Generalized Fitch Graphs II: Sets of Binary Relations that are explained by Edge-labeled Trees

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Abstract

Fitch graphs $G = (X, E)$ are digraphs that are explained by $\{0, 1\}$-edge-labeled rooted trees $T$ with leaf set $X$: there is an arc $(x, y) \in E$ if and only if the unique path in $T$ that connects the last common ancestor $\text{lca}(x, y)$ of $x$ and $y$ with $y$ contains at least one edge with label “1”. In practice, Fitch graphs represent xenology relations, i.e., pairs of genes $x$ and $y$ for which a horizontal gene transfer happened along the path from $\text{lca}(x, y)$ to $y$.

In this contribution, we generalize the concept of Fitch graphs and consider trees $T$ that are equipped with edge-labeling $\lambda : E \to \mathcal{P}(\mathcal{M})$ that assigns to each edge a subset $M' \subseteq M$ of colors. Given such a tree, we can derive a map $\varepsilon_{(T, \lambda)}$ (or equivalently a set of not necessarily disjoint binary relations), such that $i \in \varepsilon_{(T, \lambda)}(x, y)$ (or equivalently $(x, y) \in R_i$) with $x, y \in X$, if and only if there is at least one edge with color $i$ from $\text{lca}(x, y)$ to $y$.

The central question considered here: Is a given map $\varepsilon$ a Fitch map, i.e., is there there an edge-labeled tree $(T, \lambda)$ with $\varepsilon_{(T, \lambda)} = \varepsilon$, and thus explains $\varepsilon$? Here, we provide a characterization of Fitch maps in terms of certain neighborhoods and forbidden submaps. Further restrictions of Fitch maps are considered. Moreover, we show that the least-resolved tree explaining a Fitch map is unique (up to isomorphism). In addition, we provide a polynomial-time algorithm to decide whether $\varepsilon$ is a Fitch map and, in the affirmative case, to construct the (up to isomorphism) unique least-resolved tree $(T^*, \lambda^*)$ that explains $\varepsilon$.

Keywords: Labeled trees; Fitch map; Forbidden subgraphs; Phylogenetics; Recognition algorithm

1 Introduction

Labeled rooted trees arise naturally as models of evolutionary processes in mathematical biology. Both vertex and edge labels are used to annotate classes of evolutionary events. The
Figure 1: The evolution of gene families is modeled as an embedding of a gene tree (thin lines, and r.h.s. panel, with four genes $a$, $b$, $b^*$ and $c$) into a species tree (shown as tubes with fat outlines with three species A, B, and C). At each speciation (gray ellipses), each gene present in the genome is transmitted into both descending lineages, corresponding to a speciation even in the gene tree (shown as •). Horizontal gene transfer consists in a duplication of a gene, one copy of which “jumps” into a different lineage. The corresponding edge in the gene tree is marked with label 1. The corresponding Fitch digraph has an edge from $x$ to $y$ if there is at least one HGT event on the path from the last common ancestor $\text{lca}(x, y)$ and $y$ in the gene tree.

connection to both empirically accessible data and to key biological concepts is given by binary relations on the leaves that are specified in terms of the labels encountered in certain substructures within the underlying tree. The practical importance of this type of models derives from the fact that the relations can be inferred directly from empirical data, such as gene sequences, without knowledge of the tree [29, 31, 32]. From a mathematical perspective, a rich set of interrelated graph-theoretical problems arises from the questions which relations on the leaves can be obtained from labeled trees under a given set of rules.

Relations and edge-labeled graphs defined in terms of vertex-labeled trees have been widely studied since the 1970’s and range from cographs [4, 21, 27, 28] and di-cographs [5] to 2-structures [7–9], symbolic ultrametrics [1, 22] or three-way symbolic tree-maps [17, 26]. In contrast, relations and edge-labeled graphs that are defined in terms of edge-labeled trees have just been explored recently. Edge-labels may represent the number of events, in which case they lead to pairwise compatibility graphs (PCGs) and their variants: here, an edge is drawn if the total weight along the path connecting $x$ and $y$ lies between $a$ priori defined bounds [3]. Leaf power graphs specify either only an upper or a lower bound [11]. While PCGs are defined with strictly positive edge weights, an extension to zero weights – the absence of evolutionary events along an edge – is required in models of evolution focused on rare events [23].

Fitch graphs were introduced to model so-called horizontal transfer events [15] based on the seminal work by Walter M. Fitch [12], see Fig. 1 for an illustration of the model. Fitch graphs can be seen as directed generalizations of lower bound leaf power graphs: a directed edge connects $x$ and $y$ if at least one of the tree edges connecting the last common ancestor $\text{lca}(x, y)$ and the “target” leaf $y$ carries a “horizontal transfer” label [15]. Modeling different types of events by different labels yields a multi-colored generalization of Fitch graphs that can be regarded as a collection of edge-disjoint sets of Fitch graphs [20]. The colors can be used e.g. to distinguish genomic locations where the horizontally transferred gene copy is inserted, and adds to the information that can be extracted for the colored Fitch graphs compared to their color-free version. Here, we further relax the compatibility conditions and consider sets of Fitch maps and trees whose edges are labeled by finite sets. Conceptually, the construction explored in this contribution can be seen as an edge-centered analog of the 2-structures explored in [7, 8, 22].

An uncolored Fitch graph is explained by an unique least-resolved trees which, in the context of gene families, is obtained by a series of edge-contractions from the true gene tree. Fitch graphs therefore encode constraints on the evolutionary history. From a mathematical point of view, Fitch graphs are a subclass of the directed cographs [5] characterized by a small set of forbidden induced subgraphs [15]. An alternative characterization [18] makes use of certain
neighborhood systems that will also play a key role here.

This contribution is organized as follows. In Section 2, we provide most of the necessary definitions needed here, and continue to characterize Fitch maps in Section 3. To this end, we introduce the notion of (complementary) neighborhoods that additionally provide the necessary information to reconstruct a tree that explains a given Fitch map. In addition, we provide a so-called inequality-condition that is needed to obtain a correct edge-labeling of the underlying trees. In Section 4, we utilize the latter results and show that every Fitch map is explained by a (up to isomorphism) unique least-resolved tree. Moreover, we show that every Fitch map is characterized in terms of so-called forbidden submaps. In Section 5, we consider $k$-restricted Fitch maps, i.e., Fitch maps that are explained by edge-labeled trees for which the number of colors on their edges does not exceed a prescribed integer $k$. We provide a constructive characterization of $k$-restricted Fitch maps, and show that, in general, $k$-restricted Fitch maps cannot be characterized in terms of forbidden submaps. In Section 6, we finally provide a polynomial-time algorithm to recognize Fitch maps $\mathcal{E}$ and, in the affirmative case, to reconstruct the unique least-resolved tree that explains $\mathcal{E}$. We complete this work with a short outlook where we provide a couple of open questions for further research.

2 Preliminaries

**Basics** For a finite set $X$ we put $|X \times X|_{\text{irr}} := X \times X \setminus \{(x, x) : x \in X\}$, and $\binom{X}{2} := \{X' \subseteq X : |X'| = 2\}$. The power set $2^X$ is $X$ comprises all subsets of $X$. In the following, we consider maps $f : X \to Y$ that associate to every element of the set $X$ exactly one element of the set $Y$. Moreover, we consider (undirected) graphs, resp., di-graphs $G = (V, E)$ with finite vertex set $V$ and edge set $E \subseteq \binom{V}{2}$, resp., arc set $E \subseteq [X \times X]_{\text{irr}}$. Hence, the graphs considered here do not contain loops or multiple edges. A graph $H = (W, F)$ is a subgraph of $G = (V, E)$, denoted by $H \subseteq G$, if $W \subseteq V$ and $F \subseteq E$.

**Trees** A rooted tree is a connected, cycle-free graph with a distinguished vertex $\rho_T \in V$, called the root of $T$. Let $T = (V, E)$ be a rooted tree. Then, the unique path from the vertex $v \in V$ to the vertex $w \in V$ is denoted by $P_T(v, w)$. A leaf of $T$ is a vertex $v \in V \setminus \{\rho_T\}$ such that $\deg_T(v) = 1$. The set of all leaves of $T$ will be denoted by $L(T)$. The vertices in $\tilde{V}(T) := V \setminus L(T)$ are called inner vertices. All edges in $\tilde{E}(T) := \{(v, w) \in E : v, w \in \tilde{V}(T)\}$ are called inner edges. Edges of $T$ that are not contained in $\tilde{E}(T)$ are called outer edges. Every rooted tree carries a natural partial order $\preceq_T$ on the vertex set $V$ that can be obtained by setting $v \preceq_T w$ if and only if the path from $\rho_T$ to $w$ contains $v$. In this case, we call $v$ an ancestor of $w$, $w$ a descendant of $v$, and say that $v$ and $w$ are comparable. Instead of writing $v \preceq_T w$ and $v \not\preceq_T w$, we will use $v \prec_T w$.

It will be convenient to use a notation for edges $\{v, w\} \in E$ that implies which one of the vertices in $\{v, w\}$ is closer to the root. Therefore, we always write $(v, w) \in E$ to indicate that $v \prec_T w$. In this case, the unique vertex $v$ is called parent of $w$, denoted by $\text{par}_T(w)$. For a non-empty subset $V' \subseteq V$ of vertices, the last common ancestor of $V'$, denoted by $\text{lca}_T(V')$, is the unique $\preceq_T$-maximal vertex of $T$ that is an ancestor of every vertex in $V'$. We will make use of the simplified notation $\text{lca}_T(x, y) := \text{lca}_T(\{x, y\})$ for $V' = \{x, y\}$. We will omit the explicit reference to $T$ for $\preceq_T$, $\text{par}_T(w)$ and $\text{lca}_T$, whenever it is clear which tree is considered.

A phylogenetic tree $T$ on $X$ is a rooted tree $T$ with leaf set $L(T) = X$, with the degree $\deg_T(\rho_T) \geq 2$, and the degree $\deg_T(v) \geq 3$ for every inner vertex $v \in \tilde{V}(T) \setminus \{\rho_T\}$.

A rooted triple, denoted by $xy|z$, is a phylogenetic tree on $\{x, y, z\}$ with $\text{lca}(x, y, z) \prec_T \text{lca}(x, y)$. A triple $xy|z$ is displayed by a rooted tree $T$, if $\text{lca}_T(x, y, z) \prec_T \text{lca}_T(x, y)$. We denote with $\mathcal{R}(T)$ the set of all triples that are displayed by $T$. A set $R$ of triples is called compatible if $\langle R \rangle \neq \emptyset$, where $\langle R \rangle$ denotes the set of all trees that display $R$. In other words, $R$ is compatible if there is a tree $T$ with $R \subseteq \mathcal{R}(T)$, see Figure 2 for an illustrative example. Moreover, the closure $\overline{R}$ of an
Figure 2: Shown are two (phylogenetic) trees $T$ and $T'$ on $X = \{a, b, c, d\}$ that display the set $R = \{ac, bd\}$ of rooted triples. For the set $R' = \{abc, acd, bc, ab\}$, there is only the tree $T$ that displays $R'$. Thus, $\overline{R} = \mathcal{R}(T) = \{abc, acd, bc, ab\}$. In particular, $ab$ is not displayed by $T'$. In this example, $\mathcal{C}(T) = \{X, \{a, b, c\}, \{a, b\}, \{b\}, \{c\}, \{d\}\}$ and $\mathcal{C}(T') = \mathcal{C}(T) \setminus \{\{(a, b)\}\}$.

arbitrary compatible set $R$ of triples is defined by $\overline{R} = \bigcap_{T \in \mathcal{R}} \mathcal{R}(T)$. In other words, $\overline{R}$ contains all triples that are displayed by every tree that also display $R$, see e.g. [2, 16, 33] for further details. In fact, $\overline{R}$ satisfies the usual properties for a closure operator [2], i.e., $R \subseteq \overline{R}$, $\overline{R} = \overline{\overline{R}}$, and if $R' \subseteq R$, then $\overline{R'} \subseteq \overline{R}$.

Clusters and Hierarchies Let $X$ be a finite set, and let $\mathcal{H} \subseteq \mathcal{P}(X)$ be a set system on $X$. Then, we say that $\mathcal{H}$ is hierarchy-like if $P \cap Q \in \mathcal{H}$ for all $P, Q \in \mathcal{H}$. The set system $\mathcal{H}$ is a hierarchy (on $X$) if it is hierarchy-like and in addition satisfies $X \in \mathcal{H}$ and $\{x\} \in \mathcal{H}$ for all $x \in X$.

Given a phylogenetic tree $T = (V, E)$, we define for each vertex $v \in V$ the set of descendant leaves as $C_T(v) := \{x \in \mathcal{L}(T) : v \preceq_T x\}$. We say that $C_T(v)$ is a cluster of $T$. Moreover, the cluster set of $T$ is $\mathcal{C}(T) := \{C_T(v) : v \in V\}$. In this context, it is well-known that $\mathcal{C}(T)$ forms a hierarchy and that there is a one-to-one correspondence between (isomorphism classes of) rooted trees and their cluster sets:

**Lemma 2.1** ([34, Thm. 3.5.2]). For a given subset $H \subseteq \mathcal{P}(X)$, there is a phylogenetic tree $T$ on $X$ with $H = \mathcal{C}(T)$ if and only if $H$ is a hierarchy on $X$. Moreover, if there is such a phylogenetic tree $T$ on $X$, then, up to isomorphism, $T$ is unique.

