathcal{P}$, a contradiction to the assumption.

In case (2'), we have $Y^* \in H$. Together with the facts that $Y^*$ is inclusion-minimal for $A$ in $H^*_P$ and that $H \subseteq H^*_P$, $Y^* \in H$ implies that $Y^*$ is also inclusion-minimal for $A$ in $H$, i.e. $Y^* = A_H$. Analogous arguments imply $Y^* = B_H$. Since $Y^* \cap B \neq \emptyset$ we conclude that $A \in \mathcal{P}$. Therefore, we have added a set $Y_A$ that satisfies both $A \subseteq Y_A$ and, by the arguments above, $Y_A \subseteq Y^*$. Therefore, $Y^*$ is not inclusion-minimal for $A$ in $H^*_P$; a contradiction.

In summary, $H^*_P$ is a hierarchy on $X$ such that Conditions (i) and (ii) in Thm. 4.5 are satisfied for all $A, B \in \mathcal{P}$. Thus $\mathcal{P}$ is compatible with the refinement $H^*_P$ of $H$.

**Theorem 5.7.** A hierarchy $H$ and a partition $\mathcal{P}$ on $X$ are $r$-compatible if and only if no set $Y \in H$ overlaps with two distinct sets $A, B \in \mathcal{P}$.

**Proof.** The only-if-direction follows from Lemma 5.2. Conversely, if no set $Y \in H$ overlaps with two distinct sets $A, B \in \mathcal{P}$, then Lemma 5.5(2) and 5.6 imply that the hierarchy $H^*_P$ is compatible with $\mathcal{P}$. By construction, $H \subseteq H^*_P$ and thus, $H^*_P$ is a refinement of $H$, which completes the proof.

It is worth noting that the characterization of $r$-compatibility in Thm. 5.7 implies neither Property (i) nor Property (ii) in Thm 4.5. As a counterexample to (i), consider the hierarchy $H$ on $X = \{a, a', b, b'\}$ that comprises in addition to $X$ and the singletons only the set $Y = \{a, a', b\}$, and the partition $\mathcal{P} = \{A, B\}$ with $A = \{a, a'\}$ and $B = \{b, b'\}$. We have $A_H = Y$ and $B_H = X$. Clearly, $Y = A_H$ overlaps $B$ and thus violates (i). On the other hand, it admits the refinement $H^* = H \cup \{A\}$, which is compatible with $\mathcal{P}$. As a counterexample to (ii), consider $H'$ comprising only $X$ and the singletons. Here, we have $A_H = B_H = X$, while both refinements $H' \cup \{A\}$ and $H' \cup \{B\}$ are compatible with $\mathcal{P}$.

We continue with considering systems $\mathfrak{P} = \{\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_k\}$ of partitions of $X$ rather then single partitions. By definition, $T$ (or equivalently the hierarchy $H(T)$) and each $\mathcal{P}_i$ are compatible if and only if $\mathcal{P}_i = \mathcal{F}(T, H_i)$ for some subset $H_i \subseteq E(T)$, $1 \leq i \leq k$. In this case, we say that $T$ (equiv. $H(T)$) and $\mathfrak{P}$ are compatible. It is natural, then, to ask whether for a given system of partitions $\mathfrak{P}$, there exists a tree $T$ such that $\mathfrak{P}$ and $T$ are compatible.

**Proposition 5.8.** Let $H$ be a hierarchy on $X$ and $\mathfrak{P} = \{\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_k\}$ be a collection of partitions of $X$. The following two statements are equivalent

1. There is a refinement $H^*$ of $H$ that is compatible with $\mathfrak{P}$.
2. Each $\mathcal{P}_i \in \mathfrak{P}$ admits a compatible refinement $H^*_i$ of $H$ such that $\bigcup_{i=1}^k H^*_i$ is a hierarchy.

**Proof.** Let $H^*$ be a refinement of $H$ that is compatible with $\mathfrak{P}$ and thus, with every $\mathcal{P}_i \in \mathfrak{P}$. Now, put $H^*_i = H^*$, $1 \leq i \leq k$. Hence, $H^* = \bigcup_{i=1}^k H^*_i$ is a hierarchy that is compatible with $\mathfrak{P}$. Conversely, if $\bigcup_{i=1}^k H^*_i$ is a hierarchy, then it is, in particular, a refinement of every $H^*_i$, $1 \leq i \leq k$. Now set $H^* = \bigcup_{i=1}^k H^*_i$. By Prop. 5.1, $H^*$ is compatible with with every $\mathcal{P}_i \in \mathfrak{P}$.

Prop. 5.8 immediately implies

**Corollary 5.9.** There is a tree $T$ that is compatible with a collection $\mathfrak{P} = \{\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_k\}$ of partitions of $X$ if and only if, for every $i \in \{1, \ldots, k\}$, there is a tree $T_i$ that is compatible with $\mathcal{P}_i$ such that $\bigcup_{i=1}^k H(T_i)$ is a hierarchy.

**Proof.** Since every tree on $X$ is a refinement of the star tree $T'$ on $X$, every hierarchy $H^*$ on $X$ is a refinement of $H(T')$. Hence, the existence of some hierarchy or, equivalently, some tree that is compatible with $\mathfrak{P}$ is equivalent to the existence of a refinement of $H^*$ of $H(T')$ that is compatible with $\mathfrak{P}$.
exists is an NP-complete problem. However, there is no refinement $H^\ast(T)$ of $H(T)$ (and thus of $H(T_1)$ and $H(T_2)$) that is compatible with both $P_1$ and $P_2$ as a consequence of Prop. 6.2 and the fact that the unrooted versions $T_1^\ast$ and $T_2^\ast$, resp., are determined by the splits $\{a,b\}\{c,d\}$ and $\{b,c\}$, resp., which cannot be represented in a common unrooted tree (cf. “Splits-Equivalence Theorem” [18, Thm. 3.1.4]).

As illustrated in Fig. 4, $H^\ast$ and $\Psi = \{P_1, P_2, \ldots, P_k\}$ might be compatible, although there are refinements $H_i^\ast$ of $H$ compatible with $P_i \in \Psi$, whose union $\bigcup_{i=1}^k H_i^\ast$ does not form a hierarchy. Fig. 7, furthermore, shows an example of a partition system $\Psi$ that is not compatible with any refinement of $H$. We will show in Section 7 that deciding whether or not such a common refinement exists is an NP-complete problem.

The partitions of a set $X$ form a complete lattice [2, Sect. 4.9]. The common refinement $P_1 \wedge P_2$ of two partitions $P_1$ and $P_2$ of $X$ is

$$P_1 \wedge P_2 := \{A_1 \cap A_2 \mid A_1 \in P_1, A_2 \in P_2, A_1 \cap A_2 \neq \emptyset\}. \quad (6)$$

The common refinement operation is associative and commutative. The common refinement of an arbitrary system $\Psi$ of partitions, therefore, consists of all distinct sets $P_x = \bigcap_{A \in P} \chi_{x \in A} A$. The following statements are equivalent.

**Proposition 5.10.** Let $T$ be a tree with leaf set $X$ and $\Psi = \{P_1, P_2, \ldots, P_k\}$ a collection of partitions on $X$ that are all compatible with $T$. Then, $\bigwedge_{i=1}^k P_i$ is compatible with $T$.

**Proof.** Let $T$ be a tree with leaf set $X$. We show first that for all subsets $H_1, H_2 \in E(T)$ it holds that

$$F(T, H_1 \cup H_2) = F(T, H_1) \cap F(T, H_2). \quad (7)$$

To see this, let $A \in F(T, H_1) \cap F(T, H_2)$. Then, for all $a, a' \in A$ there is a separating edge in $H_1$ and in $H_2$ that is on the path between $a$ and $a'$ in $T$.

1. $a, a' \in A = A_1 \cap A_2$ for some $A_1 \in F(T, H_1), A_2 \in F(T, H_2)$,
2. there is no separating edge in $H_1$ and in $H_2$ that is on the path between $a$ and $a'$ in $T$,
3. there is no separating edge in $H_1 \cup H_2$ that is on the path between $a$ and $a'$ in $T$, and
4. $a, a' \in B \in F(T, H_1 \cup H_2)$.

Hence, $A \subseteq B \in F(T, H_1 \cup H_2)$. Similarly, the latter equivalent statements hold for all $a, a' \in B \in F(T, H_1 \cup H_2)$ and thus, $A = B$.

