Best Match Graphs with Binary Trees

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Abstract

Best match graphs (BMG) are a key intermediate in graph-based orthology detection and contain a large amount of information on the gene tree. We provide a near-cubic algorithm to determine whether a BMG can be explained by a fully resolved gene tree and, if so, to construct such a tree. Moreover, we show that all such binary trees are refinements of the unique binary-resolvable tree (BRT), which in general is a substantial refinement of the also unique least resolved tree of a BMG.

Keywords: Best match graphs, Binary trees, Rooted triple consistency, Polynomial-time algorithm

1 Introduction

The evolutionary history of a gene family can be described by a gene tree $T$, a species tree $S$, and an embedding of the gene tree into the species tree (Fig. 1A). The latter is usually formalized as a reconciliation map $\mu$ that locates gene duplication events along the edges of the species tree, identifies speciation events in $T$ as those that map to vertices in $S$, and encodes horizontal gene transfer as edges in $T$ that cross from one branch of $S$ to another. Detailed gene family histories are a prerequisite for studying associations between genetic and phenotypic innovations. They also encode orthology, i.e., the fact that two genes in distinct species arose from a speciation event, a notion that is of key importance in genome annotation and phylogenomics. Two conceptually distinct approaches have been developed to infer orthology and/or complete gene family histories from sequence data. Tree-based methods explicitly construct the gene tree $T$ and the species tree $S$, and then determine the reconciliation map $\mu$ as an optimization problem. Graph-based methods, on the other hand, start from best matches, i.e., by identifying for each gene its closest relative or relatives in every other species. Due to the page limits, we only refer to a few key reviews and the references therein [12, 13, 20].

Best match graphs (BMGs) have only very recently been introduced as mathematical objects to formalize the idea of pairs of evolutionarily most closely related genes in two species [6]. The gene tree is modeled as a rooted, leaf-colored phylogenetic tree $(T, \sigma)$ (Fig. 1B). Its leaf set $L(T)$ denotes the extant genes, and each gene $x \in L(T)$ is colored by the species $\sigma(x)$ in whose genome it resides. A gene tree $T$, we denote the ancestor order on its vertex set by $\preceq_T$. That is, we have $v \preceq_T u$ if $u$ lies along the unique path connecting $v$ to the root $\rho_T$ of $T$, in which case we call $u$ an ancestor of $v$. The least common ancestor $\text{lca}_T(A)$ is the unique $\preceq_T$-smallest vertex that is an ancestor of all genes in $A$. Writing $\text{lca}_T(x, y) := \text{lca}_T(\{x, y\})$, we have

Definition 1.1. Let $(T, \sigma)$ be a leaf-colored tree. A leaf $y \in L(T)$ is a best match of the leaf $x \in L(T)$ if $\sigma(x) \neq \sigma(y)$ and $\text{lca}_T(x, y) \preceq_T \text{lca}_T(x, y')$ holds for all leaves $y'$ of color $\sigma(y') = \sigma(y)$.

The best match graph (BMG) of a leaf-colored tree $(T, \sigma)$, denoted by $G(T, \sigma)$, is a vertex-colored digraph with vertex set $L(T)$ and arcs $(x, y)$ if and only if $y$ is a best match of $x$ (Fig. 1C).
Figure 1: (A) An evolutionary scenario consisting of a gene tree \((T, \sigma)\) (whose topology is again shown in (B)) together with an embedding into a species tree \(S\). The coloring \(\sigma\) of the leaves of \(T\) represents the species in which the genes reside. Speciation vertices (●) of the gene tree coincide with the vertices of the species tree, whereas gene duplications (□) are mapped to the edges of \(S\). (C) The best match graph \((G, \sigma)\) explained by \((T, \sigma)\). (D) The unique least resolved tree \((T^*, \sigma)\) explaining \((G, \sigma)\). (E) An hourglass, i.e. the smallest example for a BMG that is not binary-explainable. (F) The (unique) tree that explains the hourglass.

An arbitrary vertex-colored graph \((G, \sigma)\) is a best match graph if there exists a leaf-colored tree \((T, \sigma)\) such that \((G, \sigma) = G(T, \sigma)\). In this case, we say that \((T, \sigma)\) explains \((G, \sigma)\).