3 Characterization of Generalized Fitch maps

3.1 Definitions

**Definition 3.1.** Let $M$ be an arbitrary finite set of colors. An edge-labeled (phylogenetic) tree $(T, \lambda)$ on $X$ (with $M$) is a phylogenetic tree $T = (V, E)$ on $X$ together with a map $\lambda : E \to \mathcal{P}(M)$ that assigns to every edge $e \in E$ exactly one subset $\lambda(e) \subseteq M$ of colors.

We will often refer to the map $\lambda$ as the edge-labeling and call $e$ an $m$-edge if $m \in \lambda(e)$. Note that the choice of $m \in \lambda(e)$ may not be unique. An edge can be an $m$- and $m'$-edge at the same time.

To avoid trivial cases, we assume from here on that both the set $X$ of leaves and the set $M$ of colors is non-empty.

**Definition 3.2.** Let $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ be a map that assigns to every pair $(x, y) \in [X \times X]_{irr}$ a unique subset $M' \subseteq M$, where $M' = \emptyset$ may possible. Then, $\varepsilon$ is a Fitch map if there is an edge-labeled tree $(T, \lambda)$ with leaf set $X$ and edge labeling $\lambda : E(T) \to \mathcal{P}(M)$ such that for every pair $(x, y) \in [X \times X]_{irr}$ holds

$$m \in \varepsilon(x, y) \iff \text{there is an } m\text{-edge on the path from lca}(x, y) \text{ to } y.$$ 

In this case we say that $(T, \lambda)$ explains $\varepsilon$. 

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We write for a map \( \varepsilon : [X \times X]_{\text{irr}} \rightarrow \mathcal{P}(M) \) with the color set \( M = \{1, 2, 3, 4\} \) on the right. It is easy to see that Fitch maps are not necessarily symmetric as e.g. \( \varepsilon(a, b) \neq \varepsilon(b, a) \). Moreover, we can observe that \( 1 \in \varepsilon(a, c) \), \( 1 \in \varepsilon(c, b) \) but \( 1 \notin \varepsilon(a, b) = \emptyset \). Therefore, Fitch maps are not “transitive” in general.

Figure 3 provides an illustrative example of a Fitch map \( \varepsilon \) and its corresponding tree \((T, \lambda)\). A map \( \varepsilon : [X \times X]_{\text{irr}} \rightarrow \mathcal{P}(M) \) is called \emph{monochromatic} if \( |M| = 1 \). Monochromatic Fitch maps are equivalent to the “Fitch relations” studied by Geiß et al. [15], and Hellmuth and Seemann [18].

The map \( \varepsilon \) can also be interpreted as a set of \( |M| \) not necessarily disjoint binary relations (or equivalently graphs) on \( X \) defined by the sets of pairs \( \{(x, y) \in [X \times X]_{\text{irr}} : m \in \varepsilon(x, y)\} \) (or equivalently arcs) for each fixed color \( m \in M \). These relations are disjoint if and only if \( |\varepsilon(x, y)| \leq 1 \) for every \( (x, y) \in [X \times X]_{\text{irr}} \), in which case we call \( \varepsilon \) a \emph{disjoint} map. Disjoint Fitch maps are equivalent to “multi-colored Fitch graphs” studied by Hellmuth [20].

The Fitch maps defined here correspond to directed multi-graphs with the restriction that there are no parallel arcs of the same color. Note, we may also allow parallel arcs with the same color \( m \) provided that this still means that there is an \( m \)-edge along the path from \( \text{lca}(x, y) \) to \( y \). However, we must omit parallel edges with the same color \( m \) whenever the multiplicity \( k \) of a parallel \( m \)-edge implies that at least \( k \) \( m \)-edges must occur along the path from \( \text{lca}(x, y) \) to \( y \), an issue that may be part of future research.

### 3.2 Characterization in Terms of Neighborhoods

We start by generalizing the approach developed by Hellmuth and Seemann [18] for the monochromatic case.

**Definition 3.3.** For a map \( \varepsilon : [X \times X]_{\text{irr}} \rightarrow \mathcal{P}(M) \), the set

\[
\mathcal{N}_{-m}[y] := \{x \in X \setminus \{y\} : m \notin \varepsilon(x, y)\} \cup \{y\}
\]

is the \emph{(complementary) neighborhood} \( y \in X \) for a color \( m \in M \) \((\text{w.r.t. } \varepsilon)\).

We write \( \mathcal{N}[\varepsilon] := \{\mathcal{N}_{-m}[y] : y \in X, m \in M\} \) for the set of complementary neighborhoods of \( \varepsilon \).

The set \( \mathcal{N}_{-m}[y] \subseteq X \) contains vertex \( y \) and all vertices \( x \in X \setminus \{y\} \) for which the color \( m \) is \emph{not} contained in \( \varepsilon(x, y) \). Informally speaking, if one thinks about a di-graph that contains all arcs \((u, v)\) whenever \( m \in \varepsilon(u, v) \), then \( \mathcal{N}_{-m}[y] \) contains, in particular, all vertices \( x \) that do not form an arc \((x, y)\). This fact justifies the name “complementary” neighborhood. Before we give an illustrative example, we generalize the key conditions characterizing Fitch relations in [18] in terms of complementary neighborhoods.

**Definition 3.4.** A map \( \varepsilon : [X \times X]_{\text{irr}} \rightarrow \mathcal{P}(M) \) satisfies

- the \emph{hierarchy-like-condition (HLC)} if \( \mathcal{N}[\varepsilon] \) is hierarchy-like; and
- the \emph{inequality-condition (IC)} if for every neighborhood \( N := \mathcal{N}_{-m}[y] \in \mathcal{N}[\varepsilon] \) and every \( y' \in N \), we have \( |\mathcal{N}_{-m}[y']| \leq |N| \).

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**Figure 3:** The edge-labeled tree \((T, \lambda)\) with the leaf set \( \mathcal{L}(T) = \{a, b, c\} \) on the left explains the displayed Fitch map \( \varepsilon : [X \times X]_{\text{irr}} \rightarrow \mathcal{P}(M) \) with the color set \( M = \{1, 2, 3, 4\} \) on the right. It is easy to see that Fitch maps are not necessarily symmetric as e.g. \( \varepsilon(a, b) \neq \varepsilon(b, a) \). Moreover, we can observe that \( 1 \in \varepsilon(a, c) \), \( 1 \in \varepsilon(c, b) \) but \( 1 \notin \varepsilon(a, b) = \emptyset \). Therefore, Fitch maps are not “transitive” in general.
The example in Fig. 3 gives some intuition for the definition of the sets $N_m[y]$ and $N[e]$:

Here, we have $N_{-1}[b] = \{a, b\}$ and $N_{-4}[b] = \{a, b, c\}$. In this example, we obtain all clusters of size at least 2, and thus, all clusters that are needed to recover the tree that explains the map $\varepsilon$.

In fact, $N[e]$ is hierarchy-like. However, even if $N[e]$ is hierarchy-like it may be the case that there is no tree that can explain $\varepsilon$, as we shall see below. As in [18] the IC will turn out to be necessary as well.

The following proposition is crucial for the remaining part of this paper as it provides a quite powerful characterization of neighborhoods and edge-labeled trees that explain a Fitch map.

**Proposition 3.5.** Let $(T, \lambda)$ be an edge-labeled tree explaining the Fitch map $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$. Then, for every leaf $y \in X$ and every color $m \in M$ there is a vertex $v \in V(T)$ such that the following two equivalent statements are satisfied:

1. a) There is no $m$-edge on the path from $v$ to $y$ and 
b) the edge $(\text{par}(v), v)$ is an $m$-edge unless $v = \rho_T$.
2. $N_{-m}[y] = C_T(v)$.

**Proof.** Let $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ be a Fitch map that is explained by $(T, \lambda)$. Furthermore, let $y \in X$ be an arbitrary leaf and $m \in M$ be an arbitrary color.

First, we show that there is a vertex $v \in V(T)$, which satisfies Statement (1). Let $v \in V(T)$ be the vertex that is an ancestor of $y$ and is closest to the root $\rho_T$ such that there is no $m$-edge on the path from $v$ to $y$. Note that $v = y$ is possible. By the choice of $v$, Statement (1a) is trivially satisfied. Now, assume that $v \neq \rho_T$. This, together the the fact that $v$ is closest to the root among all ancestors of $y$ that satisfies that there is no $m$-edge on the path from $v$ to $y$, implies that $(\text{par}(v), v)$ is an $m$-edge. Therefore, Statement (1b) is also satisfied.

Next, we show that Statement (1) implies Statement (2). For fixed $m$ and $y$, consider a vertex $v \in V(T)$ satisfying (1a) and (1b).

First, we establish $v \preceq y$. Since $y$ is a leaf, we either have $v \preceq y$ or $v$ and $y$ are not comparable. Assume for contradiction that $v$ and $y$ are not comparable, and thus $v \neq \rho_T$. Therefore, Statement (1b) implies that $(\text{par}(v), v)$ is an $m$-edge. However, $(\text{par}(v), v)$ lies on the path from $v$ to $y$; a contradiction to Statement (1a). Thus, $v$ and $y$ must be comparable, and therefore $v \preceq y$.

In order to see that $C_T(v) \subseteq N_{-m}[y]$, we consider $x \in C_T(v)$, i.e. $v \preceq x$. This, together with $v \preceq y$ implies that $v \preceq \text{lca}(x, y) \preceq y$. Hence, $P_T(\text{lca}(x, y), y) \subseteq P_T(v, y)$. This, together with Statement (1a), implies that there is no $m$-edge on the path from $\text{lca}(x, y)$ to $y$. Since $(T, \lambda)$ explains $\varepsilon$, we have $v \in N_{-m}[y]$.

Next, in order to see that $N_{-m}[y] \subseteq C_T(v)$, we consider $x \in N_{-m}[y]$. Note that $v \preceq y$ implies that $y \in C_T(v)$. Therefore, if $x = y$, then $x = y \in C_T(v)$. Now, assume that $x \neq y$. Hence, we have $x \in N_{-m}[y] \setminus \{ y \}$, and therefore $m \notin \varepsilon(x, y)$. Thus, since $(T, \lambda)$ explains $\varepsilon$, there is no $m$-edge on the path from $\text{lca}(x, y)$ to $y$. Note that if $\text{lca}(x, y) \prec v \preceq y$, then $v \neq \rho_T$ and Statement (1b) implies that $(\text{par}(v), v)$ is an $m$-edge that, in particular, is on the path from $\text{lca}(x, y)$ to $y$; a contradiction. Thus, $\text{lca}(x, y)$ cannot be a strict ancestor of $v$. Moreover, $v \preceq y$ and $\text{lca}(x, y) \preceq y$ imply that $\text{lca}(x, y)$ and $v$ are comparable. The latter arguments together imply that $v \preceq \text{lca}(x, y) \preceq x$. Hence, $x \in C_T(v)$.

We proceed to show that Statement (2) implies Statement (1). Suppose that Statement (2) is satisfied. If $v = y$, then Statement (1a) is trivially satisfied. Now, assume that $v \neq y$. Choose an $x \in X$ such that $\text{lca}(x, y) = v$. Note that $v \neq y$ implies that $x$ and $y$ are distinct. This and $x \in C_T(v) = N_{-m}[y]$ imply that $m \notin \varepsilon(x, y)$. This and the fact that $(T, \lambda)$ explains $\varepsilon$ imply that there is no $m$-edge on the path from $v = \text{lca}(x, y)$ to $y$. In summary, Statement (1a) is satisfied.

Now, assume that $v \neq \rho_T$. Hence, there is a parent $\text{par}(v)$ of $v$. Therefore, we can choose a vertex $x' \in C_T(\text{par}(v)) \setminus C_T(v)$. Hence, $\text{par}(v) = \text{lca}(x', y)$. Since $x' \notin C_T(v) = N_{-m}[y]$ and $x' \neq y$, we have $m \in \varepsilon(x', y)$. This, together with the fact that $(T, \lambda)$ explains $\varepsilon$, implies that there is an $m$-edge on the path from $\text{lca}(x', y) = \text{par}(v)$ to $y$. We have already shown that Statement (1a) is
satisfied, and thus, there is no \( m \)-edge on the path from \( v \) to \( y \). The latter two arguments imply that \((\text{par}(v),v)\) must be an \( m \)-edge. Therefore, Statement (1b) is also true. ■

Proposition 3.5 has several simple but important consequences.

**Corollary 3.6.** Every Fitch map \( \varepsilon \) satisfies the hierarchy-like-condition (HLC), and \( \mathcal{N}[\varepsilon] \subseteq \mathcal{C}(T) \) for every tree \((T,\lambda)\) that explains \( \varepsilon \).

**Proof.** Let \((T,\lambda)\) be an arbitrary tree that explains \( \varepsilon \). By Prop. 3.5, for every neighborhood \( N_{-m}[y] \in \mathcal{N}[\varepsilon] \) there is always a vertex \( v \in V(T) \) with \( N_{-m}[y] = C_r(v) \in \mathcal{C}(T) \). Hence, \( \mathcal{N}[\varepsilon] \subseteq \mathcal{C}(T) \). By Lemma 2.1, the set \( \mathcal{C}(T) \) forms a hierarchy. Since every subset of the cluster-set \( \mathcal{C}(T) \) of a phylogenetic tree \( T \) is hierarchy-like, the map \( \varepsilon \) satisfies HLC. ■

Moreover, Prop. 3.5 can also be used to show

**Corollary 3.7.** Every Fitch map \( \varepsilon \) satisfies the inequality-condition (IC).

**Proof.** Let \( \varepsilon: [X \times X]_{irr} \rightarrow \mathcal{P}(M) \) be a Fitch map that is explained by \((T,\lambda)\). Furthermore, let \( y \in X \) be an arbitrary leaf and \( m \in M \) be an arbitrary color; and let \( y' \in N := N_{-m}[y] \). We need to show that \( |N_{-m}[y']| \leq |N| \).