Now assume that $P_1, P_2, \ldots, P_k$ are all compatible with $T$. Hence, for each $P_i$ there is a set $H_i \subseteq E(T)$ such that $P_i = F(T, H_i)$. By the latter arguments and since $\wedge$ is commutative and associative, we can conclude that

$$\bigwedge_{i=1}^k P_i = \bigwedge_{i=1}^k F(T, H_i) = F(T, \bigcup_{i=1}^k H_i)$$

and thus, $\bigwedge_{i=1}^k P_i$ is compatible with $T$. \hfill $\square$

The converse of Prop. 5.10 is not true in general. As an example, consider the tree $T$ as shown in Fig. 7 and the two partitions $P_1 = \{\{a,b\}, \{c,d\}\}$ and $P_2 = \{\{a,c\}, \{b,d\}\}$. Both $P_1$ and $P_2$ are not compatible with $T$, however, their common refinement $P_1 \wedge P_2 = \{\{a\}, \{b\}, \{c\}, \{d\}\}$ is $F(T, E(T))$.

The refinement supremum or join $P_1 \vee P_2$ is obtained by recursively unifying any two sets $A_1, A'_1 \in P_1$ whenever there is $A_2 \in P_2$ such that $A_1 \cap A_2 \neq \emptyset$ and $A'_1 \cap A_2 \neq \emptyset$. The analogue to Prop. 5.10 does not hold for the refinement supremum. To see this, consider the tree $T$ on $X = \{a, b, c, d\}$ with hierarchy $H(T) = X \cup \{\{x\} \mid x \in X\} \cup \{\{a, b\}, \{a', b'\}\}$ and the partitions $P_1 = \{\{a, a'\}, \{b\}, \{b'\}\}$ and $P_2 = \{\{a\}, \{a'\}, \{b, b'\}\}$. Both $P_1$ and $P_2$ are compatible with $T$ (just
define the edges incident to the $x$ for respective singletons \{x\} as separating edges). However, $\mathcal{P}_1 \cup \mathcal{P}_2 = \{A := \{a,a'\}, B := \{b,b'\}\}$ is not compatible since, for the hierarchy $\mathcal{H}$ corresponding to $T$, we have $A_B = B_H$; a contradiction to Condition (ii) in Thm. 4.5. In [19], a notion of local comparability of partitions is considered: $\mathcal{P}_1 \simeq \mathcal{P}_2$ iff $A_1 \cap A_2 \subseteq \{\emptyset, A_1, A_2\}$ for all $A_1 \in \mathcal{P}_1$ and $A_2 \in \mathcal{P}_2$. The example above satisfies $\mathcal{P}_1 \simeq \mathcal{P}_2$. Hence, local comparability of partitions $\mathcal{P}_1$ and $\mathcal{P}_2$ compatible with a given hierarchy $\mathcal{H}$ is also not sufficient to imply compatibility of $\mathcal{P}_1 \cup \mathcal{P}_2$ and $\mathcal{H}$.

6 Compatibility of Partitions with Split Systems and Unrooted Trees

Throughout this section, we will assume that all unrooted trees are phylogenetic as well and have at least three leaves. In particular, therefore, they have at least one inner vertex. Not surprisingly, there is a very close connection between the case of rooted and unrooted phylogenetic trees.

**Proposition 6.1.** Let $T$ be an unrooted tree with leaf set $X$ and let $\mathcal{P}$ be a partition of $X$. Then $\mathcal{P}$ and $T$ are compatible if and only if $\mathcal{P}$ and the rooted tree $T'$ are compatible, where $T'$ is obtained by rooting $T$ at an arbitrary inner vertex.

**Proof.** Note that rooting $T$ at an arbitrary inner vertex results in a phylogenetic rooted tree $T$, since $T$ does not contain vertices of degree two. The equivalence now follows immediately from the definition and the fact that, viewed as pair of a set vertices and a set of edges, $T = T'$ and therefore, $\mathcal{P} = F(T, H) = F(T', H)$ for some subset $H \subseteq E(T)$.

In fact, it is not necessary to root $T$ at an inner vertex, we may as well place the root as a subdivision of any edge. This allows us to connect unrooted trees directly to hierarchies:

**Proposition 6.2.** Let $\mathcal{H}$ be a hierarchy with corresponding rooted tree $T$ with leaf set $X$ and let $\mathcal{P}$ be a partition of $X$. Then $\mathcal{H}$ and $\mathcal{P}$ are compatible if and only if the unrooted tree $T$ obtained from $T$ by suppressing a possible degree-two root) is compatible with $\mathcal{P}$.

**Proof.** If the root $\rho$ of $T$ has degree greater than two, then the tree $T$ is phylogenetic and thus, we can apply the same arguments as in the proof of Prop. 6.1 to establish the equivalence. If $\rho$ has degree 2, then the tree $T$ is not phylogenetic and both edges $e_1 = \{\rho, v_1\}$ and $e_2 = \{\rho, v_2\}$ that are incident to $\rho$ define the same split $S_{e_1} = S_{e_2}$. Since $\mathcal{S}(T)$ contains a split only once, the unique phylogenetic tree $\mathcal{T}$ defined by the split system $\mathcal{S}(T)$ is obtained from $T$ by suppressing the root $\rho$, i.e., $e^* := \{v_1, v_2\} \in E(T)$. Now let $H \subseteq E(T)$ be such that $F(T, H) = \mathcal{P}$. If $e_1$ or $e_2$ is contained in $H$, we add the edge $e^*$ to $H \setminus \{e_1, e_2\}$ to obtain the set $H^* \subseteq E(T)$ and, otherwise, we put $H^* = H$. It is now easy to see that $F(T, H) = F(T, H^*)$ and thus, $\mathcal{T}$ and $\mathcal{P}$ are compatible.

As outlined in Section 2, every unrooted phylogenetic tree $T$ is determined by its split system $\mathcal{S}(T) = \{S_e: e \in E(T)\}$ and for a tree-like split system $\mathcal{S}$ there is a (unique) unrooted tree $\mathcal{T}$ with $\mathcal{S}(T) = \mathcal{S}$. Since unrooted trees are so intimately related with split systems, it is interesting, therefore, to ask whether the compatibility of rooted trees or hierarchies and partitions can also be expressed in an interesting way in terms of split systems.

**Corollary 6.3.** For every partition $\mathcal{P}$ of a non-empty set $X$, the split system $\mathcal{S}_\mathcal{P} := \mathcal{S}_P \cup \{x|(X \setminus \{x\}): x \in X\}$ with

\[ \mathcal{S}_P := \{A|(X \setminus A): A \in \mathcal{P}\} \quad (8) \]

is always tree-like and compatible with $\mathcal{P}$.

**Proof.** It is easy to see that the hierarchy $\mathcal{H}_\mathcal{P}$ (as specified in Lemma 4.1) yields a rooted tree $T$ for which the unrooted version $\mathcal{T}$ (by suppressing a possible degree-two root of $T$) satisfies $\mathcal{S}(\mathcal{T}) = \mathcal{S}_\mathcal{P}$. Now apply Prop. 6.2.

Compatibility of a partition $\mathcal{P}$ with a split system $\mathcal{S}(\mathcal{T})$ of some tree, however, does not imply that $\mathcal{S}(\mathcal{T}) = \mathcal{S}_\mathcal{P}$, see Fig. 8. Suppose that $\mathcal{T}$ and $\mathcal{P}$ are compatible, i.e., that $\mathcal{P} = F(\mathcal{T}, H)$. The set $H$ of separating edges then corresponds to the set

\[ \mathcal{S}_H := \{S_e: e \in H\} \subseteq \mathcal{S}(\mathcal{T}) \]

of splits. Then we have either

\[ B \subseteq A \text{ or } B \subseteq X \setminus A \quad \text{for every } A|(X \setminus A) \in \mathcal{S}_H \text{ and every } B \in \mathcal{P} \quad (9) \]
since none of the edges \( e \in H \) separates two vertices of \( B \). Furthermore, for any two distinct sets \( A, A' \in \mathcal{P} \) there is a split \( B|B' \in \mathcal{S}_{H,T} \) such that, w.l.o.g., \( A \subseteq B \) and \( A' \subseteq B' \) because there must be an edge in \( H \) separating \( A \) and \( A' \) in \( T \). Taken together, therefore, we observe that every set \( B \in \mathcal{P} \) satisfies
\[
B = \bigcap \left\{ A \in 2^X : A|(X \setminus A) \in \mathcal{S}_{H,T}, B \subseteq A \right\}.
\] (10)

