Inference of Phylogenetic Trees from the Knowledge of Rare Evolutionary Events

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Abstract

Rare events have played an increasing role in molecular phylogenetics as potentially homoplasy-poor characters. In this contribution we analyze the phylogenetic information content from a combinatorial point of view by considering the binary relation on the set of taxa defined by the existence of single event separating two taxa. We show that the graph-representation of this relation must be a tree. Moreover, we characterize completely the relationship between the tree of such relations and the underlying phylogenetic tree. With directed operations such as tandem-duplication-random-loss events in mind we demonstrate how non-symmetric information constrains the position of the root in the partially reconstructed phylogeny.

Keywords: Phylogenetic Combinatorics; Rare events; Binary relations

1 Introduction

Shared derived characters (synapomorphies or "Hennigian markers") that are unique to specific clades form the basis of classical cladistics [22]. In the context of molecular phylogenetics rare genomic changes (RGCs) can play the same important role [32, 5]. RGCs corresponds to rare mutational events that are very unlikely to occur multiple times and thus are (almost) free of homoplasy. A wide variety
of processes and associated markers have been proposed and investigated. Well-studied RGCs include presence/absence patterns of protein-coding genes [13] as well as microRNAs [34], retroposon integrations [37], insertions and deletions (indels) of introns [31], pairs of mutually exclusive introns (NIPs) [25], protein domains [9, 43], RNA secondary structures [29], protein fusions [39], changes in gene order [33, 6, 27], metabolic networks [14, 15, 28], transcription factor binding sites [30], insertions and deletions of arbitrary sequences [38, 2, 11], and variations of the genetic code [1]. RGCs clearly have proved to be phylogenetically informative and helped to resolve many of the phylogenetic questions where sequence data lead to conflicting or equivocal results.

Not all RGCs behave like cladistic characters, however. While presence/absence characters are naturally stored in character matrices whose columns can vary independently, this is not the case e.g. for gene order characters. From a mathematical point of view, character-based parsimony analysis requires that the mutations have a product structure in which characters are identified with factors and character states can vary independently of each other [41]. This assumption is violated whenever changes in the states of two distinct characters do not commute. Gene order is of course the prime example on non-commutative events.

Three strategies have been pursued in such cases. Most importantly, the analog of the parsimony approach is considered for a particular non-commutative model. For the genome rearrangements an elaborate theory has been developed that considers various types of operations on (usually signed) permutations. Already the computation of editing distances is non-trivial. An added difficulty is that the interplay of different operations such as reversals, transpositions, and tandem-duplication-random-loss (TDRL) events is difficult to handle [3, 17]. An alternative is to focus on distance-based methods [42]. Since good rate models are usually unavailable, distance measures usually are not additive and thus fail to precisely satisfy the assumptions underlying the most widely used methods such as neighbor joining. The third strategy is to convert the non-commutative data structure into a presence-absence structure, e.g., by using pairwise adjacencies [40] as representation of permutations or using list alignments in which rearrangements appear as pairs of insertions and deletions [16]. While this yields character matrices that can be fed into parsimony algorithms, these can only result in approximate heuristics.

While it tends to be difficult to disentangle multiple, super-imposed complex changes such as genome rearrangements or tandem duplication, it is considerably simpler to recognize whether two genes or genomes differ by a single RGC operation. It make sense therefore to ask just how much phylogenetic information can be extracted from elementary RGC events. Of course, we cannot expect that a single RGC will allow us to (re)construct a detailed phylogeny. It can, however, provide us with solid, well-founded constraints. Furthermore, we can hope that the combination of such constraints can be utilized as a practicable method for phylogenetic inference. Recently we have shown that orthology assignments in large gene families imply triples that must be displayed by the underlying species tree [23, 19]. In a phylogenomics setting a sufficient number of such triple constraints can be collected to yield fully resolved phylogenetic trees [21], see [18] for an overview.

A plausible application scenario for our setting is the rearrangement of mitogenomes [33]. Since mitogenomes are readily and cheaply available, the taxon sampling is sufficiently dense so that the gene orders often differ by only a single rearrangement or not at all. These cases are identifiable with near certainty [3]. Moreover, some RGC are inherently directional. Probably the best known example is the tandem duplication random loss (TDRL) operation [8]. We will therefore also consider a directed variant of the problem.

In this contribution, we ask how much phylogenetic information can be retrieved from single RGCs. More precisely, we consider a scenario in which we can, for every pair of taxa distinguish, for a given type of RGC, whether $x$ and $y$ have the same genomic state, whether $x$ and $y$ differ by exactly one elementary change, or whether their distance is larger than a single operation. We formalize this problem in the following way. Given a relation $\sim$ is there a phylogenetic tree $T$ with an edge labeling $\lambda$ (marking the elementary events) such that $x \sim y$ if and only if edge labeling along the unique path $p(x, y)$ for $x$ to $y$ in $T$ has a certain prescribed property $\Pi$. In this contribution we will primarily be interest in the special case where $\Pi$ is “a single event along the path”. After defining the necessary notation and preliminaries, we give a more formal definition of the general problem in section 3. Then we give characterizations for the directed and the undirected version of the “single event” relations. Finally we briefly discuss generalizations.

2 Preliminaries

2.1 Basic Notation

We largely follow the notation and terminology of [36]. Throughout, $X$ denotes always a finite set of at least three taxa. We will consider both undirected and directed graphs $G = (V, E)$ with finite vertex set $V(G) := V$ and edge set or arc set $E(G) := E$. For a digraph $G$ we write $\overline{G}$ for its underlying (undirected) graph where $V(\overline{G}) = V(G)$ and $\{x, y\} \in E(\overline{G})$ if $(x, y) \in E(G)$ or $(y, x) \in E(G)$. Thus, $\overline{G}$ is obtained from $G$ by ignoring the direction of edges. For simplicity, edges $\{x, y\} \in E(G)$ (in the undirected) and arcs $(x, y) \in E(G)$ (in the directed case) will be both denoted by $xy$.

The representation $R(G) = (V, E)$ of a relation $R \subseteq V \times V$ has vertex set $V$ and edge set $E = \{xy \mid (x, y) \in R\}$. If $R$ is irreflexive, then $G$ has no loops. If $R$ is symmetric, we regard $G(R)$ as an undirected
A clique is a complete subgraph that is maximal w.r.t. inclusion. An equivalence relation is discrete if all its equivalence classes consist of single vertices.

A tree $T = (V, E)$ is a connected cycle-free undirected graph. The vertices of degree 1 in a tree are called leaves, all other vertices of $T$ are called inner vertices. An edge of $T$ is interior if both of its end vertices are interior vertices. A star $S_m$ with $m$ leaves is a tree that has at most one inner vertex. A path $P_n$ (on $n$ vertices) is a tree with two leaves and $n - 3$ interior edges. There is a unique path $P(x, y)$ connecting any two vertices $x$ and $y$ in a tree $T$. We write $e \in P(x, y)$ if the edge $e$ connects two adjacent vertices along $P(x, y)$. We say that a directed graph is a tree if its underlying undirected graph is a tree. A directed path $P$ is a tree on vertices $x_1, \ldots, x_n$ s.t. $x_i x_{i+1} \in E(P), 1 \leq i < n - 1$. A graph is a forest if all its connected components are trees.

A tree is rooted if there is a distinguished vertex $\rho \in V$ called the root. Throughout this contribution we assume that the root is an interior vertex. In rooted trees, the first inner vertex $v$ before the root is an interior vertex. In rooted trees, the first inner vertex $v$ before the root is called the lowest common ancestor of $x$ and $y$. If $T$ is rooted, then by definition $lca(x, y)$ is a uniquely defined inner vertex along $P(x, y)$.

We write $L(v)$ for the set of leaves in the subtree below a fixed vertex $v$, i.e., $L(v)$ is the set of all leaves for which $v$ is located on the unique path from $x \in L(v)$ to the root of $T$. The children of an inner vertex $v$ are its direct descendants, i.e., vertices $w$ with $wv \in E(T)$ s.t. that $w$ is further away from the root than $v$. A rooted or unrooted tree that has no vertices of degree two (with the possible exception that $T$ is a single, distinguished root node) and leaf set $X$ is called a phylogenetic tree $T$ (on $X$) or simply an X-tree.

Suppose $X' \subseteq X$. A phylogenetic tree $T$ on $X$ displays a phylogenetic tree $T'$ on $X'$ if $T'$ can be obtained from $T$ by a series of vertex deletions, edge deletions, and suppression of vertices of degree 2 or possibly the root, i.e., the replacement of an interior vertex $u$ and its two incident edges $e'$ and $e''$ by a single edge $e$, cf. [36, Def. 6.1.2]. In the rooted case, only a vertex between two consecutive edges (as seen from the root) may be suppressed; furthermore, if $X'$ is contained in a single subtree, then the $lca(X')$ becomes the root of $T'$. It is useful to note that $T'$ is displayed by $T$ if and only if it can be obtained from $T$ step-wisely by removing an arbitrarily selected leaf $y \in X \setminus X'$, its incident edge $e = yu$, and suppression of $u$ provided $u$ has degree 2 after removal of $e$.

A partial split of $X$, or a partial X-split, is a partition of a subset of $X$ into two disjoint non-empty subsets $A$ and $B$, denoted by $A|B$. Note, there is no difference between $A|B$ and $B|A$. If $A \cup B = X$, then $A|B$ is called a (full) X-split. For a split $A|B$ with $A = \{a_1, \ldots, a_i\}$ and $B = \{b_1, \ldots, b_j\}$ we will write $a_1, a_2, \ldots, a_i, b_1, b_2, \ldots, b_j$ instead of $\{a_1, \ldots, a_i\} \cup \{b_1, \ldots, b_j\}$. A partial X-split $A|B$ is trivial if $\min|A|, |B| = 1$.

Each edge $e \in E(T)$ of a tree $T$ gives rise to a split, that is, if one removes $e$ from $T$ one obtains two distinct trees $T_1$ and $T_2$ with leaf sets $L(T_1)$ and $L(T_2)$, respectively, and thus the X-split $L(T_1) \setminus L(T_2)$. For an X-tree $T$, let $\Sigma(T)$ denote the collection of X-splits corresponding to the edges of $T$. A partial X-split $A|B$ with $A = \{a, a'\}$ and $B = \{b, b'\}$ s.t. the path from $a$ to $a'$ does not intersect the path from $b$ to $b'$ in $T$ is called quartet (of $T$).

We say that the partial split $A|B$ extends the partial split $A'|B'$ precisely if either $A' \subseteq A$ and $B' \subseteq B$ or $A' \subseteq B$ and $B' \subseteq A$. For an arbitrary collection $\Sigma$ of distinct partial X-splits, we say that a partial split $A|B \in \Sigma$ is redundant if there exists a different partial split in $\Sigma$ that extends $A|B$. It is easy to verify that for a tree $T$ the set $\Sigma(T)$ does not contain redundant splits.