By Cor. 3.6, we have \( \mathcal{N}[\varepsilon] \subseteq \mathcal{C}(T) \) and therefore, \( N_{-m}[y'], N_{-m}[y] \in \mathcal{N}[\varepsilon] \subseteq \mathcal{C}(T) \) are clusters. Hence, there are vertices \( v, y' \in V(T) \) such that \( N = C_r(v) \) and \( N_{-m}[y'] = C_r(y') \). Since \( y' \in N = C_r(v) \), and by definition \( y' \in N_{-m}[y'] = C_r(y') \), we have \( v \preceq y' \) and \( v' \preceq y' \). Hence, both \( v \) and \( v' \) are contained in the unique path from \( y' \) to the root. Thus \( v \) and \( v' \) are comparable.

Suppose that \( v' \) is a strict ancestor of \( v \), i.e., \( v' \prec v \). Then, the edge \((\text{par}(v),v)\) lies on the path \( P_r(v',y) \). Moreover, \( N_{-m}[y'] = C_r(v') \) together with Proposition 3.5 (1a, 2) implies that there is no \( m \)-edge on the path \( P_r(v',y) \). The latter arguments together imply that the edge \((\text{par}(v),v)\) is not an \( m \)-edge. However, using Proposition 3.5 (1b, 2) for \( N = C_r(v) \) implies that \((\text{par}(v),v)\) is an \( m \)-edge; this is a contradiction. Therefore we must have \( v \preceq v' \). This implies \( N_{-m}[y'] = C_r(v') \subseteq C_r(v) = N \), and thus also the desired inequality \( |N_{-m}[y']| \leq |N| \). ■

Before we show that HLC and IC are also sufficient conditions for Fitch maps, we provide the following interesting result. Although this result does not have direct impact on the proofs for HLC and IC, it provides interesting details about the relationship between Fitch maps \( \varepsilon \) and certain sets of triples that we can derive from \( \varepsilon \).

**Proposition 3.8.** Let \( \varepsilon: [X \times X]_{irr} \rightarrow \mathcal{P}(M) \) be a Fitch map, and let

\[
\mathcal{R}(\varepsilon) := \bigcup_{N \in \mathcal{N}[\varepsilon]} \{ab|c : a,b \in N \text{ and } c \in X \setminus N\}
\]

be a triple set constructed of the neighborhoods of \( \varepsilon \). Then, we have the following:

1. every edge-labeled tree \((T,\lambda)\) that explains \( \varepsilon \) displays all triples in \( \mathcal{R}(\varepsilon) \), i.e., \( \mathcal{R}(\varepsilon) \subseteq \mathcal{R}(T) \).
2. \( \mathcal{R}(\varepsilon) \) is closed, i.e., \( \overline{\mathcal{R}(\varepsilon)} = \mathcal{R}(\varepsilon) \).

**Proof.** Let \( \varepsilon: [X \times X]_{irr} \rightarrow \mathcal{P}(M) \) be a Fitch map, and let \((T,\lambda)\) be a tree that explains \( \varepsilon \). Then, assume that \( ab|c \in \mathcal{R}(\varepsilon) \). Thus, there is a neighborhood \( N \in \mathcal{N}[\varepsilon] \) with \( a,b \in N \) and \( c \in X \setminus N \). By Prop. 3.5, we conclude that \( N = C_r(v) \) for some \( v \in V(T) \). Moreover, \( c \in X \setminus N \) implies that there is a vertex \( w \in V(T) \) with \( w = \text{lca}_T(a,b,c) \), and thus \( C_r(v) \subseteq C_r(w) \). The latter directly implies that \( \text{lca}_T(a,b,c) = w \prec_T v \preceq_T \text{lca}_T(a,b) \), and thus \( ab|c \) is displayed by \( T \).

We proceed with showing that \( \mathcal{R}(\varepsilon) \) is closed. First, we apply Corollary 3.6 to conclude that \( \mathcal{N}[\varepsilon] \) is hierarchy-like. Thus, \( \mathcal{N} := \mathcal{N}[\varepsilon] \cup \{X\} \cup \{\{x\} : x \in X\} \) is a hierarchy. By Lemma 2.1, there is a (unique) tree \( T \) such that \( \mathcal{C}(T) = \mathcal{N} \). By construction, we conclude that \( \mathcal{R}(\varepsilon) = \mathcal{R}(T) \), and thus \( \overline{\mathcal{R}(\varepsilon)} = \mathcal{R}(T) \). Due to the definition of a closure, we have \( \mathcal{R}(\varepsilon) = \mathcal{R}(T) \subseteq \mathcal{R}(T) \).

However, since \( T \in \mathcal{R}(T) \) and due to the definition of a closure, we obtain \( \overline{\mathcal{R}(T)} = \mathcal{R}(T) \). Therefore, \( \mathcal{R}(\varepsilon) = \mathcal{R}(T) = \overline{\mathcal{R}(T)} = \mathcal{R}(\varepsilon) \). Hence, \( \mathcal{R}(\varepsilon) \) is closed. ■
In order to show that HLC and IC are also sufficient conditions for Fitch maps, we define a particular edge-labeled tree \( \mathcal{T}(\varepsilon) = (T, \lambda) \) and proceed by proving that \( \mathcal{T}(\varepsilon) \) explains \( \varepsilon \).

**Definition 3.9.** Let \( \varepsilon : [X \times X]_{irr} \to \mathcal{P}(M) \) be a map that satisfies HLC. The edge-labeled tree \( \mathcal{T}(\varepsilon) = (T, \lambda) \) on \( X \) (with \( M \)), called \( \varepsilon \)-tree, has the cluster set
\[
\mathcal{C}(T) = N[\varepsilon] \cup \{X\} \cup \\{\{x\} : x \in X\}
\]
and each edge \((\text{par}(v), v)\) of \( T \) obtains the label
\[
\lambda((\text{par}(v), v)) := \{m \in M : \text{there is a } y \in X \text{ with } C_{\triangleright \downarrow}(v) = N_{-m}[y]\}. \tag{b}
\]

We first note that the \( \varepsilon \)-tree \( \mathcal{T}(\varepsilon) = (T, \lambda) \) is well-defined: If there is a map \( \varepsilon : [X \times X]_{irr} \to \mathcal{P}(M) \) that satisfies HLC, then \( \mathcal{C}(T) \) is indeed a hierarchy. This, together with Lemma 2.1, implies that the phylogenetic tree \( T \) on \( X \) is well-defined. The edge-labeling \( \lambda : E \to \mathcal{P}(M) \) in Def. 3.9 requires only the existence of vertices \( y \in X \) with \( C_{\triangleright \downarrow}(v) = N_{-m}[y] \) for some \( m \in M \), and thus, \( \lambda \) is also well-defined.

Now, we are in the position to show that HLC and IC are sufficient for Fitch maps.

**Lemma 3.10.** Let \( \varepsilon : [X \times X]_{irr} \to \mathcal{P}(M) \) be a map that satisfies HLC and IC. Then, \( \varepsilon \) is a Fitch map explained by \( \mathcal{T}(\varepsilon) \).

**Proof.** Let \( \varepsilon : [X \times X]_{irr} \to \mathcal{P}(M) \) be a map that satisfies HLC and IC, and let \( \mathcal{T}(\varepsilon) = (T, \lambda) \) be the \( \varepsilon \)-tree. To show that \( \varepsilon \) is a Fitch map it suffices to show that \( \mathcal{T}(\varepsilon) \) explains \( \varepsilon \). To this end, we will show that for every \((x, y) \in [X \times X]_{irr}\) we have the following:
\[
m \in \varepsilon(x, y) \iff \text{there is an } m\text{-edge on the path from lca}(x, y) \text{ to } y.
\]

Let \((x, y) \in [X \times X]_{irr}\), and suppose that \( m \in \varepsilon(x, y) \). Hence, \( x \notin N_{-m}[y] \). By construction of \( \mathcal{T}(\varepsilon) \), the set \( N_{-m}[y] \in N[\varepsilon] \subseteq \mathcal{C}(T) \) is a cluster. Hence, there is a vertex \( v \in V \) with \( N_{-m}[y] = C_{\triangleright \downarrow}(v) \). Since \( y \in N_{-m}[y] = C_{\triangleright \downarrow}(v) \), i.e. \( v \preceq y \), and \( \text{lca}(x, y) \preceq y \), we conclude that \( v \) and \( \text{lca}(x, y) \) are comparable. Moreover, since \( x \notin N_{-m}[y] = C_{\triangleright \downarrow}(v) \), i.e. \( v \not\preceq x \), and \( \text{lca}(x, y) \preceq x \), we can conclude that \( v \not\preceq \text{lca}(x, y) \). The latter two arguments imply that \( \text{lca}(x, y) \prec v \); and therefore, \( \text{lca}(x, y) \preceq \text{par}(v) \prec v \preceq y \). Hence, the edge \((\text{par}(v), v)\) lies on the path from \( \text{lca}(x, y) \) to \( y \). Since \( C_{\triangleright \downarrow}(v) = N_{-m}[y], v \neq \rho_{\triangleright \downarrow} \) and by the construction of \( \mathcal{T}(\varepsilon) \), we have \( m \in \lambda((\text{par}(v), v)) \), i.e. \((\text{par}(v), v)\) is an \( m\)-edge. Hence, there is the \( m\)-edge \((\text{par}(v), v)\) that lies on the path from \( \text{lca}(x, y) \) to \( y \).

Conversely, suppose that there is an \( m\)-edge \((\text{par}(v), v)\) on the path from \( \text{lca}(x, y) \) to \( y \) in \( \mathcal{T}(\varepsilon) \), and that \((x, y) \in [X \times X]_{irr}\). By construction of \( \mathcal{T}(\varepsilon) \), cf. Def. 3.9 (b), there is a leaf \( y' \in X \) with \( C_{\triangleright \downarrow}(v) = N_{-m}[y'] = N \).

We continue to show that \( N_{-m}[y] \subseteq C_{\triangleright \downarrow}(v) \). Since \( v \) lies on the path \( P_{\triangleright \downarrow}(\text{lca}(x, y), y) \), we have \( v \preceq y \), and thus \( y \in C_{\triangleright \downarrow}(v) \). By the construction of \( \mathcal{T}(\varepsilon) \), we have \( N[\varepsilon] \subseteq \mathcal{C}(T) \); and therefore, \( N_{-m}[y], C_{\triangleright \downarrow}(v) \subseteq \mathcal{C}(T) \) are clusters. This, together with \( y \in C_{\triangleright \downarrow}(v) \cap N_{-m}[y] \neq \emptyset \), implies either \( N_{-m}[y] \subseteq C_{\triangleright \downarrow}(v) \) or \( C_{\triangleright \downarrow}(v) \subseteq N_{-m}[y] \). Moreover, since \( \varepsilon \) satisfies the IC and \( y \in N = \text{lca}(x, y) \) it must hold that \( |N_{-m}[y]| = |N| = |C_{\triangleright \downarrow}(v)| \). The latter two arguments immediately imply \( N_{-m}[y] \subseteq C_{\triangleright \downarrow}(v) \). Furthermore, since \((\text{par}(v), v)\) lies on the path from \( \text{lca}(x, y) \) to \( y \), we can conclude that \( x \notin C_{\triangleright \downarrow}(v) \). This and \( N_{-m}[y] \subseteq C_{\triangleright \downarrow}(v) \) imply that \( x \notin N_{-m}[y] \). Hence, by definition of \( N_{-m}[y] \) we must have \( m \in \varepsilon(x, y) \).

To summarize, for any pair \((x, y) \in [X \times X]_{irr}\) we have \( m \in \varepsilon(x, y) \) if and only if there is an \( m\)-edge on the path from \( \text{lca}(x, y) \) to \( y \) in \( \mathcal{T}(\varepsilon) \). Therefore, \( \mathcal{T}(\varepsilon) \) explains \( \varepsilon \); and thus, \( \varepsilon \) is a Fitch map.

**Theorem 3.11.** A map \( \varepsilon : [X \times X]_{irr} \to \mathcal{P}(M) \) is a Fitch map if and only if
Based on Lemma 3.13, there are five forbidden (not necessarily induced) submaps on one or two colors. The colored graph-representation of these maps are shown here. Solid edges indicate that the particular color must occur, while dashed edges indicate that the particular color must not occur. Note, $m,m'$ are not necessarily distinct except for the Cases (3) and (4).

1. $N[e]$ is hierarchy-like (HLC); and
2. for every neighborhood $N := N_m[y] \in N[e]$ and every leaf $y' \in N$, we have $|N_m[y']| \leq |N|$ (IC).

Note that Theorem 3.11 and [18, Thm. 4] are equivalent in case that $\varepsilon$ is a monochromatic Fitch map. In particular, for a Fitch map $\varepsilon$, Theorem 3.11 implies that $N_m[y] \subseteq N$ for every neighborhood $N := N_m[y] \in N[\varepsilon]$ and every leaf $y' \in N$, since $N[\varepsilon]$ must be hierarchy-like.