A best match \((x, y)\) is reciprocal if \((y, x)\) is also a best match. We will call a pair of reciprocal arcs \((x, y)\) and \((y, x)\) in a graph \((G, \sigma)\) an edge, denoted by \(xy\). In the absence of horizontal gene transfer, all pairs of orthologous genes form reciprocal best matches. That is, the undirected orthology graph is always a subgraph of the best match graph [7]. This simple observation has stimulated the search for computational methods to identify the "false-positive" edges in a BMG, i.e., edges that do not correspond to a pair of orthologous genes [15]. This requires a better understanding of the set of trees that explain a given BMG.

In this contribution we derive an efficient algorithm for the construction of a binary tree that explains a BMG if and only if such a tree exists. Such BMGs will be called binary-explainable. This problem can be expressed as a consistency problem involving certain sets of both required and forbidden triples. It is therefore related to the Most Resolved Compatible Tree and Forbidden Triples (restricted to binary trees) problems, both of which are NP-complete [2]. However, binary-explainable BMGs are characterized in [15] as those BMGs that do not contain a certain colored graph on four vertices, termed hourglass, as induced subgraph (Fig. 1E,F). The presence of an induced hourglass in an arbitrary vertex-colored graph \((G = (V, E), \sigma)\) can be checked in \(O(|E|^2)\) [15]. This characterization, however, is not constructive and it remained an open problem how to construct a binary tree that explains a BMG.

This contribution is organized as follows. In Sec. 2, we introduce some notation and review key properties of BMGs that are needed later on. In Sec. 3, we derive a constructive algorithm for this problem that runs in near-cubic time \(\tilde{O}(|V|^3)\). It produces a unique tree, the binary-refinable tree (BRT) of a BMG show in Fig. 3. The BRT has several interesting properties that are studied in detail in Sec. 4. Simulated data are used in Sec. 5 to show that BRTs are much better resolved than the least resolved trees of BMGs.

2 Best Match Graphs

By construction, no vertex \(x\) of a BMG \((G, \sigma)\) has a neighbor with the same color, i.e., the coloring \(\sigma\) is proper. Furthermore, every vertex \(x\) has at least one out-neighbor (i.e., a best match) \(y\) of
every color \( \sigma(y) \neq \sigma(x) \). We call such a proper coloring sink-free and say that \((G, \sigma)\) is sf-colored.

We write \( v \prec_T u \) for \( v \preceq_T u \) and \( v \neq u \) and use the convention that the vertices in an edge \( uv \in E(T) \) are ordered such that \( u \prec_T v \). Thus \( u \) is the unique parent of \( v \), and \( v \) is a child of \( u \). The set of all children of a vertex \( u \) is denoted by \( chd_T(u) \). The subtree of a tree \( T \) rooted at a vertex \( u \) is induced by the set of vertices \( \{x \in V(T) \mid x \preceq_T u\} \) and will be denoted by \( T(u) \).

A triple \( ab|c \) is a rooted tree \( t \) on three pairwise distinct vertices \( \{a, b, c\} \) such that \( lca_t(a, b) \prec_T lca_t(b, c) = \rho \), where \( \rho \) denotes the root of \( t \). A tree \( T' \) is displayed by a tree \( T \), in symbols \( T' \preceq_T T \), if \( T' \) can be obtained from a subtree of \( T \) by contraction of edges \([19]\). Conversely, a tree \( T \) is a refinement of \( T' \) if \( T' \preceq_T T \) and additionally \( L(T) = L(T') \). We denote by \( r(T) \) the set of all triples that are displayed by a tree \( T \), and write \( R[L] := \{xy|z \in R : x, y, z \in L\} \) for the restriction of a triple set \( R \) to a set \( L \) of leaves.

A leaf-colored tree \((T, \sigma)\) explaining a BMG \((G, \sigma)\) is least resolved if every tree \( T' \) obtained from \( T \) by edge contractions no longer explains \((G, \sigma)\). Thus, \((T, \sigma)\) does not display a tree with fewer edges that explains \((G, \sigma)\). As shown in \([6]\), every BMG is explained by a unique least resolved tree. We will need the following technical result relating induced subgraphs of BMGs to subtreess of their explaining trees:

**Lemma 2.1.** \([14, \text{Lemma 22}]\) Let \((G, \sigma)\) be a BMG explained by a tree \((T, \sigma)\). Then, for every \( u \in V(T) \), it holds \( G(T(u), \sigma|_{L(T(u))}) = (G[L(T(u))], \sigma|_{L(T(u))}) \).