Conversely, suppose that an arbitrary split system \( \mathcal{S} \) satisfies Eqs. (9) and (10) (replace \( \mathcal{S}_{H,T} \) by \( \mathcal{S} \) in the equations). By Eq. (10), for every \( B' \in \mathcal{P} \) with \( B \neq B' \) and thus \( B \cap B' = \emptyset \), there is a split \( A|(X \setminus A) \) such that \( B \subseteq A \) and \( B' \subseteq X \setminus A \) and thus there is an edge \( e_{B,B'} \in E(T) \) that separates \( B \) and \( B' \) in \( T \). Add all these edges to the set \( H \). Eq. (9) ensures that no two elements in \( B \) are separated by an edge in \( H \). Thus, \( B \in \mathcal{F}(T,H) \) for every \( B \in \mathcal{P} \). Hence, \( \mathcal{P} \) and \( T \) are compatible if and only if \( \mathcal{S} \subseteq \mathcal{S}(T) \) satisfies Eqs. (9) and (10). Recall that splits on \( X \) are partitions of \( X \) and that the common refinement of a set \( \mathcal{P} \) of partitions of \( X \) is the partition \( \bigwedge \mathcal{P} \) whose sets are the intersections \( B_x := \bigcap \{ B \in \mathcal{P} \in \mathcal{F}(T) \text{ s.t. } x \in B \} \) of sets appearing in any of the partitions in the system \( \mathcal{P} \) that have a least one point \( x \in X \) in common. Thus, \( \mathcal{S} \subseteq \mathcal{S}(T) \) satisfies Eqs. (9) and (10) if and only if \( \mathcal{P} = \bigwedge \mathcal{S} \). We summarize this discussion as

**Theorem 6.4.** Let \( \mathcal{P} \) be a partition and \( \mathcal{S} \) be a tree-like split system. Then \( \mathcal{P} \) and \( \mathcal{S} \) are compatible if and only if there is a subset \( \mathcal{S} \subseteq \mathcal{S} \) such that \( \mathcal{P} \) is the common refinement of \( \mathcal{S} \). In this case, \( \mathcal{P} = \mathcal{F}(T,H) \) for the tree \( T \) with \( \mathcal{S}(T) = \mathcal{S} \) and \( H = \{ e \in E(T), S_x \subseteq \mathcal{S} \} \).

Since every refinement \( T' \) of a tree \( T \) corresponds to a tree-like split system \( \mathcal{S}(T') \) that satisfies \( \mathcal{S}(T) \subseteq \mathcal{S}(T') \), we immediately obtain a characterization of tree-like split systems that admit a refinement that is compatible with a partition \( \mathcal{P} \).

**Corollary 6.5.** Let \( \mathcal{P} \) be a partition and \( \mathcal{S}(T) \) be the split system associated with a tree \( T \). Then \( \mathcal{P} \) is compatible with a refinement of \( T \) if and only if there is a set of splits \( \mathcal{S} \) such that (i) \( \mathcal{P} \) is the common refinement of \( \mathcal{S} \) and (ii) \( \mathcal{S}(T) \cup \mathcal{S} \) is tree-like.

The characterizations in Thm. 6.4 and Cor. 6.5 are not constructive, i.e., they do not provide recipes to construct \( \mathcal{S} \). Clearly, we can directly employ Prop. 6.1 and the linear-time algorithm provided in Section 7 to check whether a split system and a partition are compatible or not. Nevertheless, we provide the following two lemmas to provide a further constructive characterization that makes use of a step-wise decomposition and might be of further theoretical interest.

**Definition 6.6 ([18, Def. 6.1.1]).** Let \( T \) be an unrooted phylogenetic tree with leaf set \( X \) and corresponding split system \( \mathcal{S}(T) \). Then the restriction \( T|_Y \) of \( T \) to a non-empty subset \( Y \subseteq X \) of leaves is the tree for which
\[
\mathcal{S}(T|_Y) = \{(A \cap Y)|(Y \setminus A) : A|(X \setminus A) \in \mathcal{S}(T), A \cap Y \neq \emptyset, Y \setminus A \neq \emptyset \}.
\]

Somewhat surprisingly, it suffices to check whether there is a single element \( A \in \mathcal{P} \) such that \( \mathcal{P} \setminus \{A\} \) and \( T|_{X \setminus A} \) are compatible, to determine whether \( \mathcal{P} \) and \( T \) are compatible as shown in the next

**Lemma 6.7.** Let \( T \) be an unrooted tree with leaf set \( X \) and let \( \mathcal{P} \) be a partition of \( X \). Then \( \mathcal{P} \) and \( T \) are compatible if and only if \( |\mathcal{P}| = 1 \), or there is a set \( A \in \mathcal{P} \) such that (i) \( A|(X \setminus A) \in \mathcal{S}(T) \) and (ii) \( \mathcal{P} \setminus \{A\} \) and \( T|_{X \setminus A} \) are compatible.

**Proof.** Clearly, every tree on \( X \) is compatible with the partition \( \mathcal{P} = \{X\} \) since \( \{X\} = \mathcal{F}(T, \emptyset) \). Thus, assume \( |\mathcal{P}| > 1 \) in the following. First suppose that \( T \) and \( \mathcal{P} \) are compatible. We first show that there is a set \( A \in \mathcal{P} \) such that \( A|(X \setminus A) \in \mathcal{S}(T) \). Since \( T \) and \( \mathcal{P} \) are compatible, there is an edge set \( H \subseteq E(T) \) such that \( \mathcal{F}(T,H) = \mathcal{P} \) and a corresponding set of splits \( \mathcal{S} := \mathcal{S}_{H,T} \subseteq \mathcal{S}(T) \).
Since $|\mathcal{P}| > 1$ by assumption, both sets $H$ and $\mathcal{S}$ are non-empty. Therefore, we can pick an arbitrary split $S_1|\{X \setminus S_1\} \in \mathcal{S}$. By Eq. (9), every $A \in \mathcal{P}$ satisfies either $A \subseteq S_1$ or $A \subseteq X \setminus S_1$. In particular, there must be some $A \in \mathcal{P}$ with $A \subseteq S_1$. If there is no other split $S_2|\{X \setminus S_2\} \in \mathcal{S}$ with $S_2 \subseteq S_1$, then $S_1 \in \mathcal{P}$ and we are done. Otherwise consider the split $S_2|\{X \setminus S_2\} \in \mathcal{S}$ with $S_2 \subseteq S_1$. Then either there is another split $S_3|\{X \setminus S_3\} \in \mathcal{S}$ with $S_3 \subseteq S_2$ or $S_3 \in \mathcal{P}$. Since $\mathcal{S}$ is finite, we eventually reach a split $S_j|\{X \setminus S_j\} \in \mathcal{H}$ with $S_j \in \mathcal{P}$, i.e., we can choose $A = S_j$ in Condition (i). Now let $e_A \in H$ be the edge in $\mathcal{T}$ with $S_e = A|\{X \setminus A\}$. The restriction $\mathcal{T}_{|Y} = \mathcal{T}$ to $Y = X \setminus A$ is therefore simply the connected component $\mathcal{T}'$ of $\mathcal{T} - e_A$ that does not intersect $A$. Thus $\mathcal{F}(\mathcal{T}_{|X \setminus A}, H \setminus \{e_A\}) = \mathcal{P} \setminus \{A\}$, i.e., Condition (ii) is satisfied.

Conversely, suppose there is an $A \in \mathcal{P}$ such that $\mathcal{P} \setminus \{A\}$ and $\mathcal{T}_{|X \setminus A}$ is compatible and $A|\{X \setminus A\}$ is a split corresponding to an edge in $\mathcal{T}$. Then there is an edge set $H' \subseteq E(\mathcal{T}_{|X \setminus A})$ such that $\mathcal{F}(\mathcal{T}_{|X \setminus A}, H') = \mathcal{P} \setminus \{A\}$. Since $A|\{X \setminus A\} \in \mathcal{S}(\mathcal{T})$, there is an edge $e_A$ in $E(\mathcal{T}) \setminus E(\mathcal{T}_{|X \setminus A})$ connecting the subtrees $\mathcal{T}_{|X \setminus A}$ and $\mathcal{T}_{|A}$. In particular $e_A \notin H'$. Therefore, we have $\mathcal{F}(\mathcal{T}, H' \cup \{e_A\}) = \mathcal{F}(\mathcal{T}_{|X \setminus A}, H') \cup \{A\} = \mathcal{P} \cup \{A\} = \mathcal{T}$ and $\mathcal{T}$ and $\mathcal{P}$ are compatible. □

**Lemma 6.8.** Let $\mathcal{P}$ be a partition of $X$, and $\mathcal{T}$ an unrooted tree with leaf set $X$. Then $\mathcal{T}$ admits a refinement $\mathcal{T}^*$ compatible with $\mathcal{P}$ if and only if $|\mathcal{P}| = 1$, or there is an $A \in \mathcal{P}$ such that (i) for every $B_1|B_2 \in \mathcal{S}(\mathcal{T})$ we have at least one of $A \subseteq B_1$, $A \subseteq B_2$, $B_1 \subseteq A$, or $B_2 \subseteq A$ and (ii) the restriction $\mathcal{T}_{|X \setminus A}$ admits a refinement $\mathcal{T}'_{|X \setminus A}$ that is compatible with $\mathcal{P} \setminus \{A\}$.