### 3.3 Characterization in Terms of Forbidden Submaps

Monochromatic Fitch maps $\varepsilon : [X \times X]_{irr} \rightarrow \mathcal{P}(M)$ with $|M| = 1$ are characterized by a small set of forbidden subgraphs [15, 23]. In what follows, we show that also non-monochromatic Fitch maps have a forbidden submap characterization as defined as follows:

**Definition 3.12.** Let $\varepsilon : [X \times X]_{irr} \rightarrow \mathcal{P}(M)$ and $\varepsilon' : [X' \times X']_{irr} \rightarrow \mathcal{P}(M')$ be two maps. Then, the map $\varepsilon'$ is a submap of $\varepsilon$ if $X' \subseteq X$, and $\varepsilon'(x,y) \subseteq \varepsilon(x,y)$ for every $(x,y) \in [X' \times X']_{irr}$. In addition, a submap $\varepsilon'$ is an induced submap of $\varepsilon$ if $\varepsilon'(x,y) = \varepsilon(x,y)$ for every $(x,y) \in [X' \times X']_{irr}$.

For the characterization in terms of forbidden submaps, we first provide the next lemma, which is illustrated in Fig. 4.

**Lemma 3.13.** A map $\varepsilon : [X \times X]_{irr} \rightarrow \mathcal{P}(M)$ is not a Fitch map if and only if there are (not necessarily distinct) colors $m,m' \in M$ and

- there is a subset $\{a,b,c\} \in \binom{X}{3}$ with $m \notin \varepsilon(c,b)$ and $m' \notin \varepsilon(a,b)$ that satisfies one of the following conditions
  1. $m \notin \varepsilon(c,a)$, or
  2. a) $m' \notin \varepsilon(a,c)$ and $m' \notin \varepsilon(b,c)$, or
     b) $m' \in \varepsilon(a,c)$ and $m' \notin \varepsilon(b,c)$, or
  3. $m \neq m'$, $m' \notin \varepsilon(c,b)$ and $m' \notin \varepsilon(a,b)$; or
- there is a subset $\{a,b,c,d\} \in \binom{X}{4}$ with $m \notin \varepsilon(c,b)$ and $m \notin \varepsilon(a,b)$ that satisfies
  4. $m \neq m'$, $m' \notin \varepsilon(b,d) \cup \varepsilon(c,d)$ and $m' \in \varepsilon(a,d)$. 
Proof. Let $\varepsilon : [X \times X]_{irr} \rightarrow \mathcal{P}(M)$ be an arbitrary map. First, suppose that $\varepsilon$ is not a Fitch map. Thus, Theorem 3.11 implies that $\varepsilon$ does not satisfy HLC or IC.

First, suppose that $\varepsilon$ does not satisfy IC. Hence, there is a neighborhood $N_{-m}[b] \in \mathcal{N}[\varepsilon]$ and a vertex $a \in N_{-m}[b]$ such that $|N_{-m}[a]| > |N_{-m}[b]|$. Hence, $a \neq b$ and there is a vertex $c \in N_{-m}[a] \setminus N_{-m}[b]$. Since $a,b \in N_{-m}[b]$, we have $c \neq a$ and $c \neq b$, and hence $\{a,b,c\} \in \binom{X}{3}$. Since $c \notin N_{-m}[b]$, it must hold that $m \notin \varepsilon(c,b)$. Since $a \in N_{-m}[b]$, it must hold that $m \notin \varepsilon(a,b)$. Since $c \in N_{-m}[a]$, it must hold that $m \notin \varepsilon(c,a)$. The last three observations imply that Condition (1) is satisfied.

Now, assume that $\varepsilon$ does not satisfy HLC, and thus that $\mathcal{N}[\varepsilon]$ is not hierarchy-like. Hence, there are two neighborhoods $N_{-m}[y], N_{-m'}[y'] \in \mathcal{N}[\varepsilon]$ such that $N_{-m}[y] \cap N_{-m'}[y'] \neq \emptyset$. This, together with the fact that $y \in N_{-m}[y]$ and $y' \in N_{-m'}[y']$, implies that there are three mutually exclusive cases that need to be examined:

(A) neither of $y$ and $y'$ is contained in $N_{-m}[y] \cap N_{-m'}[y']$,
(B) exactly one element of $\{y,y'\}$ is contained in $N_{-m}[y] \cap N_{-m'}[y']$,
(C) both $y$ and $y'$ are contained in $N_{-m}[y] \cap N_{-m'}[y']$.

First, consider Case (A). This case is equivalent to $y \in N_{-m}[y] \setminus N_{-m'}[y']$ and $y' \in N_{-m'}[y'] \setminus N_{-m}[y]$. Since $N_{-m}[y] \cap N_{-m'}[y'] \neq \emptyset$, there is a vertex $a \in N_{-m}[y] \cap N_{-m'}[y']$ with $y,y' \neq a$. Thus, $a,y$ and $y'$ are pairwise distinct. Since $y \notin N_{-m'}[y']$, we have $m' \notin \varepsilon(y,y')$, and since $y' \notin N_{-m}[y]$, we have $m \notin \varepsilon(y',y)$. Moreover, since $a \in N_{-m}[y] \cap N_{-m'}[y']$, we have $m \notin \varepsilon(a,y')$ and $m' \notin \varepsilon(a,y)$. Now, put $b := y$ and $c := y'$. Then, we have found a subset $\{a,b = y,c = y'\} \in \binom{X}{3}$ such that $m \notin \varepsilon(c,b)$, $m \notin \varepsilon(a,b)$, $m' \notin \varepsilon(a,c)$ and $m' \notin \varepsilon(b,c)$. Hence, Condition (2a) is satisfied.

Now, consider Case (B). We can assume w.l.o.g. that $y \in N_{-m}[y] \cap N_{-m'}[y']$ and $y' \notin N_{-m'}[y'] \setminus N_{-m}[y]$. Since $N_{-m}[y] \setminus N_{-m'}[y'] \neq \emptyset$, there is a vertex $a \in N_{-m}[y] \setminus N_{-m'}[y']$ with $y,y' \neq a$. Thus, $a,y$ and $y'$ are pairwise distinct. Since $y \in N_{-m'}[y']$, we have $m' \notin \varepsilon(y,y')$, and since $y' \notin N_{-m}[y]$, we have $m \notin \varepsilon(y',y)$. Moreover, since $a \in N_{-m}[y] \setminus N_{-m'}[y']$, we have $m \notin \varepsilon(a,y)$ and $m' \notin \varepsilon(a,y')$. Now, put $b := y$ and $c := y'$. Then, we have found a subset $\{a,b = y,c = y'\} \in \binom{X}{3}$ such that $m \notin \varepsilon(c,b)$, $m \notin \varepsilon(a,b)$, $m' \notin \varepsilon(a,c)$ and $m' \notin \varepsilon(b,c)$. Hence, Condition (2b) is satisfied.

Next, consider Case (C). Here we consider the two subcases (i) $y = y'$ and (ii) $y \neq y'$. Let us start with Subcase (C.i) and suppose that $y = y'$. Since $N_{-m}[y] \cap N_{-m'}[y] \neq \emptyset$, we can directly conclude that $m \neq m'$. Moreover, since $N_{-m}[y] \setminus N_{-m'}[y] \neq \emptyset$ and $N_{-m'}[y'] \setminus N_{-m}[y] \neq \emptyset$, there are two distinct vertices $a \in N_{-m}[y] \setminus N_{-m'}[y]$ and $c \in N_{-m'}[y] \setminus N_{-m}[y]$. Hence, $a,c$ and $y$ are pairwise distinct. Since $a \in N_{-m}[y] \setminus N_{-m'}[y]$, we have $m \notin \varepsilon(a,y)$ and $m' \notin \varepsilon(a,y')$. Moreover, since $c \in N_{-m'}[y] \setminus N_{-m}[y]$, we have $m' \notin \varepsilon(c,a)$ and $m \notin \varepsilon(c,y)$. Now, put $b := y$. Then, we have found a subset $\{a,b = y,c = y\} \in \binom{X}{3}$ such that $m \notin \varepsilon(c,b)$, $m \notin \varepsilon(a,b)$, $m' \notin \varepsilon(c,b)$ and $m' \notin \varepsilon(a,b)$. This, together with $m \neq m'$, implies that Condition (3) is satisfied.

Finally, consider Subcase (C.ii) and suppose that $y \neq y'$. Since $N_{-m}[y] \setminus N_{-m'}[y'] \neq \emptyset$ and $N_{-m'}[y'] \setminus N_{-m}[y] \neq \emptyset$, there are two distinct vertices $x \in N_{-m}[y] \setminus N_{-m'}[y']$ and $x' \in N_{-m'}[y'] \setminus N_{-m}[y]$. Hence, $x,x',y$ and $y'$ are pairwise distinct, since $y,y' \in N_{-m}[y] \cap N_{-m'}[y']$ are distinct. Since $x \in N_{-m}[y] \setminus N_{-m'}[y']$, we have $m \notin \varepsilon(x,y)$ and $m' \notin \varepsilon(x',y)$. Since $y \in N_{-m'}[y']$, we have $m' \notin \varepsilon(x,y')$. Moreover, since $x' \in N_{-m'}[y'] \setminus N_{-m}[y]$, we have $m' \notin \varepsilon(x',y')$ and $m \notin \varepsilon(x',y)$. Thus, we have found a subset $\{a = x,b = y,c = x'\} \in \binom{X}{3}$ such that $m = m' \notin \varepsilon(c,b)$, $m = m' \notin \varepsilon(a,b)$, $m \notin \varepsilon(c,a)$. Hence, Condition (1) is satisfied.

Next, assume that $m \neq m'$. Then, put $a := x,b := y,c := x'$ and $d := y'$. Then, we have found a subset $\{a = x,b = y,c = x',d = y'\} \in \binom{X}{4}$ such that $m \notin \varepsilon(c,b)$, $m \notin \varepsilon(a,b)$, $m' \notin \varepsilon(b,d) \cup \varepsilon(c,d)$ and $m' \notin \varepsilon(a,d)$. This, together with $m \neq m'$, implies that Condition (4) is satisfied.

In summary, if $\varepsilon$ is not a Fitch map, then at least one of the Conditions (1), (2), (3) or (4) must be satisfied.

Conversely, suppose that $\varepsilon : [X \times X]_{irr} \rightarrow \mathcal{P}(M)$ satisfies at least one of the Conditions (1), (2), (3) or (4). First, assume that Condition (1) holds. Then, $a \in N_{-m}[a] \cap N_{-m}[b]$ and $c \in N_{-m}[a] \setminus N_{-m}[b]$. Then, put $c := a$. Then, we have found a subset $\{a,b = y,c = y'\} \in \binom{X}{3}$ such that $m = m' \notin \varepsilon(c,b)$, $m = m' \notin \varepsilon(a,b)$, $m \notin \varepsilon(c,a)$. Hence, Condition (1) is satisfied.
$N_{=m}[b]$. If $N_{=m}[b] \not\subseteq N_{=m}[a]$, then $N[\varepsilon]$ is not hierarchy-like; and therefore, Theorem 3.11 implies that $\varepsilon$ is not a Fitch map. Since $c \in N_{=m}[a] \setminus N_{=m}[b]$ implies that $N_{=m}[a] \neq N_{=m}[b]$, we can now assume that $N_{=m}[b] \subseteq N_{=m}[a]$. Hence, there is a neighborhood $N := N_{=m}[b]$ and a vertex $a \in N$ such that $|N_{=m}[a]| > |N|$; and therefore, $\varepsilon$ does not satisfy the inequality-condition (IC). Theorem 3.11 implies that $\varepsilon$ is not a Fitch map. Hence, either way, if $\varepsilon$ satisfies Condition (1), then $\varepsilon$ is not a Fitch map.

Now, if Condition (2a) is satisfied, then $a \in N_{=m}[b] \cap N_{=m}[c]$, $b \in N_{=m}[b] \setminus N_{=m}[c]$ and $c \in N_{=m}[c] \setminus N_{=m}[b]$. If Condition (2b) is satisfied, then $a \in N_{=m}[b] \cap N_{=m}[c]$, $b \in N_{=m}[b] \cap N_{=m}[c]$ and $c \in N_{=m}[c] \setminus N_{=m}[b]$. Moreover, if Condition (4) is satisfied, then $a \in N_{=m}[b] \setminus N_{=m}[d]$, $b \in N_{=m}[b] \cap N_{=m}[d]$ and $c \in N_{=m}[d] \setminus N_{=m}[b]$. It is easy to see that in neither case the set $N[\varepsilon]$ is hierarchy-like, and Thm. 3.11 implies that $\varepsilon$ is not a Fitch map.

In summary, if one of the Conditions (1), (2), (3) or (4) is satisfied, then $\varepsilon$ is not a Fitch map.

Application of simple Boolean conversion on Lemma 3.13 implies

**Theorem 3.14.** A map $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ is a Fitch map if and only if for every (not necessarily distinct) colors $m, m' \in M$, and

- for every subset $\{a, b, c\} \in \binom{X}{3}$ with $m \in \varepsilon(c, b)$ and $m \notin \varepsilon(a, b)$ we have
  1. $m \in \varepsilon(c, a)$, and
  2. $m' \in \varepsilon(c, a)$ if and only if $m' \in \varepsilon(b, c)$, and
  3. if $m \neq m'$ and $m' \notin \varepsilon(c, b)$, then $m' \notin \varepsilon(a, b)$; and
- for every subset $\{a, b, c, d\} \in \binom{X}{4}$ with $m \in \varepsilon(c, b)$ and $m \notin \varepsilon(a, b)$ we have
  4. if $m \neq m'$ and $m' \notin \varepsilon(b, d) \cup \varepsilon(c, d)$, then $m' \notin \varepsilon(a, d)$.