An X-tree displays $A|B$ if there is an edge $e \in E(T)$ of $T = (V, E)$ such that, in $(V, E \setminus \{e\})$, the sets $A$ and $B$ are subsets of the vertex sets of different connected components. A collection $\Sigma$ of partial X-splits is said to be compatible if there exists an X-tree that displays every X-split in $\Sigma$. This is equivalent to requiring that every split in $\Sigma$ is either contained in $\Sigma(T)$ or extended by a split in $\Sigma(T)$. The mathematical theory of systems of partial splits has been explored in [4, 35, 24, 12].

For later reference, we state the following well-know results [35].

**Lemma 1.** Let $A_1|B_1$ and $A_2|B_2$ be partial X-splits. The following statements are equivalent:

(i) $A_1|B_1$ and $A_2|B_2$ are compatible.

(ii) At least one of the sets $A_1 \cap A_2$, $A_1 \cap B_2$, $B_1 \cap A_2$, and $B_1 \cap B_2$ is empty.

**Lemma 2.** Let $\Sigma$ be a set of partial X-splits and $A_1|B_1, A_2|B_2 \in \Sigma$ that satisfy

\[ \emptyset \notin \{A_1 \cap A_2, A_1 \cap B_2, B_1 \cap A_2, B_1 \cap B_2\}, \quad A_2 \cap B_1 = \emptyset. \]

Furthermore, let

\[ \Sigma' := \Sigma \setminus \{A_1|B_1, A_2|B_2\} \cup \{(A_1 \cup A_2)|B_1, A_2|(B_1 \cup B_2)\}, \]

and $\Sigma'$ denote the set $\Sigma'$ after removing of any redundant partial splits from $\Sigma'$. Then an X-tree $T$ displays $\Sigma$ if and only if $T$ displays $\Sigma'$.

We say that a rooted tree $T$ contains or displays the triple $xy|z$ if $x, y,$ and $z$ are leaves of $T$ and the path from $x$ to $y$ does not intersect the path from $z$ to the root of $T$. A set of triples $\mathcal{R}$ is consistent if there is a rooted tree that contains all triples in $\mathcal{R}$. For a given leaf set $L$, a triple set $\mathcal{R}$ is said to be strict dense if for any three distinct vertices $x, y, z \in L$ we have $\{(xy|z, xz|y, yz|x) \cap \mathcal{R}\} = 1$. It is well-known that any consistent strict-dense triple set $\mathcal{R}$ has a unique representation as a binary tree [21, Suppl. Material]. For a consistent set $R$ of rooted triples we write $R^+(xy|z)$ if any phylogenetic tree that displays all triples of $R$ also displays $(xy|z)$. In a work of Bryant and Steel [7], in which the authors
extend and generalize the work of Dekker [10], it was shown under which conditions it is possible to infer triples by using only subsets $R' \subseteq R$, i.e., under which conditions $R \vdash (xy|z) \Rightarrow R' \vdash (xy|z)$ for some $R' \subseteq R$. In particular, we will use the following inference rules:

\begin{align*}
\{(ab|c), (ad|c)\} & \vdash (bd|c) \\
\{(ab|c), (ad|b)\} & \vdash (bd|c), (ad|c) \\
\{(ab|c), (cd|b)\} & \vdash (ab|d), (cd|a).
\end{align*}

(iii)

3 Path Relations and Phylogenetic Trees

Let $\Lambda$ be a non-empty set. Throughout this contribution we consider an X-tree $T = (V, E)$ with edge-labeling $\lambda: E \to \Lambda$. An edge $e$ with label $\lambda(e) = k$ will be called a $k$-edge. We interpret $(T, \lambda)$ so that a RGC occurs along edge $e$ if and only if $\lambda(e) = 1$. Let $\Pi$ be a subset of the set $\Lambda$-labeled paths. We interpret $\Pi$ as a property of the path and its labeling. The tree $(T, \lambda)$ and the property $\Pi$ together define a binary relation $\sim_\Pi$ on $X$ by setting

$$x \sim_\Pi y \iff (P(x, y), \lambda) \in \Pi$$

The relation $\sim_\Pi$ has the graph representation $G(\sim_\Pi)$ with vertex set $X$ and edges $xy \in E(G(\sim_\Pi))$ if and only if $x \sim_\Pi y$.

**Definition 3.** Let $(T, \lambda)$ be a $\Lambda$-labeled X-tree with leaf set $L(T)$ and let $G$ be a graph with vertex set $L(T)$. We say that $(T, \lambda)$ explains $G$ (w.r.t. to the path property $\Pi$) if $G = G(\sim_\Pi)$.

For simplicity we also say “$(T, \lambda)$ explains $\sim$” for the binary relation $\sim$.

We consider in this contribution the conceptually “inverse problem”: Given a definition of the predicate $\Pi$ as a function of edge labels along a path and a graph $G$, is there an edge-labeled tree $(T, \lambda)$ that explains $G$? Furthermore, we ask for a characterization of the class of graph that can be explained by edge-labeled trees and a given predicate $\Pi$.

A straightforward biological interpretation of the edge labeling $\lambda$ is that a certain type of evolutionary event has occurred along edge $e$ if and only if $\lambda(e) = 1$. This suggests that in particular the following path properties and their associated relations on $X$ are of practical interest:

- **(i)** $x \sim_0 y$ if and only if all edges in $P(x, y)$ are labeled 0; For convenience we set $x \sim_0 x$ for all $x \in X$.
- **(ii)** $x \sim_1 y$ if and only if all but one edges along $P(x, y)$ are labeled 0 and at exactly one edge is labeled 1;
- **(iii)** $x \sim_k y$ with $k > 1$ if and only if and at least $k$ edges are labeled 1;
- **(iv)** $x \sim y$ if the path from $\text{lca}(x, y)$ to $x$ has all edges labeled 0 and there are one or more edges along the path from $\text{lca}(x, y)$ to $y$ with a non-zero label, i.e., $\text{lca}(x, y) \sim_k y$ where $k \geq 1$.

We will call the relation $\sim_k$ the single-$k$-relation. It will be studied in detail in the following section. Its directed variant $\rightarrow_k$ will be investigated in Section 5. The more general relations $\sim_k$ and $\rightarrow_k$ will be studied elsewhere.

These (and many other) combinations of labeling systems and path properties have nice properties:

1. **(L1)** The label set $\Lambda$ is endowed with a semigroup $\oplus: \Lambda \times \Lambda \to \Lambda$.
2. **(L2)** There is a subset $\Lambda_{\Pi} \subseteq \Lambda$ of labels such that $(P(x, y), \lambda) \in \Pi$ if and only if $\lambda(P(x, y)) := \bigoplus_{e \in P(x, y)} \lambda(e)$ or $\lambda(P(x, y)) := \bigoplus_{e \in P(x, y)} \lambda(e)$

For instance, we may set $\Lambda = \mathbb{N}$ and use the usual addition for $\oplus$. Then $\sim_0$ corresponds to $\Lambda_{\Pi} = \{0\}$, $\sim_1$ corresponds to $\Lambda_{\Pi} = \{1\}$, etc.

We now extend the concept of an X-tree displaying another one to the $\Lambda$-labeled case.

**Definition 4.** Let $(T, \lambda)$ and $(T', \lambda')$ be two X-trees with $L(T') \subseteq L(T)$. Then $(T, \lambda)$ displays $(T', \lambda')$ if (i) $T'$ displays $T'$ and (ii) $(P_T(x, y), \lambda) \in \Pi$ if and only if $(P_{T'}(x, y), \lambda) \in \Pi$ for all $x, y \in L(T')$.

The definition is designed to ensure that the following property is satisfied:

**Lemma 5.** Suppose $(T, \lambda)$ displays $(T', \lambda')$ and $(T, \lambda)$ explains a graph $G$. Then $(T', \lambda')$ explains the induced subgraph $G[L(T')]$.

**Lemma 6.** Let $(T, \lambda)$ display $(T', \lambda')$. Assume that the labeling system satisfies (L1) and (L2) and suppose $\lambda'(e) = \lambda(e') \oplus \lambda(e'')$ whenever $e$ is the edge resulting from suppressing the interior vertex between $e'$ and $e''$. If $T'$ is displayed by $T$ then $(T', \lambda')$ is displayed by $(T, \lambda)$.

**Proof.** Suppose $T'$ is obtained from $T$ by removing a single leaf $w$. By construction $T'$ is displayed by $T$ and $\lambda(P_T(x, y))$ is preserved upon removal of $w$ and suppression of its neighbor. Thus (L2) implies that $(T, \lambda)$ displays $(T', \lambda')$. For arbitrary $T'$ displayed by $T$ this argument can be repeated for each individual leaf removal on the editing path from $T$ to $T'$.
Let us now turn to the properties of the specific relations that are of interest in this contribution.

**Lemma 7.** The relation $\sim_0$ is an equivalence relation.

*Proof.* By construction, $\sim_0$ is symmetric and reflexive. To establish transitivity, suppose $x \sim_0 y$ and $y \sim_0 z$, i.e., $\lambda(e) = 0$ for all $e \in \mathbb{P}(x, y) \cup \mathbb{P}(y, z)$. By uniqueness of the path connecting vertices in a tree, $\mathbb{P}(x, z) \subseteq \mathbb{P}(x, y) \cup \mathbb{P}(y, z)$, i.e., $\lambda(e) = 0$ for all $e \in \mathbb{P}(x, z)$ and therefore $x \sim_0 z$. \qed

Since $\sim_0$ is an equivalence relation, the graph $G(\sim_0)$ is a disjoint union of complete graphs, or in other words, each connected component of $G(\sim_0)$ is a clique.

We are interested here in characterizing the pairs of trees and labeling functions $(T, \lambda)$ that explain a given relation $\rho$ as its $\sim_0$, $\sim_1$ or $\sim_\Lambda$ relation. More precisely, we are interested in the least resolved trees with this property.

**Definition 8.** Let $(T, \lambda)$ be an edge-labeled phylogenetic tree with leaf set $X = L(T)$. We say that $(T', \lambda')$ is edge-contraction from $(T, \lambda)$ if the following conditions hold: (i) $T' = T/e$ is the usual graph-theoretical edge contraction for some interior edge $e = \{u, v\}$ of $T$. (ii) The labels satisfy $\lambda'(e') = \lambda(e)$ for all $e' \neq e$.

Note that we do not allow the contraction of terminal edges, i.e., of edges incident with leaves.

**Definition 9** (Least Resolved Tree). A pair $(T, \lambda)$ is least resolved for a prescribed relation $\sim_0$, $\sim_1$ or $\sim_\Lambda$ if no edge contraction leads to a tree $(T', \lambda')$ of $(T, \lambda)$ that explains $\sim_0$, $\sim_1$ or $\sim_\Lambda$, respectively.

### 4 The single-1-relation

The single-1-relation does not convey any information on the location of the root and the corresponding partial order on the tree. Where therefore regard $T$ as unrooted in this section.