BMGs can be characterized in terms of informative and forbidden triples \([6, 14, 16]\). Given a vertex-colored graph \((G, \sigma)\), we define

\[
\begin{align*}
\mathcal{R}(G, \sigma) := \{ab|b' : \sigma(a) \neq \sigma(b) = \sigma(b'), (a, b) \in E(G); (a, b') \notin E(G)\}, \\
\mathcal{F}(G, \sigma) := \{ab|b' : \sigma(a) \neq \sigma(b) = \sigma(b'), b \neq b'; (a, b), (a, b') \in E(G)\}.
\end{align*}
\]

We refer to \(\mathcal{R}(G, \sigma)\) as the informative triples and to \(\mathcal{F}(G, \sigma)\) as the forbidden triples of \((G, \sigma)\). We will regularly make use of the observation that, as a direct consequence of their definition, forbidden triples always come in pairs:

**Observation 2.2.** Let \((G, \sigma)\) be a vertex-colored digraph. Then \(ab|b' \in \mathcal{F}(G, \sigma)\) with \(\sigma(b) = \sigma(b')\) if and only if \(ab'|b \in \mathcal{F}(G, \sigma)\).

**Definition 2.3.** A pair of triple sets \((\mathcal{R}, \mathcal{F})\) is consistent if there is a tree \(T\) that displays all triples in \(\mathcal{R}\) but none of the triples in \(\mathcal{F}\). In this case, we say that \(T\) agrees with \((\mathcal{R}, \mathcal{F})\).

For \(\mathcal{F} = \emptyset\) this definition reduces to the usual notion of consistency of \(\mathcal{R}\) \([19]\). In general, consistency of \((\mathcal{R}, \mathcal{F})\) can be checked in polynomial time. The algorithm MTT, named for mixed triplets problem restricted to trees, constructs a tree \(T\) that agrees with \((\mathcal{R}, \mathcal{F})\) or determines that no such tree exists \([9]\). It can be seen as a generalization of BUILD, which solves the corresponding problem for \(\mathcal{F} = \emptyset\) \([1]\). Given a consistent triple set \(\mathcal{R}\) on a set of leaves \(L\), BUILD constructs a deterministic tree on \(L\) known as the Aho tree, and denoted here as \(Aho(\mathcal{R}, L)\).

Two characterizations of BMGs given in \([14, \text{Thm. 15}]\) and \([16, \text{Lemma 3.4 and Thm. 3.5}]\) can be summarized as follows:

**Proposition 2.4.** Let \((G, \sigma)\) be a properly colored digraph with vertex set \(L\). Then the following three statements are equivalent:

1. \((G, \sigma)\) is a BMG.
2. \(\mathcal{R}(G, \sigma)\) is consistent and \(G(Aho(\mathcal{R}(G, \sigma), L), \sigma) = (G, \sigma)\).
3. \((G, \sigma)\) is sf-colored and \((\mathcal{R}(G, \sigma), \mathcal{F}(G, \sigma))\) is consistent.

In this case, \((Aho(\mathcal{R}(G, \sigma), L), \sigma)\) is the unique least resolved tree for \((G, \sigma)\), and a leaf-colored tree \((T, \sigma)\) on \(L\) explains \((G, \sigma)\) if and only if it agrees with \((\mathcal{R}(G, \sigma), \mathcal{F}(G, \sigma))\).

### 3 Binary Trees Explaining a BMG in Near Cubic Time

We start with a few technical results on the structure of the triples sets \(\mathcal{R}(G, \sigma)\) and \(\mathcal{F}(G, \sigma)\).

**Lemma 3.1.** Let \((G, \sigma)\) be explained by a binary tree \((T, \sigma)\). If \(ab|b' \in \mathcal{F}(G, \sigma)\) with \(\sigma(b) = \sigma(b')\), then \((T, \sigma)\) displays the triple \(bb'|a\).
Lemma 3.3 implies that we can infer a set of additional triples that would be required for a binary tree to explain a vertex-colored graph \((G, \sigma)\). This motivates the definition of an extended informative triple set

\[
\mathcal{R}^B(G, \sigma) := \mathcal{R}(G, \sigma) \cup \{bb'|a: ab|b' \in \mathcal{F}(G, \sigma) \text{ and } \sigma(b) = \sigma(b')\}.
\] (2)

Since informative and forbidden triples are defined by the presence and absence of certain arcs in a vertex-colored digraph, this leads to the following

**Observation 3.2.** Let \((G, \sigma)\) be a vertex-colored digraph and \(L' \subseteq V(G)\). Then \(R(G, \sigma)|_{L'} = R(G[L'], \sigma|_{L'})\) holds for any \(R \in \{\mathcal{R}, \mathcal{F}, \mathcal{R}^B\}\).