**Proof.** For brevity, we write $\mathcal{S} := \mathcal{S}(\mathcal{T})$ and $\mathcal{S}^* := \mathcal{S}(\mathcal{T}^*)$ for the split systems of the two trees $\mathcal{T}$ and $\mathcal{T}^*$. Clearly, every tree on $X$ is compatible with the partition $\mathcal{P} = \{X\}$ since $\{X\} = \mathcal{F}(\mathcal{T}, \emptyset)$. Thus, assume $|\mathcal{P}| > 1$ in the following. Suppose the refinement $\mathcal{T}^*$ (with corresponding split system $\mathcal{S}^*$) of $\mathcal{T}$ is compatible with $\mathcal{P}$. By Lemma 6.7, there is an $A \in \mathcal{P}$ such that $A|\{X \setminus A\}$ is a split in $\mathcal{S}^*$ and $\mathcal{T}'_{|X \setminus A}$ is compatible with $\mathcal{P} \setminus \{A\}$. Clearly, $\mathcal{T}'_{|X \setminus A}$ is a refinement of $\mathcal{T}_{|X \setminus A}$, i.e., $\mathcal{T}_{|X \setminus A}$ admits a refinement that is compatible with $\mathcal{P} \setminus \{A\}$. Since $\mathcal{S}^*$ identifies the tree $\mathcal{T}^*$, it is in particular a tree-like split system. Since $\mathcal{T}^*$ is a refinement of $\mathcal{T}$, we have $\mathcal{S} \subseteq \mathcal{S}^*$. In particular, therefore $A|\{X \setminus A\}$ and every split $B_1|B_2 \in \mathcal{S}$ must have at least one empty intersection $A \cap B_1$, $A \cap B_2$, $(X \setminus A) \cap B_1$, or $(X \setminus A) \cap B_2$. Depending on which of the four intersections is empty, we have one of the following situations $A \subseteq B_2$, $A \subseteq B_1$, $B_2 \subseteq A$, $B_1 \subseteq A$, respectively.

Conversely, suppose there is an $A \in \mathcal{P}$ satisfying conditions (i) and (ii). Then $\mathcal{S}' := \mathcal{S} \cup \{A|\{X \setminus A\}\}$ is a tree-like split system because $\mathcal{S}$ has this property and, for any $B_1|B_2 \in \mathcal{S} \setminus \{A|\{X \setminus A\}\}$, the alternatives in (i) amount to $A \cap B_2 = \emptyset$, $A \cap B_1 = \emptyset$, $(X \setminus A) \cap B_1 = \emptyset$, or $(X \setminus A) \cap B_2 = \emptyset$, respectively. Moreover, $\mathcal{S}$ and thus $\mathcal{S}'$ contains the singleton splits $\{x\}|\{X \setminus \{x\}\}$ for all $x \in X$. The split system $\mathcal{S}'$ therefore defines a refinement $\mathcal{T}'$ of $\mathcal{T}$. Furthermore, we have $\mathcal{T}'_{|X \setminus A} = \mathcal{T}'_{|X \setminus A}$ and $\mathcal{T}'_{|A} = \mathcal{T}'_{|A}$ since either $\mathcal{T} = \mathcal{T}'$ or the difference between $\mathcal{T}$ and $\mathcal{T}'$ is only the expansion or contraction of the edge $e_A$ identified by the additional split $A|\{X \setminus A\}$. By condition (ii), there is a refinement $\mathcal{T}'_{|X \setminus A}$ of the restriction $\mathcal{T}_{|X \setminus A} = \mathcal{T}'_{|X \setminus A}$ that is compatible with the partition $\mathcal{P} \setminus \{A\}$ of $X \setminus A$. Thus there is also a refinement $\mathcal{T}''_{|X \setminus A}$ of $\mathcal{T}$ such that the restriction $\mathcal{T}''_{|X \setminus A} = \mathcal{T}'_{|X \setminus A}$ is compatible with $\mathcal{P} \setminus \{A\}$. Let $H^*$ be the corresponding set of separating edges. Then $\mathcal{F}(\mathcal{T}'^*, H^* \cup \{e_A\}) = \mathcal{F}(\mathcal{T}''_{|X \setminus A}, H^*) \cup \{A\} = \mathcal{T}$. Thus $\mathcal{T}$ and $\mathcal{P}$ are compatible. □

**Lemma 6.7 and Lemma 6.8 are associated with a simple algorithmic intuition. Among the sets $A \in \mathcal{P}$, at least one corresponds (at least in a refinement) to a connected component in the forest obtained by deletion of a single edge, and thus to a split $A|\{X \setminus A\}$ that is either already contained in $\mathcal{S}(\mathcal{T})$ or that can be used to refine the tree $\mathcal{T}$. This immediately yields an algorithm on the split systems that, in each step, finds a set $A \in \mathcal{P}$ that satisfies condition (i) and then proceeds to checking the restriction to $X \setminus A$. While the formulation in terms of tree-like split systems is of some theoretical interest, it seems to be of little practical use compared to the linear-time algorithms described in the following section.**

### 7 Algorithms and Complexity

In the following, we will first derive results for the complexity of checking whether $\mathcal{P}$ and $\mathcal{T}$ are $r$-compatible and the construction of the edge coloring $\gamma_{\mathcal{T};\mathcal{P}}$ which we then use for the special case of compatibility of $\mathcal{P}$ and $\mathcal{T}$. Finally, we investigate the complexity of finding a refinement that is
compatible with a system $\mathcal{P}$ of partitions. In view of Prop. 6.2, we will assume that $T$ is a rooted tree in this section unless explicitly stated otherwise.

Recall that, for a tree $T$ on $X$ and a partition $\mathcal{P}$ of $X$, the map $\gamma_{T,\mathcal{P}}$ assigns to $e \in E(T)$ as “colors” all sets $A \in \mathcal{P}$ for which $e$ lies on a path connecting two elements $x, x' \in A$.

**Observation 7.1.** Let $T$ be a tree on $X$ and $\mathcal{P}$ a partition of $X$, $v \neq \mu_T$, and $e = \{\text{par}(v), v\} \in E(T)$. Then

\[ A \in \gamma_{T,\mathcal{P}}(e) \iff A \cap L(T(v)) \neq \emptyset \text{ and } A \setminus L(T(v)) \neq \emptyset. \]

**Lemma 7.2.** Let $\mathcal{H}$ be a hierarchy on $X$, $T$ the corresponding tree on $X$, and $\mathcal{P}$ a partition of $X$. Moreover, let $Y \in \mathcal{H}$. Then, $Y$ overlaps with two distinct sets $A, B \in \mathcal{P}$ if and only if $A, B \in \gamma_{T,\mathcal{P}}(\{\text{par}(|\text{lca}_T(Y)|), \text{par}_T(Y)\})$ with $A \neq B$.

**Proof.** Since $Y \in \mathcal{H}$, there is a unique vertex $v \in V(T)$ with $Y = L(T(v))$ and thus, $v = \text{lca}_T(Y)$. First assume that $Y \in \mathcal{H}$ overlaps with two distinct sets $A, B \in \mathcal{P}$. Thus, we have $C \cap L(T(v)) \neq \emptyset$ and $\emptyset = C \setminus L(T(v)) \neq \emptyset$ for $C \in \{A, B\}$. By Obs. 7.1, this implies $A, B \in \gamma_{T,\mathcal{P}}(\{\text{par}(v), v\})$. For the converse, assume that $A, B \in \gamma_{T,\mathcal{P}}(\{\text{par}(v), v\})$ with $A \neq B$. By Obs. 7.1, we have $C \setminus Y \neq \emptyset$ and $\emptyset = C \cap Y$ for $C \in \{A, B\}$. Since, in addition, $A$ and $B$ are disjoint, we have $Y \setminus C \neq \emptyset$ for $C \in \{A, B\}$. In summary, $Y$ overlaps with the two distinct sets $A$ and $B$. \qed

Lemma 7.2 together with Thm. 5.7 immediately implies

**Proposition 7.3.** Let $T$ be a tree on $X$ and $\mathcal{P}$ a partition of $X$. $\mathcal{P}$ and $T$ are $r$-compatible if and only if $|\gamma_{T,\mathcal{P}}(e)| \leq 1$ for every $e \in E(T)$.