**Lemma 10.** Let $(T, \lambda)$ be an edge-labeled $X$-tree with resulting relations $\sim_1$ and $\sim_0$ over $X$. Assume that $A, B$ are distinct cliques in $G(\sim_0)$ and suppose $x \sim_1 y$ where $x \in A$ and $y \in B$. Then $x' \sim_0 y'$ holds for all $x' \in A$ and $y' \in B$.

*Proof.* First, observe that $\mathbb{P}(x', y') \subseteq \mathbb{P}(x', x) \cup \mathbb{P}(x, y) \cup \mathbb{P}(y, y')$ in $T$. Moreover, $\mathbb{P}(x', x)$ and $\mathbb{P}(y, y')$ have only edges with label 0. As $\mathbb{P}(x, y)$ contains exactly one non-0-label, thus $\mathbb{P}(x', y')$ contains at most one non-0-label. If there was no non-0-label, then $\mathbb{P}(x, y) \subseteq \mathbb{P}(x, x') \cup \mathbb{P}(x', y') \cup \mathbb{P}(y, y')$ would imply that $\mathbb{P}(x, y)$ also has only 0-labels, a contradiction. Therefore $x' \sim_0 y'$.

As a consequence it suffices to study the single-1-relation on the quotient graph $G(\sim_1)/\sim_0$. To be more precise, $G(\sim_1)/\sim_0$ has as vertex set the equivalence classes of $\sim_0$ and two vertices $c_1$ and $c_2$ are connected by an edge if there are vertices $x \in c_1$ and $y \in c_2$ with $x \sim_1 y$. Analogously, the graph $G(\sim_1)/\sim_1$ is defined.

For a given $(T, \lambda)$ and its corresponding relation $\sim_1$ consider an arbitrary nontrivial equivalence class $c_i$ of $\sim_0$. Since $\sim_0$ is an equivalence relation, the induced subtree $T'$ with leaf set $c_i$ and interior vertices $lca(c_i)$ for any subset $c \subseteq c_i$ contains only 0-edges and is maximal w.r.t. this property. Hence, we could remove $T'$ from $T$ and identify the root $lca(c_i)$ of $T'$ in $T$ by a representative of $c_i$, while keeping the information of $\sim_0$ and $\sim_1$. Let us be a bit more explicit about this point. Consider trees $(T_Y, \lambda_Y)$ displayed by $(T, \lambda)$ with leaf sets $Y$ such that $Y$ contains exactly one (arbitrarily chosen) representative from each $\sim_0$ equivalence class of $(T, \lambda)$. For any such trees $(T_Y, \lambda_Y)$ and $(T_Y', \lambda_Y')$ with the latter property, there is an isomorphism $\alpha : T_Y \rightarrow T_Y'$ such that $\alpha(y) \sim_0 y$ and $\lambda_Y'(\alpha(e)) = \lambda_Y(e)$. Thus, all such $(T_Y, \lambda_Y)$ are isomorphic and differ basically only in the choice of the particular representatives of the equivalence classes of $\sim_0$. Furthermore, $T_Y$ is isomorphic to the quotient graph $T'/\sim_0$ obtained from $T$ by replacing the (maximal) subtrees where all edges are labeled with 0 by a representative of the corresponding $\sim_0$-class.

Suppose $(T, \lambda)$ explains $G$. Then $(T_Y, \lambda_Y)$ explains $G[Y]$ for a given $Y$. Since all $(T_Y, \lambda_Y)$ are isomorphic, all $G[Y]$ are also isomorphic, and thus $G[Y] = G/\sim_0$ for all $Y$.

To avoid unnecessarily clumsy language we will say that “$(T, \lambda)$ explains $G(\sim_1)/\sim_0$” instead of the more accurate wording “$(T, \lambda)$ displays $(T_Y, \lambda_Y)$ where $Y$ contains exactly one representative of each $\sim_0$ equivalence class such that $(T_Y, \lambda_Y)$ explains $G(\sim_1)/\sim_0$”.

In contrast to $\sim_0$, the single-1-relation $\sim_1$ is not transitive. As an example, consider the star $S_5$ with leaf set $\{x, y, z\}$, interior vertex $v$, and edge labeling $\lambda(v, x) = \lambda(v, z) = 1 \neq \lambda(v, y) = 0$. Hence $x \sim_1 y$, $y \sim_1 z$ and $x \not\sim_1 z$. In fact, a stronger property holds that forms the basis for understanding the single-1-relation:

**Lemma 11.** If $x \sim_1 y$ and $x \sim_1 z$, then $y \not\sim_1 z$. 


Proof. Uniqueness of paths in $T$ implies that there is a unique interior vertex $u$ in $T$ such that $P(x, y) = P(x, u) \cup P(y, u)$, $P(x, z) = P(x, u) \cup P(z, u)$, and $P(y, z) = P(y, u) \cup P(z, u)$. By assumption, each of the three sub-paths $P(x, u)$, $P(y, u)$, and $P(z, u)$ contains at most one 1-label. There are only two cases: (i) There is a 1-edge in $P(x, u)$. Then neither $P(y, u)$ nor $P(z, u)$ may have another 1-edge, and thus $y \not\sim z$, which implies that $y \not\sim z$. (ii) There is no 1-edge in $P(x, u)$. Then both $P(y, u)$ and $P(z, u)$ must have exactly one 1-edge. Thus $P(y, z)$ harbors exactly two 1-edges, whence $y \not\sim z$.

Lemma 11 can be generalized as follows.

Lemma 12. Let $x_1, \ldots, x_n$ be vertices s.t. $x_i \not\sim x_{i+1}$, $1 \leq i \leq n - 1$. Then, for all $i, j, x_i \not\sim x_j$ if and only if $|i - j| = 1$.

Proof. For $n = 3$, we can apply Lemma 11. Assume the assumption is true for all $n < K$. Now let $n = K$. Hence, for all vertices $x_i, x_j$ along the paths from $x_1$ to $x_{K-1}$, as well as the paths from $x_2$ to $x_K$ it holds that $|i - j| = 1$ if and only if we have $x_i \not\sim x_j$. Thus, for the vertices $x_i, x_j$ we have $|i - j| > 1$ if and only if we have $x_i \not\sim x_j$. Therefore, it remains to show that $x_1 \not\sim x_n$.

Assume for contradiction, that $x_1 \sim x_n$. Uniqueness of paths on $T$ implies that there is a unique interior vertex $u$ in $T$ that lies on all three paths $P(x_1, x_2)$, $P(x_1, x_n)$, and $P(x_2, x_n)$.

There are two cases, either there is a 1-edge in $P(x_1, u)$ or $P(x_1, u')$ contains only 0-edges. If $P(x_1, u)$ contains a 1-edge, then all edges along the path $P(x_1, u)$ must be 0, and all the edge on path $P(u, x_n)$ must be 0. However, this implies that $x_2 \not\sim x_n$, a contradiction, as we assumed that $\sim$ is discrete.

Thus, there is no 1-edge in $P(x_1, u)$ and hence, both paths $P(u, x_n)$ and $P(u, x_2)$ contain each exactly one 1-edge.

Now consider the unique vertex $v$ that lies on all three paths $P(x_1, x_2)$, $P(x_1, x_n)$, and $P(x_2, x_n)$. Since $u, v \in P(x_1, x_2)$, we have either (A) $v \in P(x_1, u)$ where $u = v$ is possible, or (B) $u \in P(x_1, v)$ and $u \neq v$. We consider the two cases separately.

Case (A): Since there is no 1-edge in $P(x_1, u)$ and $x_1 \not\sim x_n$, resp., $x_1 \not\sim x_1$ there is exactly one 1-edge in $P(u, x_n)$, resp., $P(u, x_2)$.

Moreover, since $x_2 \not\sim x_3$ the path $P(x, v)$ contains only 0-edges, and thus $x_3 \not\sim x_n$, a contradiction.

Case (B): Since there is no 1-edge in $P(x_1, u)$ and $x_1 \not\sim x_n$, the path $P(u, x_n)$ contains exactly one 1-edge.

In the following, we consider paths between two vertices $x_i, x_{i-2}$ in $\{x_1, \ldots, x_n\}$ step-by-step, starting with $x_1$ and $x_{n-1}$.

The induction hypothesis implies that $x_1 \not\sim x_{n-1}$ and since $\sim$ is discrete, we can conclude that $x_i \not\sim x_{n-1}$. Let $P(x_1, x_n) = P(x_1, a) \cup ab \cup P(b, x_n)$ where $e = ab$ is the 1-edge contained in $P(x_1, x_n)$. Let $c_1$ be the unique vertex that lies on all three paths $P(x_1, x_n)$, $P(x_1, x_{n-1})$, and $P(x_{n-1}, x_n)$. If $c_1$ lies on the path $P(x_1, a)$, then $P(c_1, x_{n-1})$ contains only 0-edges, since $P(x_{n-1}, x_n) = P(x_{n-1}, c) \cup \{P(c_1, a) \cup ab \cup P(b, x_n)\}$ and $x_n \sim x_{n-1}$ in $T$. However, in this case the path $P(x_1, c_1) \cup P(c_1, x_{n-1})$ contains only 0-edges, which implies that $x_n \not\sim x_{n-1}$, a contradiction. Thus, the vertex $c_1$ must be contained in $P(b, x_n)$. Since $x_1 \sim x_n$, the path $P(c_1, x_n)$ contains only 0-edges. Hence, the path $P(c_1, x_{n-1})$ contains exactly one 1-edge, because $x_1 \not\sim x_{n-1}$. In particular, by construction we see that $P(x_1, x_n) = P(x_1, u) \cup P(u, c_1) \cup P(c_1, x_n)$.

Now consider the vertices $x_n$ and $x_{n-2}$. Let $a' b'$ be the 1-edge on the path $P(x_n, x_{n-2}) = P(c_1, a') \cup a'b' \cup P(b', x_{n-1})$. Since $x_n \not\sim x_{n-2}$ and $a \not\sim x_{n-2}$ we can apply the same argument and conclude, that there is a vertex $c_2 \in P(b', x_{n-1})$ s.t. the path $P(c_2, x_{n-2})$ contains exactly one 1-edge. In particular, by construction we see that $P(x_1, x_{n-2}) = P(x_1, u) \cup P(u, c_1) \cup P(c_1, c_2) \cup P(c_2, x_2)$ s.t. the path $P(c_1, c_2)$ contains exactly one 1-edge.

Repeating this argument, we arrive at vertices $x_2$ and $x_4$ and can conclude analogously that there is a path $P(c_{n-2}, x_2)$ that contains exactly one 1-edge and in particular, that $P(x_2, x_4) = P(x_1, u) \cup P(u, c_1) \cup P(c_1, c_2) \cup P(c_2, x_2)$ and the path $P(c_1, c_2)$ contains exactly one 1-edge. However, this contradicts that $x_1 \not\sim x_2$.

Corollary 13. The graph $G(\lesssim^1)$ is a forest, and hence all paths in $G(\lesssim^1)$ are induced paths.

Next we examine the effect of edge contractions in $T$.