Note that Theorem 3.14 and [18, Thm. 5] are equivalent in case that $\varepsilon$ is a monochromatic Fitch map. Moreover, the characterization in Theorem 3.14 directly implies the following result that shows that the recognition of Fitch maps reduces to the recognition of Fitch maps on less than five vertices and on one or two colors only.

**Corollary 3.15.** Let $X' \subseteq X$, $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ be a map, and $\varepsilon' : [X' \times X']_{irr} \to \mathcal{P}(M')$ be the submap of $\varepsilon$ defined by $\varepsilon'(x, y) := \varepsilon(x, y) \cap M'$ for every $(x, y) \in [X' \times X']_{irr}$. Then, the following statements are equivalent:

1. $\varepsilon$ is a Fitch map.
2. If $|M| \geq 2$ and $|X| \geq 4$, then for every $X' \in \binom{X}{4}$ and for every $M' \in \binom{M}{2}$ the map $\varepsilon'$ is a Fitch map.
3. If $|M| \geq 2$ and $|X| \leq 3$, then for every $M' \in \binom{M}{2}$ the map $\varepsilon'$ is a Fitch map, where $X' := X$.
4. If $|M| = 1$, then for every $X' \in \binom{X}{3}$ the map $\varepsilon'$ is a Fitch map, where $M' := M$.

In addition, we obtain the following

**Corollary 3.16.** Every induced submap of a Fitch map is a Fitch map.

**Proof.** Let $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ be a Fitch map, and let $\varepsilon' : [X' \times X']_{irr} \to \mathcal{P}(M')$ be an induced submap of $\varepsilon$. Assume for contraposition that $\varepsilon'$ is not a Fitch map. Then, Thm. 3.14 implies that $\varepsilon'$ contains a forbidden submap. Since $\varepsilon'$ is an induced submap of $\varepsilon$, this forbidden submap is also part of $\varepsilon$. Thus, Thm. 3.14 implies that $\varepsilon$ is not a Fitch map. \[\blacksquare\]
4 Uniqueness of the Least-Resolved Tree

In the following we are interested in so-called least-resolved trees that explain a given Fitch map $\varepsilon$. Roughly speaking, an edge-labeled tree $(T, \lambda)$ that explains $\varepsilon$ is least-resolved if it does not contain “unnecessary” colors along its edges and one cannot “contract” edges without destroying the property that the resulting tree still explains $\varepsilon$. To make this notion more precise, we first need a couple of definitions.

Definition 4.1. Let $(T, \lambda)$ and $(T', \lambda')$ be two edge-labeled trees on $X$ with $M$. Then, $(T', \lambda')$ is a coarse-graining of $(T, \lambda)$, denoted by $(T', \lambda') \leq (T, \lambda)$, if

- $\mathcal{C}(T') \subseteq \mathcal{C}(T)$ and
- for each $v' \in V(T') \setminus \{\rho_{T'}\}$ and for each $v \in V(T) \setminus \{\rho_T\}$ with $C_T(v) = C_T(v')$ we have $\lambda'(\text{par}_T(v'), v') \subseteq \lambda(\text{par}_T(v), v)$.

Moreover, a coarse-graining $(T', \lambda')$ of $(T, \lambda)$ is a strict coarse-graining of $(T, \lambda)$ whenever

- $\mathcal{C}(T') \subseteq \mathcal{C}(T)$ or
- for some $v' \in V(T') \setminus \{\rho_{T'}\}$ and some $v \in V(T) \setminus \{\rho_T\}$ with $C_T(v) = C_T(v')$ we have $\lambda'(\text{par}_T(v'), v') \subseteq \lambda(\text{par}_T(v), v)$.

In particular, we say $(T, \lambda)$ and $(T', \lambda')$ are isomorphic, denoted by $(T, \lambda) \cong (T', \lambda')$, if they are coarse-grainings of each other.

Definition 4.2. Let $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ be a Fitch map that is explained by some edge-labeled tree $(T^*, \lambda^*)$. Then, we say $(T^*, \lambda^*)$ is least-resolved w.r.t. $\varepsilon$ if there is no strict coarse-graining $(T', \lambda')$ of $(T^*, \lambda^*)$ that explains $\varepsilon$.

Figure 5 provides an example of coarse-graining and least-resolved edge-labeled trees.

Proposition 4.3. Let $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ be a Fitch map, let $(T, \lambda)$ be an arbitrary edge-labeled tree that explains $\varepsilon$, and let $\mathcal{S}(\varepsilon)$ be the $\varepsilon$-tree. Then, $\mathcal{S}(\varepsilon)$ is a coarse-graining of $(T, \lambda)$, i.e. $\mathcal{S}(\varepsilon) \leq (T, \lambda)$.

Proof. Let $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ be a Fitch map. Let $(T, \lambda)$ be an edge-labeled tree that explains $\varepsilon$, and let $\mathcal{S}(\varepsilon) = (\widehat{T}, \widehat{\lambda})$ be the $\varepsilon$-tree.

First, Theorem 3.11 implies that $\varepsilon$ satisfies HLC and IC. Moreover, Lemma 3.10 implies that $\mathcal{S}(\varepsilon) = (\widehat{T}, \widehat{\lambda})$ explains $\varepsilon$. By construction of $\mathcal{S}(\varepsilon)$, we have $\mathcal{C}(\widehat{T}) = N[\varepsilon] \cup \{X\} \cup \{\{x\} : x \in X\}$. Since $(T, \lambda)$ explains $\varepsilon$, we can apply Proposition 3.5 to conclude that $N[\varepsilon] \subseteq \mathcal{C}(T)$. Since $\{x\} \in \mathcal{C}(T)$ for all $x \in X$ and $X \in \mathcal{C}(T)$, we immediately obtain $\mathcal{C}(\widehat{T}) = N[\varepsilon] \cup \{X\} \cup \{\{x\} : x \in X\} \subseteq \mathcal{C}(T)$.

It remains to show that for each $\hat{v} \in V(\widehat{T}) \setminus \{\rho_{\widehat{T}}\}$ and for each $v \in V(T) \setminus \{\rho_T\}$ with $C_T(v) = C_T(v)$ we have $\widehat{\lambda}(\text{par}_T(\hat{v}), \hat{v}) \subseteq \lambda(\text{par}_T(v), v)$. Thus, let $\hat{v} \in V(\widehat{T}) \setminus \{\rho_{\widehat{T}}\}$ be an arbitrary vertex. Since $\mathcal{C}(\widehat{T}) \subseteq \mathcal{C}(T)$ there is a vertex $v \in V(T) \setminus \{\rho_T\}$ such that $C_T(v) = C_T(v)$. Let
$m \in \hat{\lambda}(\text{par}_r(\hat{v}), \hat{v})$ be an arbitrary color. By construction of $\mathcal{T}(\varepsilon)$, cf. Def. 3.9 (b), there is a leaf $y \in X$ with $C_r(\hat{v}) = N_{=m}[y]$. Hence, we have $y \in N_{=m}[y] = C_r(\hat{v}) = C_r(v)$.

Next, assume that $v \in X$ is a leaf, i.e. $\{v\} = C_r(v)$, and therefore $y = v$. Since $T$ is a phylogenetic tree, there is a leaf $z \in X$ such that lca$_r(v, z) = \text{par}_r(v)$. Moreover, $z \notin \{v\} = N_{=m}[y]$ implies $m \in \varepsilon(z, y)$. Since $(T, \hat{\lambda})$ explains $\varepsilon$, we conclude that there is an $m$-edge on the path from lca$_r(y, z) = \text{par}_r(\hat{v}) = \text{par}_r(v)$ to $v$. Hence, $m \in \hat{\lambda}(\text{par}_r(v), v)$.

Now, assume that $v \notin X$ is not a leaf. Recap, $y \in N_{=m}[y] = C_r(\hat{v}) = C_r(v)$ and $v \neq \rho_r$. This, together with the fact that $T$ is a phylogenetic tree, implies that there are two leaves $x, z \in X$ such that lca$_r(x, y) = v$ and lca$_r(y, z) = \text{par}_r(v)$. Since lca$_r(x, y) = v$ we have $x \in C_r(v) = N_{=m}[y]$. Moreover, lca$_r(y, z) = \text{par}_r(v)$ implies $z \notin C_r(v) = N_{=m}[y]$. Therefore, $x, y$ and $z$ are pairwise distinct. The latter arguments imply that $m \in \varepsilon(z, y)$ and $m \notin \varepsilon(x, y)$. This, together with the fact that $(T, \hat{\lambda})$ explains $\varepsilon$, implies that there is an $m$-edge on the path from lca$_r(x, y) = \text{par}_r(v)$ to $y$ and there is no $m$-edge on the path from lca$_r(x, y) = v$ to $y$. Therefore, we have $m \in \hat{\lambda}(\text{par}_r(v), v)$.

Thus, $m \in \hat{\lambda}(\text{par}_r(v), v)$ independent of whether $v \in X$ or $v \notin X$. Therefore, we have $\hat{\lambda}(\text{par}_r(\hat{v}), \hat{v}) \subseteq \hat{\lambda}(\text{par}_r(v), v)$. This, together with $\varepsilon(T) \subseteq \varepsilon(T)$, implies that $\mathcal{T}(\varepsilon)$ is a coarse-graining of $(T, \hat{\lambda})$.

**Theorem 4.4.** Let $\varepsilon : [X \times X]_{\text{irr}} \to \mathcal{P}(M)$ be a Fitch map and let $\mathcal{T}(\varepsilon) = (\hat{T}, \hat{\lambda})$ be the $\varepsilon$-tree. Then, $\mathcal{T}(\varepsilon)$ is the unique (up to isomorphism) least-resolved tree that explains $\varepsilon$. In particular, $\hat{T}$ has the minimum number of vertices, and the sum $\sum_{e \in E(T)} |\hat{\lambda}(e)|$ is minimum among all edge-labeled trees that explain $\varepsilon$.

**Proof.** Let $\varepsilon : [X \times X]_{\text{irr}} \to \mathcal{P}(M)$ be a Fitch map, and let $(T^*, \lambda^*)$ be a least-resolved edge-labeled tree w.r.t. $\varepsilon$. Moreover, let $\mathcal{T}(\varepsilon) = (\hat{T}, \hat{\lambda})$ be the $\varepsilon$-tree.

By Prop. 4.3, $\mathcal{T}(\varepsilon) = (\hat{T}, \hat{\lambda})$ is a coarse-graining of $(T^*, \lambda^*)$. Hence, $\mathcal{T}(\varepsilon)$ must be least-resolved. This, together with the fact that $(T^*, \lambda^*)$ is a least-resolved tree w.r.t. $\varepsilon$ and the fact that $\mathcal{T}(\varepsilon)$ explains $\varepsilon$, implies that $(T^*, \lambda^*)$ is isomorphic to $\mathcal{T}(\varepsilon)$.

Moreover, let $(T, \lambda)$ be an edge-labeled tree that explains $\varepsilon$. Then, by Prop. 4.3, $\mathcal{T}(\varepsilon) \leq (T, \lambda)$. By definition of “coarse-graining”, we have $\varepsilon(T) \subseteq \varepsilon(T)$, and hence $|\varepsilon(T)| \leq |\varepsilon(T)|$. Since $X \in \varepsilon(T) \cap \varepsilon(T)$, and since $\{x\} \in \varepsilon(T) \cap \varepsilon(T)$ for all $x \in X$, we can conclude that $|\varepsilon(T)| \leq |\varepsilon(T)|$. Since the latter is satisfied for every edge-labeled tree $(T, \lambda)$ that explains $\varepsilon$, the tree $\mathcal{T}(\varepsilon)$ must have a minimum number of vertices.

Furthermore, by definition of “coarse-graining”, we also have $\hat{\lambda}(\text{par}_r(\hat{v}), \hat{v}) \subseteq \hat{\lambda}(\text{par}_r(v), v)$ for all $\hat{v} \in V(\hat{T}) \setminus \{\rho_r\}$ and for all $v \in V(T) \setminus \{\rho_r\}$ with $C_r(\hat{v}) = C_r(v)$. Hence, the sum $\sum_{e \in E(\hat{T})} |\hat{\lambda}(e)|$ is minimum among all edge-labeled trees that explains $\varepsilon$.

Note that Theorem 4.4, together with Prop. 4.3, is equivalent to [15, Thm. 1] in case $\varepsilon$ is a monochromatic Fitch map. Moreover, Theorem 4.4 implies that one can verify whether a tree $(T, \lambda)$ is least-resolved w.r.t. a Fitch map $\varepsilon$ by checking if $(T, \lambda)$ is isomorphic to $\mathcal{T}(\varepsilon)$. An alternative way to test if a tree is least-resolved is provided by the next result.