To find a refinement of a hierarchy $\mathcal{H}$ that is compatible with $\mathcal{P}$, it is crucial to know the set $\mathfrak{g}(\mathcal{H}, \mathcal{P})$, and, in particular, the sets $A_{\mathcal{H}}$ for the $A \in \mathfrak{g}(\mathcal{H}, \mathcal{P})$. However, an explicit construction of the latter is not needed since the property of $Y \in \mathcal{H}$ being equal to $A_{\mathcal{H}}$ for some $A \in \mathfrak{g}(\mathcal{H}, \mathcal{P})$ or not is entirely determined by the colored edges incident to $\text{lca}_T(Y)$.

**Lemma 7.4.** Let $\mathcal{H}$ be a hierarchy on $X$, $T$ the corresponding tree on $X$, $\mathcal{P}$ a partition of $X$, and $Y \in \mathcal{H}$. Then, $Y = A_{\mathcal{H}}$ for some $A \in \mathfrak{g}(\mathcal{H}, \mathcal{P})$ if and only if the following two conditions are satisfied for $u := \text{lca}_T(Y)$:

(a’) $A \in \gamma_{T,\mathcal{P}}(\{u, v\})$ for some $v \in \text{child}_T(u)$ and either $u = \rho_T$ or $A \notin \gamma_{T,\mathcal{P}}(\{\text{par}_T(u), u\})$.

(b’) $B \in \gamma_{T,\mathcal{P}}(\{u, v'\})$ for some $v' \in \text{child}_T(u)$ and some color $B \neq A$.

**Proof.** Let $Y = A_{\mathcal{H}}$ for some $A \in \mathfrak{g}(\mathcal{H}, \mathcal{P}) \subseteq \mathcal{P}$. By definition, this is, if and only if, (a) $Y = A_{\mathcal{H}}$ with $A \in \mathcal{P}$ and (b) there is some $B \in \mathcal{P} \setminus \{A\}$ satisfying $B \cap Y \neq \emptyset$ and $Y \subseteq B_{\mathcal{H}}$. In particular, $u = \text{lca}_T(Y)$ is an inner vertex in this case. Thus, we have $L(T(u)) = Y = A_{\mathcal{H}}$. The definition of $\gamma_{T,\mathcal{P}}$ directly implies Condition (a’). Now, let $B \in \mathcal{P} \setminus \{A\}$ such that $B \cap Y \neq \emptyset$ and $Y \subseteq B_{\mathcal{H}}$. Hence, $B \cap L(T(u)) \neq \emptyset$, and thus, there must be a child $v' \in \text{child}_T(u)$ with $B \cap L(T(v')) \neq \emptyset$. However, since $L(T(v')) \subseteq L(T(u)) = Y \subseteq B_{\mathcal{H}}$ and since $B_{\mathcal{H}}$ is inclusion-minimal for $B$, we also have $B \setminus L(T(v')) \neq \emptyset$. Taken together, we obtain $B \in \gamma_{T,\mathcal{P}}(\{u, v'\})$ by definition of $\gamma_{T,\mathcal{P}}$ and thus Conditions (b’).

Now assume that Conditions (a’) and (b’) are satisfied. Let $A \in \gamma_{T,\mathcal{P}}(\{u, v\})$ for some $v \in \text{child}_T(u)$. Hence, $Y \subseteq A_{\mathcal{H}}$. Moreover, the two possible cases $u = \rho_T$ or $A \notin \gamma_{T,\mathcal{P}}(\{\text{par}_T(u), u\})$ imply that there must be a second edge $\{u, v''\}$ for some $v'' \in \text{child}_T(u) \setminus \{v\}$ that is colored with $A$ due to the definition of $\gamma_{T,\mathcal{P}}$ and the fact that $u = \text{lca}_T(Y)$. Therefore, $u = \text{lca}_T(A_{\mathcal{H}}) = \text{lca}_T(Y)$. This together with $Y \in \mathcal{H}$ and $Y \subseteq A_{\mathcal{H}}$ implies Condition (a) $Y = A_{\mathcal{H}}$. Condition (b’) implies that $B \cap L(T(v')) \neq \emptyset$ for some $v' \in \text{child}_T(u)$ (and thus $B \cap L(T(u)) \neq \emptyset$) and $B \setminus L(T(v')) \neq \emptyset$. Together with $v' \in \text{child}_T(u)$, these two arguments imply $u \leq_T \text{lca}_T(B)$ which is equivalent to $Y \subseteq B_{\mathcal{H}}$. In summary, Condition (b) is satisfied. \qed

We are now in the position to show that r-compatibility can be decided in linear time.

**Theorem 7.5.** Given a rooted tree $T$ on $X$ and a partition $\mathcal{P}$ of $X$, it can be decided in $O(|X|)$ time whether $\mathcal{P}$ and $T$ are r-compatible. In this case, the edge coloring $\gamma_{T,\mathcal{P}}$ and a compatible refinement can also be constructed in $O(|X|)$ time.
Proof. We employ the sparse-table algorithm described in [1], which, following an \(O(|X|)\)-preprocessing step, enables constant-time look up of \(\text{lca}_T(u, v)\) for any \(u, v \in V(T)\). We represent \(\gamma_{T, P}\) by a (hash-based) map data structure that contains the \(O(|X|)\) edges \(e \in E(T)\) as keys, and (hash-based, initially-empty) sets as values, which will be filled with the elements in \(\gamma_{T, P}(e)\). The sets in \(P\) can be represented by pointers to these sets or by integer indices when used as colors. We next show that \(\gamma_{T, P}\) can be constructed in \(O(|X|)\) time. When an edge \(e\) is colored with \(A\) (i.e., \(A\) is added to \(\gamma_{T, P}(e)\)), we check in constant time whether \(e\) still has at most one color. If this is not the case, we stop the algorithm since \(P\) and \(T\) are not \(r\)-compatible by Prop. 7.3. Conversely, Prop. 7.3 implies that if we color each edge at most once, then \(P\) and \(T\) are \(r\)-compatible.

We process every \(A = \{x_1, \ldots, x_k\} \in \mathcal{P}\) as follows. First, we initialize the set of previously visited vertices of \(V(T)\) as \(\text{visited} \leftarrow \emptyset\). Moreover, we initialize the current last common ancestor as \(\text{curLCA} \leftarrow x_1\), which we will update stepwise until it equals \(\text{lca}_T(A)\) in the end. To this end, for each leaf \(x \in \{x_2, \ldots, x_k\}\) (if any), we query \(\text{newLCA} = \text{lca}_T(x, \text{curLCA})\) and move from \(x\) upwards along the tree. Each edge \(e = \{\text{par}_T(v), v\}\) encountered during the traversal is colored with \(A\), and \(v\) is added to \(\text{visited}\). The traversal stops as soon as \(\text{par}_T(v)\) is in \(\text{visited}\) or equals \(\text{newLCA}\).

In case we have \(\text{curLCA} \leftarrow \text{newLCA}\), which by definition of \(\text{newLCA}\) holds if \(\text{curLCA} \neq \text{newLCA}\), we perform the same bottom-up traversal starting from \(\text{curLCA}\). As a final step in the processing of \(x\), we set \(\text{curLCA} \leftarrow \text{newLCA}\). One easily verifies that, after processing all vertices in \(A\), we have exactly colored the edges in the minimal subtree of \(T\) that connects all leaves in \(A\). Moreover, each edge considered in the bottom-up traversals is colored with \(A\) and required only a constant number of constant-time queries and operations. Similarly, the additional operations needed for each \(x \in A\) (i.e., set initialization, query, comparison, and update of the last common ancestor) are performed in constant time. Since the algorithm stops as soon as an edge would be colored with two colors, at most one edge is considered twice in the bottom-up traversal. Since \(T\) is a phylogenetic rooted tree, we have \(|E(T)| \leq 2|X| - 2\). In total, therefore, the traversals of the tree require \(O(|X|)\) operations.

In addition, a constant effort is required for each of the \(O(|X|)\) vertices in the disjoint sets in \(\mathcal{P}\). Thus \(\gamma_{T, P}(e)\) can be constructed in \(O(|X|)\) time.