Lemma 14. Let $(T, \lambda)$ explain $G(\lesssim^1)$ and let $(T', \lambda')$ be the result of contracting $e$ in $T$. If $\lambda(e) = 0$ then $(T', \lambda')$ explains $G(\lesssim^1)$ and if $\lambda(e) = 1$ then $(T', \lambda')$ does not explain $G(\lesssim^1)$. In particular, for connected graphs $G(\lesssim^1)$, the tree $(T, \lambda)$ is least resolved if and only if all 0-edge are incident to leaves.

Proof. Let $\lesssim_T, \lesssim_T, \lesssim_T, \lesssim_T$ be the relations explained by $T$ and $T'$, respectively. Since $(T, \lambda)$ explains $G(\lesssim^1)$ and $\lesssim_T \not\sim \lesssim_T$, we have $\lesssim_T \not\sim \lesssim_T$. Moreover, since $\lesssim_T$ is discrete, no two distinct leaves of $T$ are in relation $\lesssim_T$.\[\blacksquare\]
If $\lambda(e) = 0$, then contracting $e$ clearly preserves the property of $\sim_{T'}$ being discrete. Since only interior edges are allowed to be contracted, we have $L(T) = L(T')$. Therefore, $\sim_{T} = \sim_{T'}$, and the 1-edges along any path from $x \in L(T) = L(T')$ to $y \in L(T) = L(T')$ remains unchanged, and thus $\sim_{T} = \sim_{T'}$. Hence, $(T', \lambda')$ explains $G(\sim_{T'})$. 

If $G(\sim_{T}) / 0$ is connected, then for every 1-edge $e$ there is a pair of leaves $x'$ and $x''$ such that $x' \sim x''$ and $e$ is the only 1-edge along the unique path connecting $x'$ and $x''$. Consequently, contracting $e$ would make $x'$ and $x''$ non-adjacent w.r.t. the resulting relation. Thus no 1-edge can be contracted in $T$ without changing $G(\sim_{T}) / 0$.

If $(T, \lambda)$ is least resolved, no edge can be contracted, and thus no 0-edge can be located in the interior of $T$. For connected $G(\sim_{T}) / 0$ no interior 1-edge can be contracted in $T$ without changing the corresponding $\sim$ relation.

In order to link the relation $\sim$ to the structure of the unrooted tree $T$, we consider first paths $(x_1, x_2, x_3, x_4)$ in $G(\sim) / 0$ of length 4. Corollary 13 implies that $x_1 \sim x_2 \sim x_3 \sim x_4$. There are several possible trivial splits $\lambda|B$ with $A, B \subseteq \{x_1, x_2, x_3, x_4\}$ that might be displayed by $T$. Clearly, the trivial splits of one vertex versus the other tree are always displayed by $T$. In addition there are three further possible quartets, i.e., splits between two disjoint pairs. As we show next, only the quartet $x_1x_2|x_3x_4$ can be displayed.

**Lemma 15.** Let $(T, \lambda)$ be a tree that explains $G(\sim_{T}) / 0$. If $(x_1, x_2, x_3, x_4)$ is a path in $G(\sim_{T}) / 0$, then among all full splits of $\{x_1, x_2, x_3, x_4\}$ only the quartet $x_1x_2|x_3x_4$ is displayed in $T$.

**Proof.** Note, since $(x_1, x_2, x_3, x_4)$ is a path in $G(\sim) / 0$, we obtain that $x_1 \sim x_2 \sim x_3 \sim x_4$. Moreover, Lemma 12 implies that $x_1 \not\sim x_3, x_4$, and $x_2 \not\sim x_4$. Since by construction of $G(\sim) / 0$, neither $x_1 \sim x_3, x_4$ nor $x_2 \sim x_4$, we observe that $x_1 \sim x_3, x_4$ and $x_2 \sim x_4, k > 1$.

We first consider trivial partial splits with vertices $x_1, x_2, x_3, x_4$, and $x_4$ s.t. there is no quartet on these vertices. Note, any other trivial split is not informative, and a more refined information of the topology of the tree $T$ is encoded in the respective quartets. Assume there is such a trivial split $x_1|x_2, x_3|x_4$ with $\{i, j, k, l\} = \{1, 2, 3, 4\}$ s.t.

there is no additional quartet on these vertices. Since there is no quartet, the induced subtree on these four vertices is of the form $P(x_i, v) \cup P(x_j, v) \cup P(x_k, v) \cup P(v, x_l)$. Thus, it suffices to prove the contradiction by a star $S_r$ with inner vertex $v$ and leaves $x_1, \ldots, x_4$, edge $e_v = x_v, v, 1 \leq r \leq 4$ where $\lambda(e_v) = 0$ i.f $P(x_v, v)$ contains only 0-edges and $\lambda(e_v) = 1$ otherwise. Furthermore, the vertex $x_1$ is connected to at least one vertex $x_r$, $r \in \{j, k, l\}$ in the path $(x_1, x_2, x_3, x_4)$. W.l.o.g. assume $x_i$ is adjacent to $x_j$, and for all other vertices.

Hence, there is at least one vertex, say $x_k$ s.t. $x_k \not\sim x_k$, and since $\sim$ is assumed to be discrete $x_1 \sim x_k$. Thus, $\lambda(e_l) = \lambda(e_k) = 1$. Since $x_1 \sim x_2$, the path $\lambda(e_l) = 0$. Moreover, it must hold that $\lambda(e_l) = 1$, as otherwise $x_1 \sim x_l$, a contradiction to $\sim$ being discrete. Now it is easy to see that such a labeling cannot yield the path $(x_1, x_2, x_3, x_4)$ in $G(\sim_{T}) / 0$. Thus, whenever we have such a path in $G(\sim_{T}) / 0$ and there is a trivial split on these vertices, then there must be a quartet on these four vertices, as well.

We are now concerned with possible quartets that might be displayed in $T$. Let us denote the four terminal edges of the quadruple by $e_i$ through $e_4$, s.t. $e_i$ and $x_i$ are incident for $i = 1, 2, 3, 4$, and $e_0$ be the central edge. Here are three possibilities:

(i) $x_1x_2|x_3x_4$. Here $x_2 \sim x_1$ implies either (A) $\lambda(e_2) = 1$ and $\lambda(e_1) = 0$, or (B) $\lambda(e_2) = 0$ and $\lambda(e_1) = 1$.

(A) From $x_2 \sim x_3$ we obtain that $\lambda(e_0) = \lambda(e_3) = 0$ and $x_3 \sim x_4$ implies $\lambda(e_4) = 1$. Hence the path $P(x_1, x_4)$ along the edges $e_1, e_0, e_4$ contains exactly one 1-edge. Thus, $x_1 \sim x_4$, a contradiction to Lemma 12.

(B) We can use analogous arguments as in case (A). If $\lambda(e_3) = 1$, then $\lambda(e_0) = \lambda(e_4) = 0$, since $x_2 \sim x_3$ and $x_3 \sim x_4$. However, the latter yields $x_1 \sim x_4$; a contradiction. Therefore, $\lambda(e_3) = 0$ and $\lambda(e_4) = 1$. Since the path from $x_2$ to $x_3$ must contain a non-0-label, we must have $\lambda(e_0) = 1$. As desired this implies $x_1 \sim x_2 \sim x_3 \sim x_4$ and $x_1 \not\sim x_j$ for all $i, j$, with $|i - j| > 1$.

(ii) $x_1x_3|x_2x_4$. Since $x_1 \not\sim x_3$ and $x_1 \not\sim x_3$ we have $\lambda(e_1) = \lambda(e_3) = 1$. Analogously, $x_2 \not\sim x_4$ and $x_2 \not\sim x_4$ implies $\lambda(e_2) = \lambda(e_4) = 1$. But then there are at least two non-0-edge on the path $P(x_1, x_2)$ along the edges $e_1, e_0, e_2$, contradicting $x_1 \sim x_2$.

(iii) $x_1x_4|x_2x_3$. From $x_1 \not\sim x_4$ and $x_1 \not\sim x_4$ we obtain $\lambda(e_1) = 1$ and $\lambda(e_4) = 1$. Then $x_1 \sim x_3$ implies that $\lambda(e_2) = \lambda(e_0) = 0$ and $x_3 \sim x_4$ fixes $\lambda(e_3) = 0$. But then there is no non-0-label along $P(x_1, x_2)$, contradicting $x_2 \sim x_3$.


Figure 1: Paths in the $\sim$ relation imply unique split systems. The upper right edge labeled tree is the caterpillar $T_5^*$.

Figure 2: the simplest case of overlapping paths

Therefore a $P_4$ in $G(\sim)/\sim$ implies that a tree that explains $G(\sim)/\sim$ must contain a unique quadruple and a corresponding unique 0/1-labeling of the five edges of the quadruples:

Conversely, this quadruple explains the $P_4$. This 1-1 correspondence propagates to longer paths. A path of length 5 can be viewed as a superposition of two paths of length 4. The key observation is that there is only a single tree with 5 leaves $x_i$, $i = 1, \ldots, 5$ that displays the quadruples $x_1x_2|x_3x_4$ and $x_2x_3|x_4x_5$. To see this, we apply Lemma 2, and conclude that a tree $T$ displays $x_1x_2|x_3x_4$ and $x_2x_3|x_4x_5$ if and only if $T$ displays $x_1x_2|x_3x_4|x_7$ and $x_1x_2|x_3|x_4x_5$. It is easy to see that there is only one such (least resolved) tree, which corresponds to the tree shown in Figure 1.

By induction and repeated application of Lemma 2, we conclude that a path on $n \geq 4$ vertices $x_1, \ldots, x_n$ yields $n - 3$ non-trivial partial splits $x_1x_2|x_3 \ldots x_{n-1}x_n$, $x_1x_2x_3|x_4 \ldots x_{n-1}x_n$, $x_1x_2x_3x_4|\ldots|\ldots|x_{n-2}x_{n-1}x_n$. We will refer to this set of partial splits as $\Sigma(P)$.

We can now summarize the discussion above in the following

Lemma 16. Let $(T, \lambda)$ be a tree that explains $G(\sim)/\sim$. If $G(\sim)/\sim$ contains the path $x_1x_2 \ldots x_n$ then $T$ displays a “caterpillar” subtree $T_n^*$ consisting of $n - 2$ internal vertices $u_2u_3 \ldots u_{n-1}$ forming a path with all edges labeled 1, vertices $x_1$ and $x_n$ adjacent to $u_2$ and $u_{n-1}$, respectively, with an edge labeled 1, and $x_i$ adjacent to $u_i$ with an $\alpha$-labeled edge for $2 \leq i \leq n - 1$.

Figure 1 shows the caterpillar $T_5^*$. The latter results can also be used to establish an alternative and more elegant proof of Lemma 12 and Corollary 13.