**Lemma 3.3.** If \((T, \sigma)\) is a binary tree explaining the BMG \((G, \sigma)\), then \((T, \sigma)\) displays \(\mathcal{R}^B(G, \sigma)\).

**Proof.** Let \((T, \sigma)\) be a binary tree that explains \((G, \sigma)\). By Prop. 2.4, \((G, \sigma)\) displays all informative triples \(\mathcal{R}(G, \sigma)\). Now let \(bb'|a \in \mathcal{R}^B(G, \sigma) \setminus \mathcal{R}(G, \sigma)\). Hence, by definition and Obs. 2.2, \(ab|b'\) and \(ab|b\) are forbidden triples for \((G, \sigma)\). This together with Lemma 3.1 and the fact that \((T, \sigma)\) is binary implies that \(bb'|a\) is displayed by \((T, \sigma)\). In summary, therefore, \((T, \sigma)\) displays all triples in \(\mathcal{R}^B(G, \sigma)\).

**Lemma 3.4.** Let \((G, \sigma)\) be an sf-colored digraph with vertex set \(L\). Every tree on \(L\) that displays \(\mathcal{R}^B(G, \sigma)\) explains \((G, \sigma)\).

**Proof.** Suppose that a tree \((T, \sigma)\) on \(L\) displays \(\mathcal{R}^B(G, \sigma)\) and thus, in particular, \(\mathcal{R}(G, \sigma)\). Now suppose \(ab|b' \in \mathcal{F}(G, \sigma)\) with \(\sigma(b) = \sigma(b')\) is a forbidden triple for \((G, \sigma)\) and hence, \(bb'|a \in \mathcal{R}^B(G, \sigma)\). Clearly, \((T, \sigma)\) displays at most one of the three possible triples on \(\{a, b, b'\}\). Taken together, the latter arguments imply that \((T, \sigma)\) does not display \(ab|b'\). In summary, \((T, \sigma)\) displays all triples in \(\mathcal{R}(G, \sigma)\) and none of the triples in \(\mathcal{F}(G, \sigma)\) and thus, \(\mathcal{R}(G, \sigma), \mathcal{F}(G, \sigma)\) is consistent. Therefore and since \((G, \sigma)\) is sf-colored by assumption, we can apply Prop. 2.4 to conclude that the tree \((T, \sigma)\) on \(L\) explains the BMG \((G, \sigma)\).

Using Lemmas 3.3 and 3.4, it can be shown that consistency of \(\mathcal{R}^B(G, \sigma)\) is sufficient for an sf-colored graph \((G, \sigma)\) to be binary-explainable.

**Theorem 3.5.** A properly vertex-colored graph \((G, \sigma)\) with vertex set \(L\) is binary-explainable if and only if (i) \((G, \sigma)\) is sf-colored, and (ii) \(\mathcal{R}^B := \mathcal{R}^B(G, \sigma)\) is consistent. In this case, the BMG \((G, \sigma)\) is explained by every refinement of the tree \((\text{Aho}(\mathcal{R}^B, L), \sigma)\).

**Proof.** First suppose that \((G, \sigma)\) is sf-colored and that \(\mathcal{R}^B\) is consistent. Therefore, the tree \(T := \text{Aho}(\mathcal{R}^B, L)\) exists. By correctness of \textsc{build} \([1]\), \(T\) displays all triples in \(\mathcal{R}^B\). Clearly, every refinement \(T'\) of \(T\) also displays \(\mathcal{R}^B\). Hence, for every refinement \(T'\) of \(T\) (including \(T\) itself), we can apply Lemma 3.4 to conclude that \((T', \sigma)\) explains \((G, \sigma)\). In particular, \((G, \sigma)\) is a BMG. Since there always exists a binary refinement of \(T\), the latter arguments imply that \((G, \sigma)\) is binary-explainable.

Now suppose that \((G, \sigma)\) can be explained by a binary tree \((T, \sigma)\), and note that \((G, \sigma)\) is a BMG in this case. By Prop. 2.4, \((G, \sigma)\) is sf-colored. Moreover, the binary tree \((T, \sigma)\) displays \(\mathcal{R}^B\) as a consequence of Lemma 3.3. Therefore, \(\mathcal{R}^B\) must be consistent.