It remains to show how a compatible refinement of \(T\) can be constructed. Put \(\mathcal{H} := \mathcal{H}(T)\) and \(\mathcal{H}_P := \mathcal{H}(H, P)\). First note that all inner vertices \(u\) that need to be resolved correspond to some \(Y\) (i.e., \(u = \text{lca}_T(Y)\)) such that \(Y = A_H\) for some \(A \in \mathcal{P}\). By Lemma 7.4, it suffices to solely check the colorings for the edges incident to \(u\) according to the two conditions in Lemma 7.4. Therefore, we do not need to consider the sets \(Y = L(T(u))\) explicitly. In this way, each edge \(T\) in \(T\) and its set of colors must be checked at most twice. Since \(|\gamma_{T, P}(v)| \leq 1\) for every edge \(v \in E(T)\), this can be done in \(O(|X|)\) time. By Lemma 5.6, \(\mathcal{H}_P\) is a refinement of \(\mathcal{H}\) that is compatible with \(P\). Instead of operating on \(\mathcal{H}\) and \(\mathcal{H}_P\), we directly construct the tree \(T^*\) corresponding to \(\mathcal{H}_P\) from \(T\) in \(O(|X|)\)-time as follows. If a vertex \(u = \text{lca}_T(Y)\) satisfies Conditions (a') and (b') in Lemma 7.4, then the respective coloring of its edges imply that there is an \(A \in \mathcal{P}\) with \(A_H = Y\) for some color \(A \in \mathcal{P}\). We refine \(T\) at vertex \(u\) as follows: By definition, the sets \(W_j \in \mathcal{H}\) whose disjoint union gives the newly-created sets \(Y_A\) are child clusters of \(Y\) in \(\mathcal{H}_P\). Hence, they correspond to the children \(v_j \in \text{child}_T(u)\) for which the edge \(\{u, v_j\}\) is colored with \(A\). Therefore, we remove all of these edges \(\{u, v_j\}\), and instead add the edge \(\{u, v_{A,j}\}\) and the edges \(\{v_{A,j}, v_j\}\), where \(v_{A,j}\) is a newly-created vertex. In particular, we have \(Y_A = L(T(v_{A,j}))\). Since this is true for all sets \(Y_A \in \mathcal{H}_P \setminus \mathcal{H}\), the resulting tree \(T^*\) corresponds to the hierarchy \(\mathcal{H}_P\). Clearly, we introduce no more than \(O(|X|)\) new vertices. Since each edge has at most one color, at most \(O(|X|)\) operations are required.

We next characterize compatibility of \(\mathcal{H}\) and \(\mathcal{P}\) in terms of the edge coloring \(\gamma_{T, P}\) and show that compatibility of \(\mathcal{H}\) and \(\mathcal{P}\) can be tested in linear time.

Theorem 7.6. Let \(\mathcal{H}\) be a hierarchy on \(X\), \(T\) the corresponding tree on \(X\), and \(\mathcal{P}\) a partition of \(X\). Then \(\mathcal{H}\) and \(\mathcal{P}\) are compatible if and only if there is no vertex \(u \in V(T)\) and distinct \(A, B \in \mathcal{P}\) such that \(A \in \gamma_{T, P}(\{u, v\})\) and \(B \in \gamma_{T, P}(\{u, v'\})\) for (not necessarily distinct) children \(v, v' \in \text{child}_T(u)\). In particular, it can be decided in \(O(|X|)\) time whether \(\mathcal{P}\) and \(T\) are compatible.

Proof. First suppose, for contraposition, that there is a vertex \(u \in V(T)\) with distinct \(A, B \in \mathcal{P}\) such that \(A \in \gamma_{T, P}(\{u, v\})\) and \(B \in \gamma_{T, P}(\{u, v'\})\) for children \(v, v' \in \text{child}_T(u)\). If \(v = v'\), we can apply Prop. 7.3 to conclude that there is no refinement of \(\mathcal{H}\) that is compatible with \(\mathcal{P}\). Thus, in particular, \(\mathcal{H}\) is not compatible with \(\mathcal{P}\). Now assume that \(v\) and \(v'\) are distinct. We distinguish the three cases (a) \(u \not\in \rho_T\) and \(A, B \in \gamma_{T, P}(\{\text{par}_T(u), u\})\), (b) \(u \not\in \rho_T\) and exactly one of \(A\) and \(B\) is in \(\gamma_{T, P}(\{\text{par}_T(u), u\})\), and (c) \(u \in \rho_T\) or \(A \neq B \in \gamma_{T, P}(\{\text{par}_T(u), u\})\). In case (a), \(\gamma_{T, P}(\{\text{par}_T(u), u\})\) contains two colors and we again obtain incompatibility of \(\mathcal{H}\) and \(\mathcal{P}\) by Prop. 7.3. In case (b), we assume w.l.o.g. that \(A \not\in \gamma_{T, P}(\{\text{par}_T(u), u\})\) and \(B \in \gamma_{T, P}(\{\text{par}_T(u), u\})\). Since \(A \in \gamma_{T, P}(\{u, v\})\),...
we have $|A| > 1$ and since $A \notin \gamma_T, P(\{\text{par}_T(u), u\})$, it must hold that $A \subseteq L(T(u))$. The latter two arguments imply that there is a second edge $\{u, w\}$, $w \in \text{child}_T(u)$ with $A \notin \gamma_T, P(\{u, w\})$ and, in particular, $u = \text{lca}_T(A)$. Moreover, since $B \in \gamma_T, P(\{\text{par}_T(u), u\})$, we have $B \cap L(T(u)) \neq \emptyset$ and $B \setminus L(T(u)) \neq \emptyset$. In particular, therefore, $u$ corresponds to $A_H = L(T(u))$ and $A_H$ is not the union of sets in $\mathcal{P}$. Together with Thm. 4.5, this implies that $H$ and $\mathcal{P}$ are not compatible. In case (e), we have, by similar arguments as before, that $u = \text{lca}_T(A) = \text{lca}_T(B)$. Hence, $u$ corresponds to both $A_H$ and $B_H$ for distinct $A, B \in \mathcal{P}$, and thus, Condition (ii) in Thm. 4.5 is not satisfied. Therefore, $H$ and $\mathcal{P}$ are not compatible.

To prove the converse, suppose, for contraposition, that $H$ and $\mathcal{P}$ are not compatible. Hence, Condition (i) or (ii) in Thm. 4.5 is not satisfied. If Condition (i) is not satisfied, then there is some $A \in H$ such that $A_H$ is not the union of sets in $\mathcal{P}$. Since $A \subseteq A_H$ by definition, the latter implies that there must be some $B \in \mathcal{P} \setminus \{A\}$ such that $B \cap A_H \neq \emptyset$ and $B \setminus A_H \neq \emptyset$. Moreover, since $A$ and $B$ are disjoint and non-empty and both contain elements that are in $A_H$, the vertex $u := \text{lca}_T(A)$ corresponding to $A_H$ is an inner vertex and has (not necessarily distinct) children $v, v' \in \text{child}_T(u)$ such that $A \in \gamma_T, P(\{u, v\})$ and $B \in \gamma_T, P(\{u, v'\})$. If Condition (ii) is not satisfied, i.e., $A_H = B_H$ for two distinct $A, B \in \mathcal{P}$, we can apply similar arguments to conclude that $u := \text{lca}_T(A) = \text{lca}_T(B)$ has children $v, v' \in \text{child}_T(u)$ such that $A \in \gamma_T, P(\{u, v\})$ and $B \in \gamma_T, P(\{u, v'\})$.

It remains to show that compatibility of $\mathcal{P}$ and $T$ can be decided in $O(|X|)$ time. Compatibility implies $r$-compatibility which can be checked in $O(|X|)$ by Thm. 7.5. In particular, the edge coloring $\gamma_T, P$ can be constructed with the same complexity in this case. The condition whether or not there is a vertex $u \in V(T)$ and distinct $A, B \in \mathcal{P}$ such that $A \in \gamma_T, P(\{u, v\})$ and $B \in \gamma_T, P(\{u, v'\})$ for (not necessarily distinct) children $v, v' \in \text{child}_T(u)$ can easily be checked in $O(|X|)$ time by counting, for each vertex in an arbitrary traversal, the number of colors appearing on the edges leading to its children.

Similar to Lemma 4.6, we obtain here a result for maximum-sized sets of separating edges. Since any edge $e \in E(T)$ with $\gamma_T, P(e) = \emptyset$ cannot be a separating edge, and any edge $e$ for which $\gamma_T, P(e) = \emptyset$ can always be added as a separating edge, we obtain

**Corollary 7.7.** Suppose that $\mathcal{P}$ and $T$ are compatible. Then, there is a unique maximum-sized set of separating edges $H^*$, which is given by the set of edges $e \in E(T)$ for which $\gamma_T, P(e) = \emptyset$. This maximum-sized set $H^*$ can be computed in $O(|X|)$ time.