Alternative proof of Cor. 13. Suppose $G(\sim)/\sim$ contains a minimal length cycle $C = x_1x_2 \ldots x_n$ of length $n$. We know that $n > 3$ since $G(\sim)/\sim$ is triangle-free by Lemma 10. Thus suppose $n \geq 4$. Then $C$ contains the two paths $x_1x_2 \ldots x_n$ and $x_2 \ldots x_nx_1$ and thus by Lemma 16, $T$ displays in particular the splits $x_1x_2|x_3 \ldots x_n$ and $x_2x_3|x_4 \ldots x_{n-1}|x_nx_1$. Lemma 1 implies that these two splits are incompatible, and thus cannot be derived from the same tree. Therefore $G(\sim)/\sim$ cannot contain a cycle.

Partially overlapping paths can be understood in terms of individual paths as in Figure 2. Let $Q$ be a connected component in $G(\sim)/\sim$ with vertex set $X$. The example of Figure 2 motivates to construct an X-tree $T(Q)$ from the tree $Q$ as outlined in Algorithm 1.
Algorithm 1 Compute \((T(Q), \lambda)\)

Require: \(Q\)
Ensure: \(T(Q)\)
1: set \(T(Q) \leftarrow Q\)
2: Retain the labels of all leaves of \(Q\) in \(T(Q)\) and relabel all interior vertices \(u\) of \(Q\) as \(u'\).
3: Label all edges of the copy of \(Q\) by \(\lambda(e) = 1\).
4: For each interior vertex \(u'\) of \(Q\) add a vertex \(u\) to \(T(Q)\) and insert the edge \(uu'\).
5: Label all edges of the form \(e = uu'\) with \(\lambda(e) = 0\).

Theorem 17. Let \(Q\) be a connected component in \(G(\sim)/\sim\) with vertex set \(X\). Then the tree \(T(Q)\) constructed in Algorithm 1 is the unique least resolved tree that explains \(Q\).

Proof. We proceed by induction on the number of vertices \(|X| = n\). For \(n = 1\) and \(n = 2\) there is nothing to show, since by construction \(T(Q) = Q\) and \(Q\) must have \(|X|\) leaves. For \(n = 3\) we have \(Q = P_3 = S_2\).

Let us first consider stars \(Q = S_m, m = n + 1 \geq 3\), in general. Denote the unique central vertex by \(z\) and the leaves by \(u_i\). Then the construction of the theorem states that \(T = S_{n+1}\) and all edges \(u_iu_j\) are labeled 1, while \(\lambda(zz') = 0\). The tree \(T\) must have \(m + 1\) leaves because there are \(m + 1\) vertices in \(Q\). Hence, \(T = S_{n+1}\) is the unique least resolved tree that could possibly produce \(Q\). It is now easy to check that the edge labeling indeed yields \(Q\). Furthermore, no other edge labeling yields \(Q\). To see this, it suffices to consider explicitly all cases for \(n = 3\) since \(S_2\) is an induced subgraph of \(S_m\) corresponding to an induced subgraph \(P_3\) of \(Q\).

For \(n = 4\), we have either \(Q = S_3\) or \(Q = P_4\). For the latter case the claim coincides with the unique quadruples of Equ. (v). If the tree \(Q\) is not a star and \(n \geq 4\) then every vertex of \(Q\) is contained in at least one path on 4 vertices.

Now we proceed by induction. Suppose the claim of the theorem is true for all \(Q\) with up to \(n\) vertices. Now suppose \(Q\) has \(n + 1 \geq 5\) vertices and suppose \(Q\) is not a star, since we already know that the claim holds for all stars. Let \(u\) be a leaf of the tree \(Q\). We write \(Q \setminus \{u\}\) for the tree obtained from \(Q\) in the following way: First we remove the leaf \(u\) and the attached edge. If the vertex \(q'\) to which \(u\) was attached now has degree 2, connectedness of \(Q\) implies that at least one of its incident edges is a 0-edge. This edge is contracted. By assumption, the claim holds for \(Q'\). Let \(q\) be the unique neighbor of \(u\) in \(Q\).

We have to distinguish two cases: either (i) \(q\) is not a leaf in \(Q'\) or (ii) \(q\) is a leaf in \(Q'\).

In Case (i), the tree \(T'\) contains an interior node \(q\) as well as a leaf \(q\). Using our construction recipe to construct \(T\) we add \(q\) to \(T'\) via an edge \(qq\). If \(T'\) was least resolved, so is \(T\) since we have not added an interior vertex. We have two possibilities to label \(qq\). Of course \(\lambda(qq) = 0\) immediately yields a contradiction since the path \(q \sim q' \sim q\) would then have two edges labeled 0, but \(q\) and \(q\) are neighbors in \(Q\). One easily checks that \(\lambda(qq) = 1\) is consistent with \(Q\). There is exactly a single 1-edge along \(q \sim q' \sim q\) and two or more 1 edges along the paths to any other leaf, because all other paths either contain an interior edge (which is always labeled 1) or it connects to another neighbor of \(q\). All the latter edges, however, are also labeled 1 by our previous construction. And instead of \(q'\), \(q\) cannot be connected to any other vertex of \(T(Q)\), because of \(q \sim q'\), connected to any interior vertex of \(T(Q)\) instead of \(q'\) would either cause \(q \sim q\) or \(q \sim p\) where \(p\) is not a neighbor of \(q\) in \(Q\).

For Case (ii), first we show that \(q\) cannot be attached to any interior node of \(T'\). If \(q\) is attached to the interior node which is the unique neighbor \(q_1\) of \(q\) in \(Q'\), then the edge \(qq_1\) must be labeled by 0 to have \(q \sim q_1\). Since \(q_1\) is an interior vertex, it has neighborhoods \(Q'\). Thus \(q \sim q_2\) where \(q_2\) is any neighbor of \(q_1\). A contradiction to \(q\) be the unique neighbor of \(q\) in \(Q\). If \(q\) is attached to the interior node other than \(q_1\), then the path of \(q\) to \(q\) in \(Q\) will have at least two edges labeled by 1, a contradiction to \(q \sim q_1\).

As a consequence of the results on paths above we know that for every path \(P_4 q \sim q - q' \sim u - v\) in \(Q\) the tree \(T\) must display the quadruple \(qq'uv\). On the other hand, since \(q\) is a leaf in \(Q'\), \(u\) and \(q\) are its only neighbors in \(Q\) and thus \(qq'uv\) is a quadruple displayed by \(T\) for all \(\{r, s\} \neq \{q, q'\}\) in \(T\). Therefore \(q\) and \(q\) form a cherry in \(T\), i.e., there must be an interior vertex \(q\) that has both \(q\) and \(q\) as its neighbors. Furthermore \(q\) is necessarily connected to the rest of \(T\) by an interior edge. From the quadruple \(qq'uv\) corresponding to the path \(q \sim q' \sim u - v\), furthermore, we conclude that the interior edge must connect \(q'\) with \(u'\). It is clear that the resulting tree is least resolved: None of the new edges \(qq'\), \(qq'\), \(q' u'\) can be contracted without contradiction, and all edges in the remainder of the tree all edges are necessary due to the induction hypothesis. Therefore the tree \(T\) is uniquely defined by \(Q\).

Let us now turn to the labeling of \(T\). First we note that exactly one of the edge \(qq'\) or \(qq'\) must be labeled 1. Furthermore there must be a single 1-edge along the paths \(q \sim q' \sim u' - u\) and two or more 1's along \(q \sim q' - u' - u\). Therefore \(\lambda(qq') = 1\) and \(\lambda(qq') = 0\). Using the known constraints within \(T'\) as argued previously we see that \(\lambda(uu) = 0\), and thus \(\lambda(\bar{q} u') = 1\). Hence, the labeling of \(T\) is again unique and coincides with the labeling described in the claim of the theorem.

We therefore conclude that for all connected components \(Q\) both the least resolved tree and its labeling is uniquely determined.

We are now in the position to demonstrate how to obtain a least resolved tree that explains \(G(\sim)/\sim\) also in the case that \(G(\sim)/\sim\) itself is not connected. To this end, denote by \(Q_1, \ldots, Q_k\) the connected
components of \( G(\tilde{\approx}) \). We can construct an X-tree \( T(G(\tilde{\approx})) \) for \( G(\tilde{\approx}) \) using Alg. 2. It basically amounts to constructing a star \( S_k \) with interior vertex \( z \), where its leaves are identified with the trees \( T(Q_i) \).

**Algorithm 2** Compute \( (T(G(\tilde{\approx}))/\sim) \), \( \lambda \)

**Require:** disconnected \( G(\tilde{\approx}) \)

**Ensure:** \( T(G(\tilde{\approx}))/\sim) \)

1: \( T(G(\tilde{\approx})/\sim)) \leftarrow \{\{z\}, \emptyset\} \)

2: for Each connected component \( Q_i \) do

3: construct \( (T(Q_i), \lambda_i) \) with Alg. 1 and add to \( T(G(\tilde{\approx})/\sim)) \).

4: if \( T(Q_i) \) is the single vertex graph \( \{v\}, \emptyset \) then

5: add edge \( vz \)

6: else if \( T(Q_i) \) is the edge \( v_i, w_i \) then

7: remove the edge \( v_iw_i \) from \( T(Q_i) \), insert a vertex \( x_i \) in \( T(Q_i) \) and the edges \( x_i, v_i \), \( x_i, w_i \).

8: set either \( \lambda_i(x_i, v_i) = 1 \) and \( \lambda_i(x_i, w_i) = 0 \) or \( \lambda_i(x_i, v_i) = 0 \) and \( \lambda_i(x_i, w_i) = 1 \).

9: add edge \( x_iz \) to \( T(G(\tilde{\approx})/\sim)) \).

10: else

11: add edge edge \( zq'_i \) to \( T(G(\tilde{\approx})/\sim)) \) for an arbitrary interior vertex \( q'_i \) of \( T(Q_i) \).

12: end if

13: end for

14: Set \( \lambda(zv) = 1 \) for all edges \( zv \) and \( \lambda(e) = \lambda_z(e) \) for all edges \( e \in T(Q_i) \).

**Theorem 18.** Let \( Q_1, \ldots, Q_k \) be the connected components in \( G(\tilde{\approx})/\sim) \). Up to the choice of the vertices \( q'_i \) in Line 11 of Alg. 2, the tree \( T^* = T(G(\tilde{\approx})/\sim)) \) is the unique least resolved tree that explains \( G(\tilde{\approx})/\sim) \).

**Proof.** Since every tree \( T(Q_i) \) explains a connected component in \( G(\tilde{\approx})/\sim) \), from the construction of \( T^* \) it is easily seen that \( T^* \) explains \( G(\tilde{\approx})/\sim) \). Now we need to prove \( T^* \) is the unique least resolved tree that explains \( G(\tilde{\approx})/\sim) \).

First observe that all leaves of the trees \( T(Q_i) \) or the inner vertices of single-vertex trees must be leaves in the tree \( T^* \), as otherwise, \( T^* \) cannot explain \( G(\tilde{\approx})/\sim) \). Hence, leaves or the inner vertices of single-vertex trees \( T(Q_i) \) cannot be identified with any other vertex of a distinct tree \( T(Q_j) \). Thus, in order to connect these trees inner vertices (except the the inner vertices of single-vertex trees) must be identified or edges and possibly extra vertices must be added.