**Proposition 4.5.** Let $\varepsilon : [X \times X]_{\text{irr}} \to \mathcal{P}(M)$ be a Fitch map that is explained by $(T, \lambda)$, and let $\mathcal{T}(\varepsilon)$ be the $\varepsilon$-tree. Then, $(T, \lambda)$ is isomorphic to $\mathcal{T}(\varepsilon)$ if and only if for every inner edge $e = (\text{par}_r(v), v) \in E(T)$ the following two statements are satisfied:

1. $\lambda(e) \neq \emptyset$, and
2. for every $m \in \lambda(\text{par}(v), v)$ there is a leaf $y \in X$ such that there is no $m$-edge along the path from $v$ to $y$ in $(T, \lambda)$.

**Proof.** Let $\varepsilon : [X \times X]_{\text{irr}} \to \mathcal{P}(M)$ be a Fitch map that is explained by $(T, \lambda)$, and let $\mathcal{T}(\varepsilon) = (\hat{T}, \hat{\lambda})$ be the $\varepsilon$-tree.
First, assume that \((T, \lambda)\) is isomorphic to \(\mathcal{F}(\varepsilon)\), and thus \(\mathcal{E}(T) = \mathcal{E}(\hat{T})\). Then, we may assume w.l.o.g. that \(V(T) = V(\hat{T})\) and \(E(T) = E(\hat{T})\). Hence, by Def. 3.9, for all \(v \in V(T) \setminus \{\rho_T\}\) it holds that \(C_T(v) = N_m[y]\) for some \(y \in X\) and some \(m \in M\). Now, we can utilize the equivalence between (1) and (2) in Proposition 3.5 to conclude that Statement (1) and (2) are satisfied for \((T, \lambda)\).

Conversely, assume that \((T, \lambda)\) satisfies Statement (1) and (2). Let \(v \in \hat{V}(T) \setminus \{\rho_T\}\) be an arbitrary inner vertex. Statement (1) implies that there is an \(m \in \lambda(\text{par}_T(v), v)\), and Statement (2) implies that there is no \(m\)-edge along the path from \(v\) to \(y\) in \((T, \lambda)\). Now, we can apply Proposition 3.5 to conclude that \(C_T(v) = N_m[y]\) for some \(y \in X\) and some \(m \in M\). Hence, by Def. 3.9 (a), we have \(C_T(v) = N_m[y] \in N[\varepsilon] \subseteq N[\varepsilon] \cup \{\{x\} : x \in X\} \cup \{X\} = \mathcal{E}(\hat{T})\). This implies \(\mathcal{E}(T) \subseteq \mathcal{E}(\hat{T})\). Moreover, Prop. 4.3 implies that \(\mathcal{E}(\hat{T}) \subseteq \mathcal{E}(T)\). Hence, we obtain \(\mathcal{E}(T) = \mathcal{E}(\hat{T})\).

Now, we need to show that \(\hat{\lambda}(\text{par}_T(\hat{v}), \hat{v})\) is satisfied for every \(v \in V(T) \setminus \{\rho_T\}\) and for every \(\hat{v} \in V(\hat{T})\) with \(C_T(v) = C_T(\hat{v})\). Prop. 4.3 implies that \((\hat{T}, \hat{\lambda})\) is a coarse-graining of \((T, \lambda)\) and therefore, \(\hat{\lambda}(\text{par}_T(\hat{v}), \hat{v}) \subseteq \lambda(\text{par}_T(v), v)\). To verify that \(\hat{\lambda}(\text{par}_T(\hat{v}), \hat{v}) \subseteq \lambda(\text{par}_T(\hat{v}), \hat{v})\), let \(m \in \lambda(\text{par}_T(\hat{v}), \hat{v})\). If \(v \notin X\) is not a leaf, then Statement (2) implies that there is a leaf \(y \in X\) such that there is no \(m\)-edge on the path from \(v\) to \(y\) in \((T, \lambda)\). If \(v \in X\) is a leaf, then there is trivially no \(m\)-edge on the path from \(v\) to \(v\) in \((T, \lambda)\). In both cases, Proposition 3.5 implies that \(C_T(v) = N_m[y]\). Since \(\mathcal{E}(\hat{T}) = \mathcal{E}(T)\), as shown above, there is a vertex \(\hat{v} \in V(\hat{T}) \setminus \{\rho_T\}\) such that \(C_T(v) = C_T(\hat{v}) = N_m[y]\). By Def. 3.9, \(m \in \lambda(\text{par}_T(\hat{v}), \hat{v})\) and thus \(\hat{\lambda}(\text{par}_T(\hat{v}), \hat{v}) = \lambda(\text{par}_T(v), v)\).

In summary, \((T, \lambda)\) is isomorphic to \(\mathcal{F}(\varepsilon)\).

5 Restricted Fitch maps

In the following, we consider two typical restrictions of Fitch maps. One restricts the number of colors placed on the edges and the other is based on a “recoloring” based on subsets of the color set \(M\).

5.1 \(k\)-Restricted Fitch map

Geiß et al. [15] considered monochromatic Fitch maps and Hellmuth [20] considered disjoint Fitch maps. These special classes of Fitch maps can always be explained by edge-labeled trees \((T, \lambda)\) with \(|\lambda(e)| \leq 1\) for every \(e \in E(T)\). In view of these results, we consider here a common generalization of these ideas and ask which type of Fitch maps can be explained by edge-labeled trees \((T, \lambda)\) with \(|\lambda(e)| \leq k\) for every \(e \in E(T)\) and some fixed integer \(k\).

**Definition 5.1.** Let \(\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)\) be a Fitch map, and let \(k \in \mathbb{N}\) be an integer. Then, we call \(\varepsilon\) a \(k\)-restricted Fitch map if there is an edge-labeled tree \((T, \lambda)\) that explains \(\varepsilon\) and that satisfies \(|\lambda(e)| \leq k\) for every \(e \in E(T)\).

Note that every monochromatic Fitch map and every disjoint Fitch map is a 1-restricted Fitch map. In order to characterize \(k\)-restricted Fitch maps, we will use the \(\varepsilon\)-tree \(\mathcal{F}(\varepsilon)\), Proposition 4.3 and the following

**Definition 5.2.** A map \(\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)\) satisfies the \(k\)-edge-label-condition (\(k\)-ELC) if for every neighborhood \(N \in N[\varepsilon]\) with \(N \neq X\) we have \(|\{m \in M : \text{there is a } y \in X \text{ with } N = N_m[y]\}| \leq k\).

In other words, \(\varepsilon\) satisfies \(k\)-ELC if for every neighborhood \(N \in N[\varepsilon]\) with \(N \neq X\) there are at most \(k\) colors in \(M\) for which \(N = N_m[y]\) is satisfied.

**Proposition 5.3.** Let \(\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)\) be a Fitch map, and let \(\mathcal{F}(\varepsilon) = (\hat{T}, \hat{\lambda})\) be the \(\varepsilon\)-tree. Then, the following three statements are equivalent:

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1. $\varepsilon$ is a $k$-restricted Fitch map.
2. For every edge $e \in E(\hat{T})$ we have $|\hat{\lambda}(e)| \leq k$.
3. $\varepsilon$ satisfies $k$-ELC.

Proof. Let $\varepsilon : [X \times X]_{\text{irr}} \rightarrow \mathcal{P}(M)$ be a Fitch map, and let $\mathcal{F}(\varepsilon) = (\hat{T}, \hat{\lambda})$ be the $\varepsilon$-tree.

First, suppose that Statement (1) is satisfied. Then, there is an edge-labeled tree $(T, \lambda)$ with $|\lambda(e)| \leq k$ for every edge $e \in E(T)$. By Prop. 4.3, the tree $\mathcal{F}(\varepsilon) = (\hat{T}, \hat{\lambda})$ is a coarse-graining of $(T, \lambda)$, i.e. $\hat{\mathcal{C}}(\hat{T}) \subseteq \mathcal{C}(T)$ and for each $\hat{v} \in V(\hat{T}) \setminus \{\rho_{\hat{T}}\}$ and for each $v \in V(T) \setminus \{\rho_T\}$ with $C_T(v) = C_T(\hat{v})$ we have $\hat{\lambda}(\text{par}_{\hat{T}}(\hat{v}), \hat{v}) \subseteq \lambda(\text{par}_T(v), v)$. This, together with $|\lambda(e)| \leq k$ for every $e \in E(T)$, immediately implies Statement (2).

Next, assume that Statement (2) is satisfied. By Lemma 3.10, $\mathcal{F}(\varepsilon)$ explains $\varepsilon$. Thus, by Definition 5.1, Statement (1) is trivially satisfied. Hence, Statement (1) and (2) are equivalent.

We are still assuming that Statement (2) is satisfied, and let $N \in \mathcal{N}[\varepsilon]$ with $N \neq X$. Then, Def. 3.9 (a) implies that $N \in \mathcal{N}[\varepsilon] \subseteq \mathcal{C}(T)$ is a cluster. This, together with $N \neq X$, implies that there is a vertex $\hat{v} \in V(\hat{T})$ with $\hat{v} \neq \rho_{\hat{T}}$ such that $C_{\hat{T}}(\hat{v}) = N$. Since $\hat{v} \neq \rho_{\hat{T}}$, there is the edge $(\text{par}_{\hat{T}}(\hat{v}), \hat{v}) \in E(\hat{T})$. Then, Definition 3.9 (b), together with $C_{\hat{T}}(\hat{v}) = N$ and Statement (2), implies that

\[\{m \in M : \text{ there is a } y \in X \text{ with } N = C_{\hat{T}}(\hat{v}) = N_{-m}[y]\} = |\hat{\lambda}(\text{par}_{\hat{T}}(\hat{v}), \hat{v})| \leq k.\]

Hence, Statement (3) is satisfied.

Now, assume that Statement (3) is satisfied. Then, by Definition 3.9 (b), we immediately conclude that Statement (2) holds. Hence, Statement (2) and (3) are equivalent. \hfill \blacksquare

Proposition 5.3, together with Theorem 3.11, implies

**Theorem 5.4.** A map $\varepsilon : [X \times X]_{\text{irr}} \rightarrow \mathcal{P}(M)$ is a $k$-restricted Fitch map if and only if $\varepsilon$ satisfies HLC, IC and $k$-ELC.

Thus, we were able to adjust the characterization as in Theorem 3.11 for the special class of $k$-restricted Fitch maps. However, as we shall see later, it is not possible to derive a characterization in terms of forbidden submaps similar to Thm. 3.14. To this end, consider first the following

**Example 5.5** ($k$-restricted Fitch maps may contain induced submaps that are not $k$-restricted Fitch maps). Consider the map $\varepsilon : [X \times X]_{\text{irr}} \rightarrow \mathcal{P}(M)$ with $X = \{a, b, c, d\}$ and $M = \{1, \ldots, k, k+1\}$, $k \geq 1$ as shown in Fig. 6 (left). For the edge-labeled tree $(T, \lambda)$ as provided in Fig. 6 (middle), all dashed edges $e \in E(T)$ have label $\lambda(e) = \emptyset$. Hence, $|\lambda(e)| \leq k$ for all $e \in E(T)$. In fact, $(T, \lambda)$ explains $\varepsilon$; and therefore, $\varepsilon$ is a $k$-restricted Fitch map.

Now, consider the induced submap $\varepsilon' : [X' \times X']_{\text{irr}} \rightarrow \mathcal{P}(M)$ with $X' = \{a, b, d\}$ of $\varepsilon$, as shown in Fig. 6 (right). By Cor. 3.16, $\varepsilon'$ is also a Fitch map. For $N := \{a, b\} = N_{-1}[a] \in \mathcal{N}[\varepsilon']$
we have \(|\{m \in M: N = N_{-m}(a)\}| = |M| = k + 1 > k\). This, together with \(\{a, b\} \neq X'\), implies that \(\varepsilon'\) does not satisfy the \(k\)-ELC, cf. Def. 5.2. This, the fact that \(\varepsilon'\) is a Fitch map, and Prop. 5.3 imply that \(\varepsilon'\) is not a \(k\)-restricted Fitch map.

In summary, although \(\varepsilon\) is a \(k\)-restricted Fitch map, it contains an induced submap, which is not a \(k\)-restricted Fitch map.

Since we only consider phylogenetic trees, we can utilize Example 5.5 in order to show that there is no characterization of \(k\)-restricted Fitch maps in terms of a set of forbidden submaps. This statement can be expressed more formally as follows:

**Theorem 5.6.** There is no set of forbidden submaps such that \(\varepsilon\) is a \(k\)-restricted Fitch map if and only if \(\varepsilon\) does not contain a forbidden submap.

**Proof.** Assume for contradiction that there is a set of forbidden submaps that characterizes \(k\)-restricted Fitch maps. Let \(\varepsilon\) and \(\varepsilon'\) be chosen as in Example 5.5. Since \(\varepsilon\) is a \(k\)-restricted Fitch map, \(\varepsilon\) does not contain any of such forbidden submaps. Hence, the induced submap \(\varepsilon'\) of \(\varepsilon\) cannot contain any of these forbidden submaps. Thus, \(\varepsilon'\) must be a \(k\)-restricted Fitch map; a contradiction.

In principle it is possible to relax the restriction to phylogenetic trees. Allowing arbitrary trees, we would obtain the same characterization as for Fitch maps, i.e. Thm. 3.11 and 3.14. To assign at most \(\varepsilon\) cannot contain any of these forbidden submaps. Thus, \(\varepsilon'\) is a \(k\)-restricted Fitch map.

### 5.2 Recoloring Fitch Maps

Interpreting colors as different subclasses of horizontal transfer events it is of interest to consider different resolutions at which events are considered different. Considering certain sets of colors as equivalent thus amounts to a coarse graining. Here, we briefly show that Fitch maps are well-behaved under “recoloring” and “identification of colors”.