For a minimum-sized set of separating edges $H^*$ for compatible $\mathcal{P}$ and $T$, the cardinality of $H^*$ can be expressed as a function of $|\mathcal{P}|$ alone (cf. Lemma 4.6), and is thus independent of $T$. However, the latter is not the case for a maximum-sized $H^*$ set of separating edges. To see this, consider a partition $\mathcal{P}$ of $X$ consisting of all singletons. Clearly, we have $H^* = E(T)$ for any tree on $X$ where $|E(T)|$ varies depending on how resolved a specific tree $T$ is.

In what follows, we investigate the complexity of the problem of recognizing compatibility of systems $\mathfrak{P} = \{\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_k\}$ of partitions of $X$ with (refinements of) trees. In Section 3, we have introduced the two closely related problems asking whether a tree $T$ admits a refinement that is compatible with all partitions in $\mathfrak{P}$, COMPATP, and whether a compatible tree exists at all, EXISTTP. To this end, we first show that EXISTTP is a simple translation of the SYMM-FITCH RECOGNITION problem, which is NP-complete [12, Thm. 4.2]. In particular, this discussion will yield NP-completeness of COMPATP and EXISTTP in Thm. 7.10 below.

The concept of compatible partitions and trees is intimately related to so-called undirected Fitch graphs $G$, that is, complete multipartite graphs whose maximal independent sets form a partition $\mathcal{P}$ of $V(G)$ [10]. To be more precise, for a given tree $T$ with leaf set $X$ and subset $H \subseteq E(T)$, an undirected Fitch graph $G = (X, E)$ has an edge $\{x, y\} \in E$ if and only if there is an edge in $H$ that lies on the path between $x$ and $y$ in $T$. Therefore, $\{x, y\} \notin E$ if and only if $x$ and $y$ are contained in the same set $B \in \mathcal{P} := \mathcal{F}(T, H)$. This construction was generalized in [9, 11] to Fitch maps that allow multiple colors. In the following paragraph we briefly summarize the construction of symmetrized Fitch maps [12]. We then show that a symmetrized Fitch map $\varepsilon$ can be interpreted as a partition system $\mathfrak{P}$ on $X$ that is compatible with a suitably chosen tree $T$.

Let $M := \{1, \ldots, k\}$ be a set of colors for some $k \in \mathbb{N}$. Moreover, for a set $X$, we write $[X \times X]_{\text{irr}} := (X \times X) \setminus \{(x, x) \mid x \in X\}$. An edge-colored tree $(T, \lambda)$ is a tree $T$ together with a map $\lambda : E(T) \to 2^M$. Note that $\lambda$ can be chosen arbitrarily in contrast to the $\mathcal{P}$-coloring $\gamma_T, P$ of $T$ as in Def. 3.3. An edge $e \in E(T)$ is an $m$-edge if $m \in \lambda(e)$ for some $m \in M$.

A map $\varepsilon : [X \times X]_{\text{irr}} \to 2^M$ is a symmetrized Fitch map if there is an edge-colored tree $(T, \lambda)$ with leaf set $X$ and edge coloring $\lambda : E(T) \to 2^M$ such that for every pair $(x, y) \in [X \times X]_{\text{irr}}$ it
holds that 
\[ m \in \epsilon(x,y) \iff \text{there is an } m\text{-edge on the path from } x \text{ to } y. \]

In this case, we say that \( \epsilon : [X \times X]_{\text{irr}} \to 2^M \) is explained by \((T, \lambda)\).

For an arbitrary map \( \epsilon : [X \times X]_{\text{irr}} \to 2^M \) and each \( m \in M \), the monochromatic map (induced by \( m \)) is given by \( \epsilon_m(x,y) := \epsilon(x,y) \setminus (M \setminus \{m\}) \). By definition, we have \( \epsilon_m(x,y) \in \{0, \{m\}\} \) and, in particular, \( \epsilon_m(x,y) = \{m\} \) if and only if \( m \in \epsilon(x,y) \). If moreover \( \epsilon \) (and thus \( \epsilon_m \)) is a symmetrized Fitch map, then there is a tree \((T, \lambda)\) such that \( \epsilon_m(x,y) = \{m\} \) if and only if there is an \( m\)-edge on the path from \( x \) to \( y \). In [10], it was shown that the graph representations \( G_m = (X, E_m) \) of (monochromatic) symmetrized Fitch relations, given by \{x, y\} \( \in E \) if and only if \( \epsilon_m(x,y) = \{m\} \), coincide with the class of complete multipartite graphs. Therefore, they can uniquely be represented by a partition \( \mathcal{P}_m^\epsilon \) of \( X \) in a way that each set \( A \in \mathcal{P}_m^\epsilon \) corresponds to a maximal independent subset of \( X \), i.e. \{x, y\} \( \notin E_m \) for all \( x, y \in A \). In particular, it holds that \( x, y \in X \) are elements of distinct sets of \( \mathcal{P}_m^\epsilon \) if and only if \( m \in \epsilon(x,y) \).

Thus, if all monochromatic maps are symmetrized Fitch maps, \( \mathcal{F}^\epsilon := \{\mathcal{P}_m^\epsilon \mid m \in M\} \) is a partition system on \( X \).

**Lemma 7.8.** Let \( \epsilon : [X \times X]_{\text{irr}} \to 2^M \) be a map such that the monochromatic maps \( \epsilon_m \) are symmetrized Fitch maps for all \( m \in M \), and \( \overline{T} \) be an unrooted tree with leaf set \( X \). Then, there is an edge-coloring \( \lambda \) such that \((\overline{T}, \lambda)\) explains \( \epsilon \) if and only if the partition \( \mathcal{P}_m^\epsilon \) of \( X \) is compatible with \( \overline{T} \) for all \( m \in M \).

**Proof.** First note that, since the monochromatic maps \( \epsilon_m \) are symmetrized Fitch maps for all \( m \in M \), the partitions \( \mathcal{P}_m^\epsilon \) of \( X \) are all well-defined. For the case \(|X| \in \{1, 2\}\), the statement is trivially true since, in this case, every of the (at most two) possible partitions of \( X \) are compatible with a unique tree on \( X \). Thus, assume that \(|X| \geq 3\). Let \( T \) be any rooted version of \( \overline{T} \). Since \(|X| \geq 3\), we can apply Prop. 6.1, to conclude that \( T \) is compatible with some partition \( \mathcal{P} \) of \( X \) if and only if \( T \) is compatible with \( \overline{T} \). Hence, it suffices to show the statements for \( T \).

Assume there is an edge-coloring \( \lambda \) such that \((T, \lambda)\) explains \( \epsilon \). Put \( H_m := \{e \in E(T) \mid m \in \lambda(e)\}, m \in M \). By construction, we have for all distinct \( x, y \in X \) that \( x \) and \( y \) are in distinct sets of \( \mathcal{P}_m^\epsilon \),
\[ \iff m \in \epsilon(x,y) \]
\[ \iff m \in \lambda(e) \text{ for some } e \in E(T) \text{ on the path connecting } x \text{ and } y \]
\[ \iff \text{there is an edge in } H_m \text{ on the path connecting } x \text{ and } y \]
\[ \iff x \text{ and } y \text{ are in distinct sets of } F(T, H_m). \]

Hence, \( \mathcal{P}_m^\epsilon = F(T, H_m) \) and \( \mathcal{P}_m^\epsilon \) is compatible with \( T \) for all \( m \in M \).

Now assume that the partition \( \mathcal{P}_m^\epsilon \) of \( X \) is compatible with \( T \) for all \( m \in M \). For each \( m \in M \), define \( \lambda_m(e) = \{m\} \) for all edges \( e = \{\text{par(lca}_T(B)), \text{lca}_T(B)\} \) for some \( B \in \mathcal{P}_m^\epsilon \) with \( \text{lca}_T(B) \neq \rho_T \) and, for all remaining edges \( e \), put \( \lambda_m(e) = \emptyset \). By construction, we have for \( e \in E(T) \) that \( \lambda_m(e) = \{m\} \) if and only if \( e \) is contained the set \( H_m \) as specified in Eq. (3). By Cor. 4.7, we have \( \mathcal{P}_m^\epsilon = F(T, H_m) \). Hence, \( m \in \epsilon(x,y) \) if and only if there is an edge \( e \) along the path between \( x \) and \( y \) with \( \lambda_m(e) = \{m\} \). Now set \( \lambda(e) = \bigcup_{m \in M} \lambda_m(e) \) for all \( e \in T \) to obtain the final coloring such that \((T, \lambda)\) explains \( \epsilon \).