By Theorem 17, every tree \( T(Q_i) \) is the unique least resolved tree for the respective connected component \( Q_i \). However, if \( T(Q_i) \) is an edge, i.e., of the form \( v_iw_i \) we modify this tree in Line 8 to obtain a tree isomorphic to \( S_2 \) with inner vertex \( x_i \). Note this modification is necessary, since on the one hand, leaves cannot be identified with any other vertex of a distinct tree \( T(Q_j) \) and, on the other hand one cannot insert any edge incident to \( v_i \) and \( w_i \) to obtain connectedness in \( T^* \), otherwise the leaves become inner vertices in \( T^* \). Thus, in order to connect this tree \( T(Q_i) \) to other connected components without loosing the information about the leaves \( v_i, w_i \), it is necessary to add this extra vertex \( x_i \). By construction of \( \lambda_i \) we still have \( v_i \sim w_i \).

Hence, in what follows we can assume that the trees \( T(Q_1), \ldots, T(Q_k) \) are either single vertex graphs or have at least one inner vertex and two leaves. Moreover, after Line 8, none of such trees \( T(Q_1), \ldots, T(Q_k) \) can have less inner vertices in \( T^* \). In other words, the trees \( T(Q_1), \ldots, T(Q_k) \) must be displayed in any least resolved tree that explain \( G(\tilde{\approx})/\sim) \).

We continue to show that one cannot identify inner vertices of different trees \( T(Q_i) \) and \( T(Q_j) \) to obtain \( T^* \). Let \( q' \) and \( p' \) be arbitrary inner vertices of \( T(Q_i) \) and \( T(Q_j) \), respectively. If one of the trees, say \( T(Q_i) \), consists only of this vertex \( q' \), then identification of \( q' \) and \( p' \) leads to the loss of the leaf \( q' \) in \( T^* \), a contradiction. Otherwise, assume none of the trees is a single vertex graph. By construction, there is a leave \( q \), resp., \( p \) incident to \( q' \), resp., \( p' \) with \( \lambda_i(q, q') = \lambda_i(p, p') = 0 \). Hence, if \( q' \) and \( p' \) are identified, then \( p \sim q \) and thus, they are in the same connected component of \( G(\tilde{\approx})/\sim) \), a contradiction. Thus, none of the vertices of any \( T(Q_i) \) can be identified with any other vertex in a distinct tree \( T(Q_j) \). This also implies, that edges in \( T(Q_i) \) and \( T(Q_j) \) cannot be identified.

We continue to show that it is not possible to connect any vertex of \( T(Q_i) \) and any vertex in a distinct tree \( T(Q_j) \) by an edge. Let \( q' \) and \( p' \) be arbitrary vertices of \( T(Q_i) \) and \( T(Q_j) \), respectively. Assume one of the trees, say \( T(Q_i) \), consists only of this vertex \( q' \), and we add the edge \( e = q'p' \). If additionally \( T(Q_i) \) consists only of the vertex \( p' \), then \( p' \sim q' \) or \( q' \sim p' \) in \( T^* \), since \( \lambda(e) \in \{0, 1\} \), a contradiction. If, \( T(Q_i) \) has at least two leaves, then \( p' \) must be an inner vertex. Otherwise, the leave \( p' \) in \( T(Q_i) \) would be an inner vertex in \( T^* \) after insertion of the edge \( e \), a contradiction. By construction, there is a leave \( p \) incident to \( p' \) with \( \lambda_i(p, p') = 0 \). Since \( \lambda(e) \in \{0, 1\} \), we obtain \( p \sim q' \) or \( p \sim q' \) in \( T^* \), a contradiction.


Assume now, that none of the trees is a single vertex graph. Similarly, $q'$, resp., $p'$ must be inner vertices in $T(Q_q)$, resp., $T(Q_p)$. Again, there is a leave $q$ incident to $q'$ with $\lambda_1(q, q') = 0$ and a leave $p$ incident to $p'$ with $\lambda_1(p, p') = 0$. Thus, $p \sim q$ or $p \not\sim q$ in $T^*$, since $\lambda(e) \in \{0, 1\}$, a contradiction.

Hence, we must add a path to connect different trees in $T^*$. The way, using the least number of vertices is to add one vertex on which all those paths run. This is done by adding the tree $(z, \emptyset)$ to $T^*$. We continue to connect the different trees to $z$ by insertion of an edge $zq'$, where $q'$ is an arbitrary inner vertex of $T(Q_q)$ and label all these edges $e$ with $\lambda(e) = 1$. Thus, no two leaves $u$ and $w$ of distinct trees are in relation $\sim$ or $\not\sim$. Since we have to add at least one vertex to obtain connectedness in $T^*$, the tree $T^*$ is a least resolved tree that explains $G(z) / \sim$ and unique up to the choice of the inner vertices that are connected to the vertex $z$. 

\begin{proof}

\end{proof}

4.1 Binary trees

Instead of asking for least resolved trees that explain $G(z) / \sim$, we may also consider the other extreme and ask which binary, i.e., fully resolved tree can explain $G(z) / \not\sim$. Recall that an $X$-tree is called binary or fully resolved if the root has degree 2 while all other interior vertices have degree 3. From the construction of the least resolved trees we immediately obtain the following:

**Corollary 19.** A least resolved tree $T(Q)$ for a connected component $Q$ of $G(z) / \not\sim$ is binary if and only if $Q$ is a path.

If a least resolved tree $T(Q)$ of $G(z) / \not\sim$ is a star, we have:

**Lemma 20.** If a least resolved tree $T(Q)$ explaining $G(z) / \not\sim$ is a star with $n$ leaves, then either

(a) all edges in $T(Q)$ are 1-edges and $Q$ has no edge, or

(b) there is exactly one 0-edge in $T(Q)$ and $Q$ is a star with $n - 1$ leaves.

**Proof.** For implication in case (a) and (b) we can re-use exactly the same arguments as in the proofs of Theorem 17 and 18.

Now suppose there are at least two (incident) 0-edges in $T(Q)$, whose endpoints are the vertices $u$ and $v$. Then $u \not\sim v$, which is impossible in $G(z) / \not\sim$.

To construct the binary tree representing the star $Q = S_n$, we consider the set of all binary trees with $n$ leaves and 0/1-edge labels. If $S_n$ is of type (a) in Lemma 20, then all terminal edges are labeled 1 and all interior edges are arbitrarily labeled 0 or 1. Figure 3 shows an example for $S_5$. If $S_n$ is of type (b), we label the terminal edges in the same way as in $T(Q)$ and all interior edge are labeled 0. In this case, for each binary tree there is exactly one labeling.

![Figure 3](image)

**Figure 3:** For fixed underlying tree $T(Q)$, in this case a star $S_6$ with all 1, there are in general multiple labelings $\lambda$ that represent the same relation $Q$; here the empty relation.

In order to obtain the complete set of binary trees that explain $G$ we can proceed as follows. If $G$ is connected, there is a single least resolved tree $T(G)$ explaining $G$. If $G$ is not connected then there are multiple least resolved trees $T$. They are described by Thm. 18. For every such least resolved tree $T$ we iterate over all vertices $v_0$ of $T$ with degree $k > 3$ and perform the following manipulations:

1. Given a vertex $v_0$ of $T$ with degree $k > 3$, denote its neighbors by $v_1, v_2, \ldots, v_k$. Delete vertex $v_0$ and its attached edges from $T$, and rename the neighbors $v_i$ to $v'_i$ for all $1 \leq i \leq k$. Denote the resulting forest by $F(v_0)$.

2. Generate all binary trees with leaves $v_2, \ldots, v_k$ as described in the previous paragraph.

3. Each of these binary trees is inserted into a copy of the forest $F(v_0)$ by identify $v_i$ and $v'_i$ for all $1 \leq i \leq k$.

For a given least resolved tree $T$ this yields the set of all $\prod_{i=0}^k t(\deg(v_0))$ pairwise distinct binary trees, where $t(k)$ denotes the number of binary trees with $k$ leaves. The union of these tree sets is then the set of all binary trees explaining $G$. To establish the correctness of this procedure, we prove

**Lemma 21.** The procedure outlined above generates all binary trees representing $Q$. 

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Proof. It is easy to check that the trees we get are indeed binary trees, and any binary tree we get represents \( Q \).

On the other hand, by Theorem 18 we know that the least resolved tree representing \( Q \) is \( T(Q) \). By the definition of least resolved tree, here are two ways to get all the trees from least resolved tree. Add 0 interior edges, or add 1 interior edges in proper place. Thus if the least resolved tree has degree 2 vertices, then by adding interior edges we cannot change the degree of degree 2 vertices, so that we cannot get a binary tree. In this case there is no binary tree representation. Otherwise, whenever adding an extra vertex, we need to attach the vertex an edge, where we can only move the edges from the neighborhood. The construction goes over all the possibilities so that it gets all the binary tree with this least resolved tree.

By the proof of Lemma 21 we immediately obtain the following Corollary that characterizes the condition that \( Q \) cannot be explained by a binary tree.

**Corollary 22.** \( G(\overset{\sim}{1})/\overset{\sim}{0} \) cannot be explained by a binary tree if and only if \( G(\overset{\sim}{1})/\overset{\sim}{0} \) has exactly two connected components.

The fact that exactly two connected components appear as a special case is the consequence of a conceptually too strict definition of “binary tree”. If we allow a single “root vertex” of degree 2 in this special case, we no longer have to exclude two-component graphs.

## 5 The antisymmetric single-1 relation

The antisymmetric version \( x \overset{1}{\rightarrow} y \) of the 1-relation shares many basic properties with its symmetric cousin. We therefore will not show all formal developments in full detail. Instead, we will where possible appeal to the parallels between \( x \overset{1}{\rightarrow} y \) and \( x \overset{1}{\sim} y \). For convenience we recall the definition: \( x \overset{1}{\rightarrow} y \) if and only if all edges along \( P(u, x) \) are labeled 0 and exactly one edge along \( P(u, y) \) is labeled 1, where \( u = \text{lca}(x, y) \). As an immediate consequence we may associate with \( \overset{1}{\sim} \) a symmetrized 1-relation \( x \overset{1}{\sim} y \) whenever \( x \overset{1}{\rightarrow} y \) or \( y \overset{1}{\rightarrow} x \). Thus we can infer (part of) the underlying unrooted tree topology by considering the symmetrized version \( \overset{1}{\sim} \). On the other hand, \( \overset{1}{\sim} \) cannot convey more information on the unrooted tree from which \( \overset{1}{\rightarrow} \) and its symmetrization \( \overset{1}{\sim} \) are derived. It remains, however, to infer the position of the root from directional information. Instead of the quadruples used for the unrooted trees in the previous section, structural constraints on rooted trees are naturally expressed in terms of triples.