**Definition 5.7.** Let \(\varepsilon: [X \times X]_{irr} \to \mathcal{P}(M)\) be a map and \(P = \{M_1, \ldots, M_k\} \subseteq \mathcal{P}(M)\) be a collection of subsets of \(M\). Then, we define the \(P\)-recolored map \(\varepsilon_P: [X \times X]_{irr} \to \mathcal{P}(\{1, \ldots, k\})\) by putting for all distinct \(x, y \in X\)

\[
\varepsilon_P(x, y) := \{i \in \{1, \ldots, k\} : \varepsilon(x, y) \cap M_i \neq \emptyset\}.
\]

In other words, \(\varepsilon_P(x, y)\) contains color \(i\) if and only if \(\varepsilon(x, y) \cap M_i \neq \emptyset\). Given a Fitch map \(\varepsilon: [X \times X]_{irr} \to \mathcal{P}(M)\) explained by the edge-labeled tree \((T, \lambda)\) and given a set \(P = \{M_1, \ldots, M_k\} \subseteq \mathcal{P}(M)\), we will make use of the edge-labeled tree \((T, \lambda_P)\), where the edge-labeling \(\lambda_P: E(T) \to \mathcal{P}(\{1, \ldots, k\})\) assigns the set \(\lambda_P(e) := \{i \in \{1, \ldots, k\} : \lambda(e) \cap M_i \neq \emptyset\}\) to every edge \(e \in E(T)\).

**Proposition 5.8.** Let \(\varepsilon: [X \times X]_{irr} \to \mathcal{P}(M)\) be a Fitch map, and let \(P = \{M_1, \ldots, M_k\} \subseteq \mathcal{P}(M)\) be a collection of subsets of \(M\). Then, the \(P\)-recolored map \(\varepsilon_P\) is a Fitch map that is explained by \((T, \lambda_P)\).

**Proof.** Suppose \(\varepsilon: [X \times X]_{irr} \to \mathcal{P}(M)\) is a Fitch map explained by \((T, \lambda)\), and let \(P = \{M_1, \ldots, M_k\} \subseteq \mathcal{P}(M)\). Since \((T, \lambda)\) explains \(\varepsilon\), we have for every \(i \in \{1, \ldots, k\}\) and for every distinct \(x, y \in X\):

\[
i \in \varepsilon_P(x, y) \iff \text{there is an } m \in \varepsilon(x, y) \cap M_i
\]

\[
\iff \text{there is an edge } e \in P_i([\text{lca}(x, y), y]) \text{ with } m \in \lambda(e) \cap M_i
\]

\[
\iff \text{there is an edge } e \in P_i([\text{lca}(x, y), y]) \text{ with } i \in \lambda_P(e).
\]
Since we have chosen \( i \in \{1, \ldots, k\} \) and \( x, y \in X \) arbitrarily, we conclude that \((T, \lambda_\varphi)\) explains \( \varepsilon_\varphi \); and thus, that \( \varepsilon_\varphi \) is a Fitch map.

Note that Theorem 4.4 implies that \( \mathcal{P}(\varepsilon_\varphi) \) is a coarse-graining of \((T, \lambda_\varphi)\) for every \( P \)-recolored Fitch map \( \varepsilon_\varphi \). In particular, Proposition 5.8 allows us to identify colors. In this case \( P = \{M_1, \ldots, M_k\} \) is a partition of \( M \). Thus we have

**Corollary 5.9.** Let \( \varepsilon : [X \times X]_{irr} \rightarrow \mathcal{P}(M) \) be a Fitch map and \( P = \{M_1, \ldots, M_k\}, k \geq 1 \) be a partition of \( M \). Then, the \( P \)-recolored map \( \varepsilon_\varphi \) is a Fitch map that is explained by \((T, \lambda_\varphi)\).

In particular, therefore, the least resolved tree explaining \( \varepsilon_\varphi \) is displayed by the least resolved tree explaining \( \varepsilon \). Finally, we note that \( \varepsilon_\varphi = \varepsilon \) whenever \( P \) consists of all singletons contained in \( \mathcal{P}(M) \).

6 Algorithmic Considerations

Algorithm 2 summarizes a method to recognize Fitch maps and, in the affirmative case, to construct the corresponding (unique) least-resolved edge-labeled tree. In this algorithm it must be verified whether the computed set \( N(\varepsilon) \) forms a hierarchy or not. Although there are papers that implicitly use algorithms to test whether a set system is hierarchy-like or not based e.g.
on underlying Hasse diagrams [14, Section 5] or so-called character-compatibility [35, Section 7.2], we provide here a quite simple alternative direct algorithm (cf. Alg. 1).

**Lemma 6.1.** Given a collection \( \mathcal{C} \subseteq \mathcal{P}(X) \) of subsets of \( X \), Alg. 1 correctly determines whether \( \mathcal{C} \) is hierarchy-like or not in \( O(|\mathcal{C}||X|) \) \( \subseteq O(|X|^2) \) time.

**Proof.** First, we prove the correctness of the algorithm. Let \( X \) be a non-empty set, and let \( \mathcal{C} = \{C_1, C_2, \ldots, C_{|\mathcal{C}|}\} \subseteq \mathcal{P}(X) \) be a collection of subsets of \( X \). By [19, Lemma 1], if \( \mathcal{C} \) is a hierarchy, then \( |\mathcal{C}| \leq 2|X| - 1 \). Hence, if \( |\mathcal{C}| > 2|X| - 1 \), then \( \mathcal{C} \) cannot be a hierarchy, and thus \( \mathcal{C} \) cannot be hierarchy-like. In this case, the algorithm correctly returns \texttt{false} in Line 1.

Then, the set \( \mathcal{C} \) is ordered based on the cardinality of its elements (Line 2). Moreover, a map \( \varphi : X \rightarrow \{0,1, \ldots, |\mathcal{C}|\} \) is initialized with \( \varphi(x) = 0 \) for every \( x \in X \) (Line 3). In essence, \( \varphi(x) \) saves for each \( x \in X \) the last considered set \( C_i \) where \( x \) was discovered. The initial case \( \varphi(x) = 0 \) corresponds to the trivial case “\( x \in C_0 = X \)” in the subsequent parts of this proof.

Lines 4 to 8 iterates over all \( C_i \in \mathcal{C} \) from the largest to the smallest elements. We set \( j \leftarrow \varphi(x) \) for some arbitrary but fixed vertex \( x \in C_i \). Thus, \( j \) is now the index of the latest preceding set \( C_j \) that contains \( x \). Then, we check for all \( y \in C_j \) whether index \( \varphi(y) = j \); that is, whether \( y \in C_j \) is true for all \( y \in C_j \), i.e., whether \( C_i \subseteq C_j \). If this is the case, then the value \( \varphi(y) \) is changed to the current index \( i \); otherwise, the algorithm returns \texttt{false}.

It remains to show that Alg. 1 (Lines 4 to 8) returns \texttt{false} if and only if \( \mathcal{C} \) is not hierarchy-like. First, suppose that Alg. 1 returns \texttt{false}, which is the case if there are vertices \( x, y \in C_i \) that satisfy \( \varphi(x) = j \neq \varphi(y) \). Hence, \( x \in C_i \cap C_{\varphi(x)} \) and \( y \in C_i \cap C_{\varphi(y)} \). Note that \( \varphi(x) < \varphi(y) < i \) and we may assume w.l.o.g. that \( \varphi(x) < \varphi(y) \). Thus, \( x \notin C_{\varphi(y)} \); as otherwise, the value \( \varphi(x) \) must have been changed to the index \( \varphi(y) \) when considering \( C_{\varphi(y)} \), since \( \varphi(y) \) is considered after \( C_{\varphi(x)} \). However, in this case, \( |C_i| \leq |C_{\varphi(y)}| \), \( y \in C_i \cap C_{\varphi(y)} \neq \emptyset \) and \( x \in C_i \setminus C_{\varphi(y)} \) implies \( C_i \cap C_{\varphi(y)} \notin \{\emptyset, C_i, C_{\varphi(y)}\} \). Therefore, \( \mathcal{C} \) is not hierarchy-like.

Conversely, suppose that \( \mathcal{C} \) is not hierarchy-like. Then, there are two elements \( C_i, C_j \in \mathcal{C} \) such that \( C_i \cap C_j \notin \{\emptyset, C_i, C_j\} \). In particular, we can choose the indices \( i \) and \( j \) such \( j < i \) and \( i - j \) is minimum. Now, consider the step of the algorithm where \( C_i \) is investigated. Then, we may assume w.l.o.g. that \( x \in C_i \cap C_j \) and \( y \in C_i \setminus C_j \). Hence, by the choice of \( i \) and \( j \), we conclude that \( \varphi(x) = j \), and since \( y \notin C_j \), we conclude that \( \varphi(y) \neq j \). Thus, \( \varphi(x) \neq \varphi(y) \) and the \texttt{if}-condition in Line 7 correctly will return \texttt{false}. In summary, Alg. 1 returns \texttt{false} if and only if \( \mathcal{C} \) is not hierarchy-like.
**Algorithm 1** Test whether a set $\mathcal{C} \subseteq \mathcal{P}(X)$ is hierarchy-like

**Input:** $\mathcal{C} \subseteq \mathcal{P}(X)$.

**Output:** true, if $\mathcal{C}$ is hierarchy-like, and false, otherwise.

1: if $|\mathcal{C}| > 2|X| - 1$ then return false
2: Order $\mathcal{C} = \{C_1, \ldots, C_{|\mathcal{C}|}\}$ such that $i \leq j$ whenever $|C_i| \geq |C_j|$.
3: $\varphi(x) \leftarrow 0$ for all $x \in X$ \quad \triangleright \text{Construct a map } \varphi : X \to \{0, 1, \ldots, |\mathcal{C}|\}$
4: for all $i \in \{1, \ldots, |\mathcal{C}|\}$ do
5: \hspace{1em} $j \leftarrow \varphi(x)$ for some arbitrary $x \in C_i$
6: for all $y \in C_i$ do
7: \hspace{2em} if $\varphi(y) = j$ then $\varphi(y) \leftarrow i$
8: \hspace{1em} else return false
9: return true

We continue by investigating the running time of the algorithm. Due to the if-condition in Line 1, we can observe that $|\mathcal{C}| \in O(|X|)$. Thus, the sorting of the elements in $\mathcal{C}$ (Line 2) can be achieved in $O(|X| \log(|X|))$ time. Moreover, we iterate in Lines 4 to 8 over all $|\mathcal{C}| \in O(|X|)$ elements in $\mathcal{C}$ and all $O(|X|)$ elements in each $C_i \in \mathcal{C}$ ending an overall time complexity of $O(|\mathcal{C}| |X|) \subseteq O(|X|^2)$, which completes the proof.

Let us now consider Algorithm 2 that determines whether a given map $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ is a Fitch map or not, and that returns, in the affirmative case, the least-resolved tree that explains $\varepsilon$. We shall note first that many of the more elaborate parts of the algorithm are used to achieve the desired running time. In a nutshell, in lines 1 to 15 the collection of neighborhoods $N[\varepsilon]$ is computed. In addition, an array of sets, called label, is computed where label$_{m,y}$ contains all labels that need to be added on particular edges of the possible exiting tree that explains $\varepsilon$. Moreover, count$_{N-m}[y]$ is the number of elements in $N[\varepsilon]$ that have the same cardinality as $N_{-m}[y]$. If count$_{N-m}[y]$ is larger than some specified values, then we can directly verify that $\varepsilon$ is not a Fitch map (Line 12). Then, we continue to check in Line 16 if $N[\varepsilon]$ satisfies IC and HLC. In the affirmative case, Theorem 3.11 implies that $\varepsilon$ is a Fitch map, and we compute in lines 17 to 21 the unique least-resolved tree $\mathcal{T}[\varepsilon](\varepsilon)$ that explains $\varepsilon$.

**Theorem 6.2.** Algorithm 2 determines correctly whether a given map $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ is a Fitch map. In the affirmative case Algorithm 2 returns the least-resolved tree that explains $\varepsilon$. Algorithm 2 can be implemented to run in $O(|X|^2 \cdot |M|)$ time.

**Proof.** Let $\varepsilon : [X \times X]_{irr} \to \mathcal{P}(M)$ be a map. First, we prove the correctness of the algorithm. It is easy to verify that the block consisting of the lines 1 to 5 correctly computes $N_{-m}[y]$ for all $y \in X$ and $m \in M$.

Now, we verify that the block consisting of the lines 6 to 15 correctly computes $N[\varepsilon]$. First, for all possible cardinalities $\ell \in \{1, \ldots, |X|\}$ a counter count$[\ell] = 0$ is initialized, see Line 6. This counter will count all neighborhoods that have the same size $\ell$.