Thm. 3.5 implies that the problem of determining whether an sf-colored graph \((G, \sigma)\) is binary-explainable can be reduced to a triple consistency problem. More precisely, it establishes the correctness of Alg. 1, which in turn relies on the construction of \(\text{Aho}(\mathcal{R}^B, L)\). The latter can be achieved in polynomial time \([1]\). Making use of the improvements achievable by using dynamic graph data structures \([4, 10]\), we obtain the following performance bound:

**Corollary 3.6.** There exists an \(O(|L|^3 \log^2 |L|)\)-time algorithm that constructs a binary tree explaining a vertex-colored digraph \((G, \sigma)\) with vertex set \(L\), if and only if such a tree exists.
Algorithm 1: Construction of a binary tree explaining \((G, \sigma)\).

\[
\begin{array}{ll}
\text{Input:} & \text{A properly vertex-colored graph } (G, \sigma) \text{ with vertex set } L. \\
\text{Output:} & \text{Binary tree } (T, \sigma) \text{ explaining } (G, \sigma) \text{ if one exists.} \\
1 & \text{if } (G, \sigma) \text{ is not sf-colored then} \\
2 & \quad \text{exit false} \\
3 & \text{construct the extended triple set } \mathcal{R}^B := \mathcal{R}^B(G, \sigma) \\
4 & T \leftarrow \text{Aho}(\mathcal{R}^B, L) \\
5 & \text{if } T \text{ is a tree then} \\
6 & \quad \text{return } (T', \sigma) \\
7 & \text{else} \quad \text{exit false} \\
\end{array}
\]

Proof. For a vertex-colored digraph \((G, \sigma)\) with vertex set \(L\) it can be decided in \(O(|L|^2)\) whether it is sf-colored, i.e., whether it is properly colored and every vertex has an out-neighbor with every other color. The set \(\mathcal{R}^B := \mathcal{R}^B(G, \sigma)\) can easily be constructed in \(O(|L|^3)\) using Eqs. 1 and 2 and the number of triples in \(\mathcal{R}^B\) is bounded by \(O(|L|^3)\). Note that every triple in \(\mathcal{R}^B\) is a tree with a constant number of vertices and edges. Thus, the total number \(M\) of vertices and edges in \(\mathcal{R}^B\) is also in \(O(|L|^3)\). The algorithm \texttt{BuildST} [4] solves the consistency problem for \(\mathcal{R}^B\) and constructs a corresponding (not necessarily binary) tree \(T\) in \(O(M \log^2 M) = O(|L|^3 \log^2 |L|)\) time [4, Thm. 3]. Finally, we can obtain an arbitrary binary refinement \(T'\) of \(T\) in \(O(|L|)\). Thus there exists a version of Alg. 1 that solves the problem in \(O(|L|^3 \log^2 |L|)\) time. \(\square\)

4 The Binary-Refinable Tree of a BMG

If a graph \((G, \sigma)\) with vertex set \(L\) is binary-explainable, Thm. 3.5 implies that \(\mathcal{R}^B := \mathcal{R}^B(G, \sigma)\) is consistent and every refinement of \((\text{Aho}(\mathcal{R}^B, L), \sigma)\) explains \((G, \sigma)\). In this section, we investigate the properties of this tree in more detail.

Definition 4.1. The binary-refinable tree (BRT) of a binary-explainable BMG \((G, \sigma)\) with vertex set \(L\) is the leaf-colored tree \((\text{Aho}(\mathcal{R}^B(G, \sigma), L), \sigma)\).

The BRT is not necessarily a binary tree. However, Thm. 3.5 implies that the BRT as well as each of its binary refinements explains \((G, \sigma)\). It is well-defined since Thm. 3.5 ensures consistency of \(\mathcal{R}^B\) for binary-explainable graphs, and the Aho tree as produced by \texttt{BUILD} is uniquely determined by the set of input triples \([1]\).

Corollary 4.2. If \((G, \sigma)\) is a binary explainable BMG, then its BRT is a refinement of the LRT.