In the previous section we have considered \( \overset{1}{\sim} \) in relation to unrooted trees only. Before we start to explore \( \overset{1}{\sim} \) we first ask whether \( \overset{1}{\sim} \) contains any information about the position of the root and if it already places any constraints on \( \overset{1}{\rightarrow} \) beyond those derived for \( \overset{1}{\sim} \) in the previous section. In general the answer to this question will be negative, as suggested by the example of the tree \( T_2 \) in Figure 4. Any of its inner vertex can be chosen as the root, and each choice of a root vertex yields a different relation \( \overset{1}{\rightarrow} \).

Nevertheless, at least partial information on \( \overset{1}{\sim} \) can be inferred uniquely from \( \overset{1}{\rightarrow} \) and \( \overset{1}{\sim} \). Since all connected components in \( G(\overset{1}{\rightarrow})/\overset{1}{\sim} \) are trees, we observe that the underlying graphs \( G(\overset{1}{\rightarrow})/\overset{1}{\sim} \) of all connected components in \( G(\overset{1}{\rightarrow})/\overset{1}{\sim} \) must be trees as well. Moreover, since \( \overset{1}{\sim} \) is discrete in \( G(\overset{1}{\rightarrow})/\overset{1}{\sim} \), it is also discrete in \( G(\overset{1}{\rightarrow})/\overset{1}{\sim} \).

Let \( Q \) be a connected component in \( G(\overset{1}{\rightarrow})/\overset{1}{\sim} \). If \( Q \) is an isolated vertex or a single edge there is nothing to show. In either case there is only a single tree and the position of its root is uniquely determined. Thus we assume that \( Q \) contains at least three vertices from here on. By construction, any three vertices \( x, y, z \) in a connected component \( Q \) in \( G(\overset{1}{\rightarrow})/\overset{1}{\sim} \) either induce a disconnected graph, or a tree on three vertices. Let \( x, y, z \in V(Q) \) induce such a tree. Then there are three possibilities (up to relabeling of the vertices) for the induced subgraph contained in \( G(\overset{1}{\rightarrow})/\overset{1}{\sim} = (V, E) \):

(i) \( xy, yz \in E \) implying that \( x \overset{1}{\rightarrow} y \overset{1}{\rightarrow} z \),

(ii) \( yz, xz \in E \) implying that \( y \overset{1}{\rightarrow} x \) and \( y \overset{1}{\rightarrow} z \),

(iii) \( xz, yz \in E \) implying that \( x \overset{1}{\rightarrow} y \) and \( z \overset{1}{\rightarrow} y \).

Below, we will show that Cases (i) and (ii) both imply a unique tree on the three leaves \( x, y, z \) together with a unique 0/1-edge labeling for the unique resolved tree \( T(Q) \) that displays \( Q \), see Fig. 5. Moreover, we shall see that Case (iii) cannot occur.

**Lemma 23.** In Case (i) the unique triple \( yxz \) that must be displayed in any tree \( T(Q) \) that explains \( Q \). Moreover, the paths \( P(u, v) \) and \( P(v, z) \) in \( T(Q) \) contain both exactly one 1-edge, while the other paths \( P(u, x) \) and \( P(v, y) \) contain only 0-edges, where \( u = \text{lca}(xy) = \text{lca}(xz) \neq \text{lca}(yz) = v \).

**Proof.** Let \( x, y, z \in V(Q) \) such that \( xy, yz \in E \) and thus, \( x \overset{1}{\rightarrow} y \overset{1}{\rightarrow} z \). Notice first that there must be two distinct last common ancestors for pairs of the three vertices \( x, y, z \); otherwise, if \( u = \text{lca}(xy) = \text{lca}(xz) \neq \text{lca}(yz) \), then the path \( P(yz) \) contains a 1-edge (since \( x \overset{1}{\rightarrow} y \)) and hence \( y \overset{1}{\rightarrow} z \) is impossible. We continue to show that \( u = \text{lca}(xy) = \text{lca}(xz) \). Assume that \( u = \text{lca}(xy) \neq \text{lca}(xz) \). Hence, either the
Figure 4: Placing the root. For the tree $T_5'$ of Fig. 1 each of the tree inner vertices $a$, $b$, or $c$ can be chosen as the root, giving rise to three distinct relations $\rho$. For the “siblings” in the unrooted tree $x_1, x_2$ as well as $x_4, x_5$, it holds that $x_2 \rho x_1$ and $x_4 \rho x_3$ for all three distinct relations. Thus, there are uniquely determined parts of $\rho$ conveyed by the information of $\sim$ and $\sim$ only.

Lemma 24. In Case (ii) there is a the unique tree on the three vertices $x, y, z$ with single root $\rho$ displayed in any least resolved tree $T(Q)$ that explains $Q$. Moreover, the path $P(\rho, y)$ contains only 0-edges, while the other paths $P(\rho, x)$ and $P(\rho, z)$ must both contain exactly one 1-edge.

Proof. Assume for contradiction that there is a least resolved tree $T(Q)$ that displays $xy|z$, $yz|x$, or $xz|y$.

The choice of $xy|z$ implies $u = lca(xy) \neq lca(xz) = lca(yz) = v$. Since $y \perp x$ and $y \perp z$, $P(v, y) \subseteq P(u, y)$ contain only 0-edges, while $P(u, x)$ and $P(v, z)$ each contain exactly one 1-edge, respectively.

This leads to a tree $T'$ that yields the correct $\perp$-relation. However, this tree is not least resolved. By contracting the path $P(u, v)$ to a single vertex $\rho$ and maintaining the labels on $P(\rho, x), P(\rho, y)$, and $P(\rho, z)$ we obtain the desired labeled least resolved tree with single root.

For the triple $yz|x$ the existence of the unique, but not least resolved tree can be shown by the same argument with exchanged roles of $x$ and $y$.

For the triple $xz|y$ we $u = lca(xy) = lca(yz) \neq lca(xz) = v$. From $y \perp x$ and $y \perp z$ we see that both paths $P(u, x) = P(u, v) \cup P(v, x)$ and $P(u, z) = P(u, v) \cup P(v, z)$ contain exactly one 1-edge, while all edges in $P(u, y)$ are labeled 0. There are two cases: (1) The path $P(u, v)$ contains this 1-edge, which implies that both paths $P(v, x)$ and $P(v, z)$ contain only 0-edges. But then $x \perp z$, a contradiction to $\sim$ being discrete. (2) The path $P(u, v)$ contains only 0-edges, which implies that each of the paths $P(v, x)$ and $P(v, z)$ contain exactly one 1-edge. Again, this leads to a tree that yields the correct $\perp$-relation, but it is not least resolved. By contracting the path $P(u, v)$ to a single vertex $\rho$ and maintaining the labels on $P(\rho, x), P(\rho, y)$, and $P(\rho, z)$ we obtain the desired labeled least resolved tree with single root.

Lemma 25. Case (iii) cannot occur.

Proof. Let $x, y, z \in V(Q)$ such that $xy, yz \in E$ and thus, $x \perp y$ and $z \perp y$. Hence, in the rooted tree that represents this relationship we have the following situation: All edges along $P(u, x)$ are labeled 0;
Figure 5: There are only two possibilities for induced connected subgraphs $H$ in $G(\frac{1}{n})/\sim 0$ on three vertices, cf. Lemma 23, 24, and 25. Each of the distinct induced subgraphs imply a unique least resolved tree with a unique labeling.

exactly one edge along $P(u, y)$ is labeled 1, where $u = lca(x, y)$; all edges along $P(v, z)$ are labeled 0, and exactly one edge along $P(v, y)$ is labeled 1, where $v = lca(y, z)$. Clearly, $lca(x, y, z) \in \{u, v\}$. If $u = v$, then all edges in $P(u, x)$ and $P(u, z)$ are labeled 0, implying that $x \sim y$, contradicting that $\sim$ is discrete.

Now assume that $u = lca(x, y) \neq v = lca(y, z)$. Hence, one of the triples $xy|z$ or $yz|x$ must be displayed in $T(Q)$. W.l.o.g., we can assume that $yz|x$ is displayed, since the case $xy|z$ is shown analogously by interchanging the role of $x$ and $z$. Thus, $lca(x, y, z) = lca(x, y) = u \neq lca(yz) = v$. Hence, $P(u, y) = P(u, v) \cup P(v, y)$. Since $z \sim y$, the path $P(v, y)$ contains a single 1-edge and $P(v, z)$ contains only 0-edges. Therefore, the paths $P(u, x)$ and $P(u, v)$ contain only 0-edges, since $x \sim y$. Since $P(x, z) = P(x, u) \cup P(u, v) \cup P(v, z)$ and all edges along $P(u, x)$, $P(u, v)$ and $P(v, z)$ are labeled 0, we obtain $x \sim z$, again a contradiction.

Taken together, we obtain the following immediate implication:

**Corollary 26.** The graph $G(\frac{1}{n})/\sim$ does not contain a pair of edges of the form $xy$ and $yv$.

Recall that the connected components $Q$ in $G(\frac{1}{n})/\sim$ are trees. By Cor. 26, $Q$ must be composed of distinct paths that “point away” from each other. In other words, let $P$ and $P'$ be distinct directed path in $Q$ that share a vertex $v$, then it is never the case that there is an edge $xy$ in $P$ and an edge $yv$ in $P'$, that is, both edges “pointing” to the same vertex $v$. We first consider directed paths in isolation.

**Lemma 27.** Let $Q$ be a connected component in $G(\frac{1}{n})/\sim$ that is a directed path with $n \geq 3$ vertices labeled $x_1, \ldots, x_n$ such that $x_ix_{i+1} \in E(Q)$, $1 \leq i \leq n - 1$. Then the path $T(Q)$ explaining $Q$ must display all triples in $R_Q = \{(x_i|y, z) : i, j > l \geq 1\}$. Hence, $T(Q)$ must display $3^n$ triples and is therefore the unique (least resolved) binary rooted tree $(\ldots (x_n, x_{n-1}, x_{n-2}, \ldots) x_2) x_1$ that explains $Q$. Moreover, all inner edges in $T(Q)$ and the edge incident to $x_n$ are labeled 1 while all other edges are labeled 0.

**Proof.** Let $Q$ be a directed path as specified in the lemma. We prove the statement by induction. For $n = 3$ the statement follows from Lemma 23. Assume the statement is true for $n = k$. Let $Q$ be a directed path with vertices $x_1, \ldots, x_k, x_{k+1}$ and edges $x_ix_{i+1}$, $1 \leq i \leq k$ and let $T(Q)$ be a tree that explains $Q$. For the subpath $Q'$ on the vertices $x_2, \ldots, x_{k+1}$ we can apply the induction hypothesis and conclude that $T(Q')$ must display the triples $x_i|x_j$ with $i, j > l \geq 2$ and that all inner edges in $T(Q')$ and the edge incident to $x_{k+1}$ are labeled 1 while all other edges are labeled 0. Since $T(Q)$ must explain in particular the subpath $Q'$ and since $T(Q')$ is fully resolved, we can conclude that $T(Q)$ is displayed by $T(Q')$ and that all edges in $T(Q')$ that are also in $T(Q')$ retain the same label as in $T(Q')$.