**Lemma 7.9.** Symm-Fitch Recognition remains NP-hard if the monochromatic maps \( \epsilon_m \) are symmetrized Fitch maps for all \( m \in M \).

**Proof.** As shown in [12, Thm. 4.2], Symm-Fitch Recognition is NP-complete. Note, if for a map \( \epsilon : [X \times X]_{\text{irr}} \to 2^M \) there is an \( m \in M \) such that \( \epsilon_m \) is not a monochromatic Fitch map, then \( \epsilon \) cannot be a symmetrized Fitch map: a property that can be checked in polynomial-time for all \( m \in M \) [10]. Hence, under the assumption that \( P \neq NP \), the NP-hard instances must, in particular, be included within the instances of Symm-Fitch Recognition for which \( \epsilon_m \) is a monochromatic Fitch map for all \( m \in M \).

We are now in the position to establish NP-completeness of ExisTP and CompatP.

**Theorem 7.10.** ExisTP and CompatP are NP-complete.

**Proof.** By Thm. 7.6 and the fact that one can test in polynomial time whether \( T^* \) is a refinement of \( T \) by comparing their hierarchies, ExisTP and CompatP are contained in the class NP. By Lemma 7.8, ExisTP is equivalent to the Symm-Fitch Recognition problem restricted to a certain set of instances for which, by Lemma 7.9, the problem remains NP-hard. Asking for a tree that is compatible with \( \mathcal{P} \) is equivalent to asking whether there exists a refinement \( T^* \) of the star tree that is compatible with \( \mathcal{P} \). Therefore, ExisTP is a special instance of CompatP and
NP-hardness of EXISTTP implies that COMPATP is also NP-hard. Since both problems are in class NP, EXISTTP and COMPATP are NP-complete.

The latter problems become fixed-parameter tractable and thus, easier, if \( T \) is “almost binary”. In [17], the resolution of a rooted tree is quantified by the normalized parameter \( \text{res}(T) := (|V| - |X| - 1)/(|X| - 2) \), which varies between 0 (star tree) and 1 (binary tree). The quantity \( h(T) := 2|X| - |E(T)| - 2 = (|X| - 2)(1 - \text{res}(T)) \) accordingly measures how much \( T \) deviates from being binary. Now let \( V^* \) be the set of non-binary inner vertices of \( T \). Writing \( h_v := |\text{child}(v)| - 2 \) for the number of “excess children” at the inner vertex \( v \in V^* \), one easily checks that \( h(T) = \sum_{v \in V^*} h_v \).

Now suppose \( h(T) \leq h \). Then all possible binary refinements of \( T \) are obtained by inserting an arbitrary binary tree between each non-binary vertex \( v \) of \( T \) and its children \( \text{child}(v) \). It is well known that the number of binary rooted leaf-labeled trees on \( d_v = |\text{child}(v)| = h_v + 2 \) leaves is \((2d_v - 3)! = (2h_v + 1)! \) [6]. The total number of binary refinements is therefore \( \prod_{v \in V^*}(2h_v + 1)! \).

From the definition of the double factorial \((2n + 1)!! = 1 \cdot 3 \cdot \ldots \cdot (2n + 1)\) we see that, after omitting the leading factors 1, \((2h_v + 1)!\) has exactly \( h_v \) factors for each \( v \in V^* \), and thus, \( \prod_{v \in V^*}(2h_v + 1)! \) has exactly \( \sum_{v \in V^*} h_v \) factors. Similarly, \((2h + 1)!\) has \( h \) contributing factors.

Greater than 1. By ordering these factors in \( \prod_{v \in V^*}(2h_v + 1)! \) and \((2h + 1)!\), resp., one easily verifies that, since \( \sum_{v \in V^*} h_v \leq h \), the second product has at least as many factors as the first, and moreover, each of them is not smaller than the corresponding factor (w.r.t. the ordering) in the first product (if existent). Note that equality holds if and only if \( V^* \) comprises a single vertex with \( h + 2 \) children. Each binary refinement can be checked in \( O(|\mathcal{F}| \cdot |X|) \) time for consistency with \( \mathcal{F} \) since the consistency check for a single partition can be performed in \( O(|X|) \) time by Thm. 7.5 below. Thus there is an \( O((2h + 1)! \cdot |\mathcal{F}| \cdot |X|) \) algorithm and thus, COMPATP is FPT for the parameter \( h \).

8 Concluding Remarks

We have characterized the compatibility of a partition \( \mathcal{P} \) with a hierarchy \( \mathcal{H} \). The concept of compatibility considered here is much more general than that of a “representative partition”, i.e., the cutting of hierarchy \( \mathcal{H} \) at a particular aggregation level. Instead, it amounts to disconnecting the corresponding tree \( T \) at an arbitrary set of edges \( H \subseteq E(T) \), i.e., at a subset of the splits \( \mathcal{S}(T) \).

In Section 5, we have characterized when a refinement of \( T^* \) of a tree \( T \) exists such that \( \mathcal{P} \) and \( T^* \) are compatible. For practical application, it may be relevant to allow more general operations on the tree \( T \). A natural generalization is to allow not only refinements but also edge contraction while editing \( T \) into a tree \( T' \) that is compatible with a partition \( \mathcal{P} \) of interest. This amounts to minimizing the cardinality \(|\mathcal{S}(T) \Delta \mathcal{S}(T')|\) of the symmetric difference of the corresponding split systems, i.e., the Robinson-Foulds distance of \( T \) and \( T' \).

In Section 6, we have considered tree-like split systems, i.e., split systems that can be represented by unrooted trees. Thm. 6.4 and Cor. 6.5, however, suggest to consider the compatibility of a partition \( \mathcal{P} \) and a split system \( \mathcal{S} \) in a more general setting. These characterizations may then serve as convenient definitions in a more general context: We may say that a partition \( \mathcal{P} \) and a split system \( \mathcal{S} \) are compatible if there is a set of splits \( \mathcal{J} \) such that \( \bigwedge \mathcal{J} = \mathcal{P} \) and \( \mathcal{J} \subseteq \mathcal{S} \). In order to handle refinements in this setting, one would ask whether there is a set of splits \( \mathcal{J} \) such that \( \bigwedge \mathcal{J} = \mathcal{P} \). Without further restrictions, \( \mathcal{J} \) = \( \mathcal{S}_P \) always provides a positive answer to this question.

In analogy with our discussion above, it therefore seems natural to consider only split systems \( \mathcal{S} \) that belong to a certain class of interest. A refinement will be feasible only if the split system \( \mathcal{J} \subseteq \mathcal{S} \) again belongs to the desired class. Natural generalizations of tree-like split systems to which the notion of compatibility may be applied include circular and weakly compatible split systems [5, 18], or the even more general Teutoburan split systems considered in [13]. The suggested definition of compatibility in terms of split systems also provides the natural generalization to the framework of X-trees [5, 18], i.e., to trees in which the set of taxa \( X \) is not restricted to the leaves of \( T \) but may also appear as inner vertices of \( T \). This amounts to lifting our requirement that the trivial splits \( \{x\}\) of \( X \) must be included in \( \mathcal{S}(T) \).

We have seen in Section 7 that compatibility of \( \mathcal{P} \) and \( \mathcal{H} \) and the existence of a refinement \( \mathcal{H}^* \) can be decided in linear time, while the extension to arbitrary partition systems \( \mathcal{F} \) is NP-complete. Several interesting open questions remain concerning the computational complexity of the Compatibility of Tree and Partition System problem and the Existence of Tree compatible with Partition System problem. Do these problems remain NP-complete if the tree corresponding to \( \mathcal{H} \) has bounded degree? What if the number \(|\mathcal{F}|\) of input partitions is kept constant? Since the related Symm-Fitch Recognition problem [12] is in turn closely related to
the problem of **Unrooted Tree Compatibility** [3], which is known to be FPT in number of input trees, it is not unlikely that **Compatibility of Tree and Partition System** is FPT in the number of partitions. Furthermore, it is interesting to ask whether there are (easily recognizable) subclasses of partition systems for which **CompatTP** and **ExistTP** become tractable. Interesting candidates are the braids of partitions appearing in image analysis [15, 19], or the hierarchical partition systems considered in [14], for which \( \bigcup_{x \in X} \{ x \} \cup \bigcup_{P \in \mathcal{P}} P \cup \{ X \} \) forms a hierarchy.

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