Proof. Since each BMG has a unique LRT [6, Thm. 8], the BRT of a binary explainable BMG is necessarily a refinement of the LRT. \(\square\)

Clearly, the BRT is least resolved among the trees that display \(\mathcal{R}^B\), i.e., contraction of an arbitrary edge results in a tree that no longer displays all triples in \(\mathcal{R}^B\) [18, Prop. 4.1]. Now, we tackle the question whether the BRT is the unique least resolved tree in this sense. In other words, we ask whether every tree that displays \(\mathcal{R}^B\) is a refinement of the BRT. As we shall see, this question can be answered in the affirmative.

In order to show this, we first introduce some additional notation and concepts for sets of triples. Following [3, 17], we call the span of \(\mathcal{R}\), denoted by \(\langle \mathcal{R} \rangle\), the set of all trees with leaf set \(L_{\mathcal{R}} := \bigcup_{t \in \mathcal{R}} L(t)\) that display \(\mathcal{R}\). With this notion, we define the closure operator for consistent triple sets by

\[
\text{cl}(\mathcal{R}) = \bigcap_{T \in \langle \mathcal{R} \rangle} r(T),
\]

i.e., a triple \(t\) is contained in \(\text{cl}(\mathcal{R})\) if all trees that display \(\mathcal{R}\) also display \(t\). In particular, \(\text{cl}(\mathcal{R})\) is again consistent. The map \(\text{cl}\) is a closure in the usual sense on the set of consistent triple sets, i.e., it is extensive \([\mathcal{R} \subseteq \text{cl}(\mathcal{R})]\), monotonic \([\mathcal{R}' \subseteq \mathcal{R} \Rightarrow \text{cl}(\mathcal{R}') \subseteq \text{cl}(\mathcal{R})]\), and idempotent \([\text{cl}(\mathcal{R}) = \text{cl}(\text{cl}(\mathcal{R}))]\) [3, Prop. 4]. A consistent set of triples \(\mathcal{R}\) is closed if \(\mathcal{R} = \text{cl}(\mathcal{R})\).
Interesting properties of a triple set $\mathcal{R}$ and of the Aho tree $\text{Aho}(\mathcal{R}, L)$ can be understood by considering the Aho graph $[\mathcal{R}, L]$ with vertex set $L$ and edges $xy$ if there is a triple $xy|z \in \mathcal{R}$ with $x, y, z \in L$ [1]. It has been shown in [3] that a triple set $\mathcal{R}$ on $L$ is consistent if and only if $[\mathcal{R}, L]$ is disconnected for every subset $L' \subseteq L$ with $|L'| > 1$. The root $\rho$ of the Aho tree $\text{Aho}(\mathcal{R}, L)$ corresponds to the Aho graph $[\mathcal{R}, L]$ in such a way that there is a one-to-one correspondence between the children $v$ of $\rho$ and the connected components $C$ of $[\mathcal{R}, L]$ given by $L(T(v)) = V(C)$. The BUILD algorithm constructs $\text{Aho}(\mathcal{R}, L)$ by recursively top-down over the connected components (with vertex sets $L'$) of the Aho graphs. It fails if and only if $|L'| > 1$ and $[\mathcal{R}, L']$ is connected at some recursion step. For a more detailed description we refer to [1]. Since the decomposition of the Aho graphs into their connected components is unique, the Aho tree is also uniquely defined.

The following characterization of triples that are contained in the closure also relies on Aho graphs:

**Proposition 4.3.** [2, Cor. 3.9] Let $\mathcal{R}$ be a consistent set of triples and $L_\mathcal{R} := \bigcup_{t \in \mathcal{R}} L(t)$ the union of their leaves. Then $abc \in \text{cl}(\mathcal{R})$ if and only if there is a subset $L' \subseteq L_\mathcal{R}$ such that the Aho graph $[\mathcal{R}, L']$ has exactly two connected components, one containing both $a$ and $b$, and the other containing $c$.

The following result shows that Prop. 4.3 can be applied to the triple set $\mathcal{R}^B(G, \sigma)$ of an sf-colored graph $(G, \sigma)$ with the exception of the two trivial special cases in which either all vertices of $(G, \sigma)$ are of the same color or of pairwise distinct colors.

**Lemma 4.4.** Let $(G, \sigma)$ be an sf-colored graph with vertex set $L \neq \emptyset$, $L_{\mathcal{R}^B} := \bigcup_{t \in \mathcal{R}(G, \sigma) \cup \mathcal{F}(G, \sigma)} L(t)$ and $L_{\mathcal{R}^B} := \bigcup_{t \in \mathcal{R}^B(G, \sigma)} L(t)$. Then the following statements are equivalent:

1. $L_{\mathcal{R}^B} = L_{\mathcal{R}^B} = L$.
2. $\mathcal{R}(G, \sigma) \cup \mathcal{F}(G, \sigma) \neq \emptyset$.
3. $\mathcal{R}^B(G, \sigma) \neq \emptyset$.
4. $(G, \sigma)$ is $\ell$-colored with $\ell \geq 2$ and contains two vertices of the same color.