Thus $T(Q)$ displays in particular the triples $x_i|x_j$ with $i, j > l \geq 2$. By Lemma 23, and because there are edges $x_1x_2$ and $x_2x_3$, we see that $T(Q)$ must also display $x_2|x_3$. Take any triple $x_2|x_3, j > 3$. Application of the triple-inference rules shows that any tree that displays $x_2|x_3$ and $x_2|x_4$ must also display $x_3|x_4$ and $x_2|x_4$. Hence, $T(Q)$ must display these triples. Now we apply the same argument to the triples $x_2|x_3$ and $x_2|x_4, i, j > 2$ and conclude that in particular, the triple $x_2|x_3$ must be displayed by $T(Q)$ and thus, the the entire set of triples $\{x|x_j : i, j > l \geq 1\}$. Hence, there are $3^n$ triples and thus, the set of triples that needs to be displayed by $T(Q)$ is strictly dense. Making use of a technical result from [21, Suppl. Material], we obtain that $T(Q)$ is the unique binary tree $(\ldots (x_n, x_{n-1}, x_{n-2}, \ldots) x_2) x_1$.

Now it is an easy exercise to verify that the remaining edge containing $x_1$ must be labeled 0, while the inner edge not contained in $T(Q')$ must all be 1-edges.

If $Q$ is connected but not a simple path, it is a tree composed of the paths pointing away from each other as shown in Fig. 6. It remains to show how to connect the distinct trees that explain these paths to obtain a tree $T(Q)$ for $Q$. To this end, we show first that there is a unique vertex $v$ in $Q$ such that no edge ends in $v$.
Lemma 28. Let $Q$ be a connected component in $G(\downarrow)/\sim$. Then there is a unique vertex $v$ in $Q$ such that there is no edge $vx \in E(Q)$.

Proof. Corollary 26 implies that for each vertex $v$ in $Q$ there is at most one edge $vx \in E(Q)$. If for all vertices $w$ in $Q$ we would have an edge $vx \in E(Q)$, then $Q$ contains cycles, contradicting the tree structure of $Q$. Hence, there is at least one vertex $v$ so that there is no edge of the form $vx \in E(Q)$. If there are two vertices $v, v'$ so that there are no edges of the form $vx, vy$, then all edges incident to $v, v'$ are of the form $vx, vy$ that implies that $Q$ is not connected. Thus, there is exactly one vertex $v$ in $Q$ such that there is no edge $vx \in E(Q)$.

By Lemma 28, for each connected component $Q$ of $G(\downarrow)/\sim$ there is a unique vertex $v_Q$ s.t. all edges incident to $v_Q$ are of the form $v_Qx$. That is, all directed paths that are maximal w.r.t. inclusion start in $v_Q$. Let $P_Q$ denote the sets of all such maximal paths. Thus, for each path $P \in P_Q$ there is the triple set $R_P$ according to Lemma 27 that must be displayed by any tree that explains also $Q$. Therefore, $T(Q)$ must display all triples in $R_Q = \cup_{P \in P_Q} R_P$.

The underlying undirected graph $G(\downarrow)/\sim$ is isomorphic to $G(\downarrow)/\sim$. Thus, with Algorithm 1, one can similar to the unrooted case, first construct the tree $T(Q)$ and then set the root $\rho_Q = v_Q$ to obtain $T(Q)$. It is easy to verify that this tree $T(Q)$ displays all triples in $R_Q$. Moreover, any edge-contradiction in $T(Q)$ leads to the loss of an input triple $R_Q$ and in particular, to a wrong pair of vertices w.r.t. $\downarrow$ or $\sim$. Thus, $T(Q)$ is a least resolved tree for $R_Q$ and therefore, a least resolved tree that explains $Q$.

We summarize these arguments in

Corollary 29. Let $Q$ be a connected component in $G(\downarrow)/\sim$. Then $T(Q)$ is obtained from the unique least resolved tree $T(Q)$ by choosing the unique vertex $v$ where all edges incident to $v$ are of the form $vx$ as the root $\rho_Q$.

If $G(\downarrow)/\sim$ is disconnected, one can apply Algorithm 2, to obtain the tree $T(G(\downarrow)/\sim)$ and then chose either one of the vertices $\rho_Q$ or the vertex $z$ as root to obtain $T(G(\downarrow)/\sim)$, in which case all triples of $R_{G(\downarrow)/\sim} = \cup_Q R_Q$ are displayed. Again, it is easy to verify that any edge-contradiction leads to a wrong pair of vertices in $\downarrow$ or $\sim$. Thus, $T(G(\downarrow)/\sim)$ is a least resolved tree for $R_{G(\downarrow)/\sim}$.

To obtain uniqueness one can apply similar arguments as in the proofs of Theorems 17 and 18. This yields the following characterization:

Theorem 30. Let $Q_1, \ldots, Q_k$ be the connected components in $G(\downarrow)/\sim$. Up to the choice of the vertices $q_i$ in Line 11 of Alg. 2 for the construction of $T(Q_i)$ and the choice of the root $\rho \in \{\rho_1, \ldots, \rho_k, z\}$, the tree $T^* = T(G(\downarrow)/\sim)$ is the unique least resolved tree that explains $G(\downarrow)/\sim$. 
6 Mix of symmetric and anti-symmetric relations

In real data, e.g., in the application to mitochondrial genome arrangements, one can expect that the known relationships are in part directed and in part undirected. Such data are naturally encoded by a relation $\sim$ with directional information and a relation $\bowtie$ comprising the set of pairs for which it is unknown whether $x \sim y$, $y \sim x$, or both are true. The disjoint union $\bowtie \sqcup \sim$ of these two parts can be seen as refinement of a corresponding symmetrized relation $x \sim y$. Ignoring the directional information one can still construct the tree $T(G(\bowtie) / \sim)$. In general there will be less information of the placement of the root in $T(G(\bowtie) / \sim)$ than with a fully directed edge set. To this end we consider the symmetric pairs $(a, b) \in \bowtie$ as a pair of directed edges $ab$ and $ba$.

Given a tree $T$ we say that a directed edge $xy \in E(T)$ points away from the vertex $v$ if the unique path from $v$ to $x$ does not contain $y$. In this case the path from $v$ to $y$ contains $x$. Note that in this way we defined “pointing away from $v$” not only for the edges incident to $v$, but for all directed edges. Also note that any undirected edge in the same connected component with $v$ points away from $v$. A vertex $v$ is a central vertex if, for any two distinct vertices $x, y \in V$ that form an edge in $T$, either $xy$ or $yx$ in $T$ points away from $v$.

As an example consider the tree $a \leftrightarrow b \rightarrow c \leftrightarrow d \rightarrow e$. There is no edge containing $b$ and $c$ that points away from vertex $d$. Thus $d$ is not central. On the other hand, $b$ is a central vertex. The only possibility in this example to obtain a valid relation $\sim$ that can be displayed by rooted 0/1-edge-labeled tree is provided by removing the edge $dc$, since otherwise Cor. 26 would be violated.

In the following, for given relations $\bowtie$ and $\sim$ we will denote with $\bowtie \sim$ a relation that contains $\bowtie$ and exactly one pair, either $(x, y)$ or $(y, x)$, from $\bowtie$.

**Lemma 31.** For a given graph $G(\bowtie \sim) / \sim$ the following statements are equivalent:

(i) There is a relation $\bowtie \sim$ that is the antisymmetric single-1-relation of some 0/1-edge-labeled tree.

(ii) There is a central vertex in each connected component $Q$ of $G(\bowtie \sim) / \sim$.

**Proof.** If there is a relation $\bowtie \sim$ that can be displayed by a rooted 0/1-edge-labeled tree, then then $G(\bowtie \sim) / \sim$ consists of connected components $Q$ where each connected component is a tree composed of maximal directed paths that point away from each other. Hence, for each connected component $Q$ there is the unique vertex $v_Q$ such that all edges incident to $v_Q$ are of the form $v_Qx$ and, in particular, $v_Q$ is a central vertex in $Q$ and thus, in $G(\bowtie \sim) / \sim$.

Conversely, assume that each connected component $Q$ has a central vertex $v_Q$. Hence, one can remove all edges that do not point away from $v_Q$ and hence obtain a connected component $Q'$ that is still a tree with $V(Q') = V(Q)$ so that all maximal directed paths point away from each other and in particular, start in $v_Q$. Thus, for the central vertex $v_Q$ all edges incident to $v_Q$ are of the form $v_Qx$. Since $Q'$ is now a connected component in $G(\bowtie \sim) / \sim$, we can apply Cor. 29 to obtain the tree $T(Q')$ and Thm. 30 to obtain $T(G(\bowtie \sim) / \sim)$.

The key consequence of this result is the following characterization of the constraints on the possible placements of the root.

**Corollary 32.** Let $Q$ be a connected component in $G(\bowtie \sim) / \sim$ and let $T(Q)$ be the unique least resolved tree that explains the underlying undirected graph $Q$. Then each copy $v'$ of a vertex $v$ in $Q$ can be chosen to be the root in $T(Q)$ to obtain $T(Q)$ if and only if $v$ is a central vertex in $Q$.

7 Concluding Remarks

In this contribution we have introduced a class of binary relations deriving in a natural way from edge-labeled trees. This construction has been inspired by the conceptually similar class of relations induced by vertex-labeled trees. The latter have co-graph structure and are closely related to orthology and paralogy [19, 26, 21]. Defining $x \sim y$ whenever at least one 1-edge lies along the path from $x$ to $y$ is related to the notion of xenology: the edges labeled 1 correspond to horizontal gene transfer events, while the 0-edge encode vertical transmission. In its simplest setting, this idea can also be combined with vertex labels, leading to the directed analog of co-graphs [20]. Here, we have explored an even simpler special case: the existence of a single 1-label along the connecting path, which captures the structure of rare event data as we have discussed in the introduction. We have succeeded here in giving a complete characterization of the relationships between admissible relations, which turned out to be forests, and the underlying phylogenetic tree. Moreover, for all such cases we gave polynomial-time algorithms in order to compute the trees that explain the respective relation.

However, the analysis presented here makes extensive use of the particular properties of the single-1 relation and hence does not seem to generalize easily to other interesting cases. Horizontal gene transfer, for example, is expressed naturally in terms of the “at-least-one-1” relation $\sim$. It is worth noting that $\sim$ also has properties (L1) and (L2) and hence behaves well w.r.t. contraction of the underlying tree and
restriction to subsets of leaves. Whether this is sufficient to obtain a complete characterization remains an open question.

Several general questions arise naturally. For instance, is there a characterization of admissible relations in terms of forbidden subgraphs graphs or minors? For instance, the relation $\xrightarrow{\Delta} \xleftarrow{\Delta}$ is characterized in terms of the forbidden subgraph $x \to v \leftarrow y$. Hence, it would be of interest, whether such characterizations can be derived for arbitrary relations $\xrightarrow{\Delta}$ or for $\xleftarrow{\Delta}$. If so, can these forbidden substructures be inferred in a rational manner from properties of vertex and/or edge labels along the connecting paths in the explaining tree? Is this the case at least for labels and predicates satisfying (L1) and (L2)?

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