Then, we iterate over all $m \in M$, and over all $y \in X$. In Line 8, we check if $N_{-m}[y]$ is already contained in $N[\varepsilon]$ or not. If $N_{-m}[y]$ is not contained in $N[\varepsilon]$, then we add it to $N[\varepsilon]$. The latter, in particular, ensures that $N[\varepsilon]$ is a set and not a multi-set. Moreover, we initialize an array of sets label$_{m,y} = \{m\}$ that will contain all labels that we need to add on particular edges of the possible exiting tree that explains $\varepsilon$. Moreover, we increase count$_{[N-m][y]}$ by one, that is, we increment the number of elements in $N[\varepsilon]$ that have the same cardinality as $N_{-m}[y]$. In Line 12, we check if (i) $|N[\varepsilon]| > 2|X| - 1$ or (ii) count$_{[N-m][y]} : |N_{-m}[y]| > |X|$ is satisfied. In Case (i) we can apply [19, Lemma 1] and conclude that $N[\varepsilon]$ cannot form a hierarchy. In this case, the algorithm correctly returns \textit{“$\varepsilon$ is not a Fitch map”}. In Case (ii),
we check if the number of elements in $N[\varepsilon]$ that have the same cardinality as $N_{-m}[y]$ times the number of elements in $N_{-m}[y]$ exceeds $|X|$. Suppose that Case (ii) applies. Since the elements of $N[\varepsilon]$ are pairwise distinct, they differ in at least one element. Thus, whenever there are two elements $N', N \in N[\varepsilon]$ of the same size then $N \cap N' = \emptyset$ if $N[\varepsilon]$ forms a hierarchy. But, then count$(|N_{-m}[y]|) \cdot |N_{-m}[y]| > X$, if $N[\varepsilon]$ forms a hierarchy. By contraposition, if Case (ii) applies, then $N[\varepsilon]$ cannot form a hierarchy. Hence, in both Cases (i) and (ii), the algorithm correctly returns “$\varepsilon$ is not a Fitch map”.

If $N_{-m}[y]$ is already contained in $N[\varepsilon]$ (else-case), then there is a unique neighborhood $N_{-m'}[y'] \in N[\varepsilon]$ with $N_{-m}[y] = N_{-m'}[y']$. In this case, we simply save the particular color $m$, and add $m$ to the label$[m', y']$. Clearly, $N[\varepsilon] = \{N_{-m}[y] : y \in X, m \in M\}$ is correctly computed.

According to Thm. 3.11, $\varepsilon$ is a Fitch Map if and only if $\varepsilon$ satisfies IC and HLC. Thus, the algorithm correctly returns “$\varepsilon$ is not a Fitch map”, in case $\varepsilon$ does not satisfy IC or HLC. Hence, if $\varepsilon$ is a Fitch map, then we can compute the edge-labeled tree $\mathcal{T}(\varepsilon) = (T, \lambda)$ according to Def. 3.9, which is done in lines 17 to 21. In particular, for a vertex $v \in V(T) \setminus \{\rho_x\}$ the pre-computed set label$[m', y']$ consists of all colors $m$ for which there is a $y$ with $C_r(v) = N_{-m}[y]$. Hence, $\lambda(\text{par}(v), v)$ is correctly computed in lines 18 to 21. Thm. 4.4 states that $\mathcal{T}(\varepsilon)$ is the least-resolved tree that explains $\varepsilon$. In summary, Algorithm 2 is correct.

Now, we investigate the running time of the algorithm. To this end, we assume w.l.o.g. that $X = \{1, \ldots, |X|\}$ and $M = \{1, \ldots, |M|\}$ are the ordered sets of positive integers from 1 to
Consider the block consisting of the lines 1 to 5 that computes \( N_{=\text{in}}[y] = \{ x \in X \setminus \{ y \} : m \notin \varepsilon(x, y) \} \cup \{ y \} \). First, we initialize \( N_{=\text{in}}[y] = \emptyset \) for all \( y \in X \) and \( m \in M \), a task that can be done in \( O(|X||M|) \) time. Then, we iterate in Line 2 over all \( y \in X \) and \( x \in X \setminus \{ y \} \) in the order they appear in \( X \). Then, we check for all \( m \in M \) if \( m \notin \varepsilon(x, y) \) and, in the affirmative case, add \( x \) to \( N_{=\text{in}}[y] \). Note that the resulting set \( N_{=\text{in}}[y] \) will then already be ordered. To check if \( m \notin \varepsilon(x, y) \), we may first compute \( \overline{M}_{xy} := M \setminus \varepsilon(x, y) \) in \( O(|M|) \) time and, afterwards, iterate over all elements \( m \in \overline{M}_{xy} \), which are precisely those \( m \in M \) with \( m \notin \varepsilon(x, y) \). The computation of \( \overline{M}_{xy} \) can be achieved in \( O(M) \) time for a fixed \( y \in X \) and \( x \in X \setminus \{ y \} \). Thus, the entire for-loop in Line 2 runs in \( O(|X|^2|M|) \) time. Finally, we add \( y \) to \( N_{=\text{in}}[y] \) for all \( y \in X \) and all \( m \in M \) in such a way that \( N_{=\text{in}}[y] \) remains an ordered set which can be done in \( O(|X|) \) time for a fixed \( y \in X \) and \( m \in M \). Thus, the latter task can be achieved in \( O(|X|^2|M|) \) time for all \( y \in X \) and all \( m \in M \).

Next, consider the block consisting of the lines 7 to 15 where the set \( N[\varepsilon] = \{ N_{=\text{in}}[x] : x \in X, m \in M \} \) is computed.

First, we show that the if-condition in Line 8 can be computed in \( O(|X|) \). Recalling that the neighborhoods \( N_{=\text{in}}[y] \) are already ordered. Hence, checking \( N_{=\text{in}}[y] = N \) for some \( N \in N[\varepsilon] \) can be done in \( O(|N_{=\text{in}}[y]|) \) time. Clearly, we only need to verify \( N_{=\text{in}}[y] = N \) for those \( N \in N[\varepsilon] \) with \( |N_{=\text{in}}[y]| = |N| \). Hence, testing if \( N_{=\text{in}}[y] \neq N[\varepsilon] \), can be done in \( O(\text{count}(|N_{=\text{in}}[y]|) \cdot |N_{=\text{in}}[y]| + |N[\varepsilon]|) \) time. Due to conditions in Line 12, \( O(\text{count}(|N_{=\text{in}}[y]|) \cdot |N_{=\text{in}}[y]| + |N[\varepsilon]|) \subseteq O(|X|) \). Therefore, the if-condition in Line 8 can be computed in time \( O(|X|) \).

Line 9 can be evaluated in \( O(|N_{=\text{in}}[y]|) \) time and the lines 10 to 12 require only constant time. In Line 14, finding the particular neighborhood \( N_{=\text{in}}[y'] \in N[\varepsilon] \) with \( N_{=\text{in}}[y'] = N_{=\text{in}}[y'] \) has already been done in the if-condition in Line 8, and thus requires only the constant effort for a look-up.

Since we iterate over all \( m \in M \) in the given order of \( M \), the set \( \text{label}[m', y'] \) is already sorted. In particular, if \( m \) is already contained in \( \text{label}[m', y'] \), then \( m \) must be the last element of this set. Hence, the union in Line 15 can be constructed in constant time.

In summary, each individual step within the for-loops in Line 7 can be accomplished in \( O(|X|) \) time. Since the for-loop has \( O(|X||M|) \) iterations, we achieve a total running time of \( O(|X|^2|M|) \) for the block consisting of the lines 7 to 15.

In Line 16, we check if \( \varepsilon \) satisfies IC and HLC. To check HLC, we can use Alg. 1 to verify if \( N[\varepsilon] \) is hierarchy-like in \( O(|N[\varepsilon]| |X|) \) time. Since we are in this step only if \( |N[\varepsilon]| \leq 2|X| - 1 \in O(|X|) \) (cf. Line 12), the latter task requires \( O(|X|^2|M|) \) time. To verify IC, we check whether \( |N_{=\text{in}}[y']| \leq |N| \) for every neighborhood \( N := N_{=\text{in}}[y] \) with \( m \in M \) and \( y \in X \) and for every \( y' \in N \). This requires \( O(|X|^2|M|) \) time.

Finally, we compute \( \mathcal{S}(\varepsilon) = (T, \lambda) \) in Lines 17 to 21. To this end, we build \( T \) based on the set \( \mathcal{C}(T) = N[\varepsilon] \cup \{ X \} \cup \{ \{ x \} : x \in X \} \). Since \( N[\varepsilon] \) is hierarchy-like, we have \( |N[\varepsilon]| \in O(|X|) \).

Hence, the hierarchy \( \mathcal{C}(T) \) can be computed in \( O(|X|) \) time. Moreover, \( T \) can be computed in \( O(|\mathcal{C}(T)|) \subseteq O(|X|) \) time, cf. [30]. While doing this, we also save the information, which vertex \( v \in T \) corresponds to which cluster \( C_T(v) = N_{=\text{in}}[y] \).

To compute \( \lambda : E(T) \rightarrow \mathcal{P}(M) \), we iterate over all \( |V(T)| - 1 \in O(|X|) \) edges in \( T \) and check if there is a (unique) \( N_{=\text{in}}[y] \in N[\varepsilon] \) with \( C_T(v) = N_{=\text{in}}[y] \) in constant time based on the latter step, and then set \( \lambda(\text{par}(v), v) = \text{label}[m, y] \). The latter can be done in \( O(|M|) \) time for a fixed vertex \( v \in T \). Thus, computing \( \lambda(\text{par}(v), v) \) for all \( v \in V(T) \setminus \{ r_T \} \) takes \( O(|X||M|) \) time.

In summary, Alg. 2 can be implemented to run in \( O(|X|^2|M|) \) time. ☑
7 Summary and Outlook

Fitch maps $\varepsilon$ are map $\varepsilon: [X \times X]_{irr} \rightarrow \mathcal{P}(M)$ that are explained by edge-labeled trees $(T, \lambda)$ where $\lambda: E(T) \rightarrow \mathcal{P}(M)$ assigns a subset of colors in $M$ to each edge of $T$. The main result of this contribution is to show that Fitch maps $\varepsilon$ are characterized by the two simple conditions HLC and IC, which are both defined in terms of (complementary) neighborhoods in the multi-edge-colored graph representation of $\varepsilon$ (cf. Thm. 5.4). Additionally, we provided a characterization via forbidden submaps (cf. Thm. 3.14). Moreover, we demonstrated that there is always a unique least-resolved tree for a Fitch map (cf. Thm. 4.4). Finally, we gave a polynomial-time algorithm to verify whether a given map $\varepsilon$ is a Fitch map, and, in the affirmative case, to construct the underlying least-resolved tree that explains $\varepsilon$.

Monochromatic Fitch maps have an additional characterization as a subclass of so-called directed cographs [15]. This, in particular, enables Geiß et al. [15] to establish a linear-time recognition algorithm as well as a linear-time tree reconstruction method for monochromatic Fitch maps. We suspect that there is a similar close relationship between the Fitch maps defined here and so-called unp-2 structures [7, 8, 10, 22], which form a natural generalization of directed cographs to edge-colored graphs. In particular, we expect that, using the theory of unp-2 structures, the recognition of Fitch maps and the reconstruction of the least-resolved trees is possible in a more efficient way.

As part of future research, it will be of interest to understand symmetrized Fitch maps in more detail. A map $\varepsilon: [X \times X]_{irr} \rightarrow \mathcal{P}(M)$ is a symmetrized Fitch map if there is an edge-labeled tree $(T, \lambda)$ such that $m \in \varepsilon(x, y)$ if and only if there is an $m$-edge along the unique path from $x$ to $y$ in $(T, \lambda)$. A characterization of symmetrized monochromatic Fitch maps can be found in [13]. Note that both, monochromatic Fitch maps and their symmetrized versions, form a special subclass of (directed) cographs, which are graphs that can be explained by vertex-labeled trees [13, 15]. A first attempt to understand symmetrized Fitch maps can be found in [24]. There, a characterization in terms of quartets (unrooted phylogenetic trees on four leaves) is provided, and it was shown that the recognition of symmetrized Fitch maps is NP-complete.

The Fitch maps defined here correspond to directed multi-graphs with the restriction that there are no parallel arcs of the same color. However, as already outlined in Section 3, we may also allow parallel arcs of the same color. That is, we may force to have $k m$-edges along the path from lca$(x, y)$ to $y$, whenever there are $k$ edges with color $m$ connecting $x$ and $y$ in the graph representation of $\varepsilon$. To our knowledge, this generalization has not been considered so far.

Finally, we have considered here only maps that are explained by trees. Generalizations to maps that are defined by (vertex-labeled) networks can be found in [25]. Thus, a general question arises: Can a map $\varepsilon: [X \times X]_{irr} \rightarrow \mathcal{P}(M)$ that is not a Fitch map, and thus cannot be explained by an edge-labeled tree, be explained by (rooted) edge-labeled networks instead? What are the “minimal” or “least-resolved” networks that explain such a map?

At present, there is no tool available to estimate the Fitch relation directly from data. There are, however, methods to retrieve partial information such as the fact that a given gene has undergone horizontal transfer [6]. On the one hand, the result reported here suggests that such partial information can help constrain gene trees. On the other hand, our results show that Fitch maps contain a wealth of information on the gene tree and its embedding into the species tree, providing a strong motivation to investigate ways to infer them from data directly. In this context, it is interesting to note that the phylogenetic signal to infer the edge-labeled trees is entirely contained in the collection $N[\varepsilon]$ of “complementary” neighborhoods $N_{-m}[y]$. In other words, to reconstruct such trees it is not necessary to find those pairs $(x, y)$ for which some type of transfer happened, that is, $m \in \varepsilon(x, y)$, but only to determine those pairs $(x, y)$ for which such an event has not occurred, i.e., $m \notin \varepsilon(x, y)$. Sloppy speaking, the phylogenetic signal to infer such trees is entirely contained in the non-HGT events.
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