If these statements are not satisfied, then $(G, \sigma)$ is a BMG that is explained by any tree $(T, \sigma)$ on $L$.

**Proof.** It was shown in [16, Lemma 3.6] that Statements 2 and 4, and $L_{\mathcal{R}^B} = L$ are equivalent. One easily verifies using Eqs. 1 and 2 that there is a triple on $\{a, b, c\}$ in $\mathcal{R}(G, \sigma) \cup \mathcal{F}(G, \sigma)$ if and only if there is a triple on $\{a, b, c\}$ in $\mathcal{R}^B(G, \sigma)$. Therefore, Statements 2 and 3 are equivalent and we always have $L_{\mathcal{R}^B} = L_{\mathcal{R}^B}$. Thus all statements are equivalent. If the statements are not satisfied, i.e., in particular, Statement (4) is not satisfied, then the vertices in $L$ are all either of the same or of different color. In both cases, $(G, \sigma)$ is explained by any tree on $L$. \(\square\)

Lemma 4.4 holds for BMGs since these are sf-colored by Prop. 2.4. The following result is essential for the application of Prop. 4.3 to a triple set $\mathcal{R}^B(G, \sigma)$.

**Lemma 4.5.** Let $(G, \sigma)$ be a binary-explainable BMG with vertex set $L$ and $\mathcal{R}^B := \mathcal{R}^B(G, \sigma)$. Then, for any two distinct connected components $C$ and $C'$ of the Aho graph $H := [\mathcal{R}^B, L]$, the subgraph $H[L']$ induced by $L' := V(C) \cup V(C')$ satisfies $H[L'] = [\mathcal{R}^B(L'), L'] = C \cup C'$.

**Proof.** Since $(G, \sigma)$ is binary-explainable, $\mathcal{R}^B$ is consistent by Thm. 3.5. Thus $H := [\mathcal{R}^B, L]$ contains at least two connected components. If $H$ contains exactly two connected components $C$ and $C'$, the statement trivially holds. Hence, assume that $H$ contains at least three connected components. Let $C$ and $C'$ be two distinct connected components of $H$, and set $L' := V(C) \cup V(C')$ and $H' := [\mathcal{R}^B, L']$. Note, $H[L'] = V(H') = L'$, and $H[L'] = C \cup C'$ is the induced subgraph of $H$ that consists precisely of the two connected components $C$ and $C'$. From $\mathcal{R}^B(L') \subseteq \mathcal{R}^B$ and the construction of $H$ we immediately observe that $H'$ is a subgraph of $H[L']$. Hence, it remains to show that every edge $xy$ in $H[L']$ is also an edge in $H'$.

To this end, we consider the BRT $(T, \sigma)$ of $(G, \sigma)$, which exists since $\mathcal{R}^B$ is consistent and explains $(G, \sigma)$ by Thm. 3.5. By construction, there is a one-to-one correspondence between the connected components of $H$ and the children of the root $\rho$ of $T$. Thus, let $v$ and $v'$ be the distinct children of $\rho$ such that $L(T(v)) = V(C)$ and $L(T(v')) = V(C')$ and let $xy$ be an edge in $H[L']$. Since $x$ and $y$ lie in the same connected component of $H$ and $x, y \in L'$, we can assume w.l.o.g. that $x, y \in L(T(v))$. It suffices to show that there is a triple $xy|z \in \mathcal{R}^B$ with $z \in L'$, since in this case, we obtain $xy|z \in \mathcal{R}^B(L')$ and thus $xy \in E(H')$. \(\square\)
We assume, for contradiction, that there is no \( z \in L' \) with \( xy|z \in \mathcal{R}^B \). Then, by construction of \( H \) and since \( xy \) is an edge therein, \( \mathcal{R}^B \) contains a triple \( xy|z \in L(T(v')) \) for some \( v' \in \text{child}_T(p) \setminus \{v, v'\} \) and a connected component \( C'' \) of \( H \) with \( V(C'') = L(T(v'')) \). By Eqs. 1 and 2, there are exactly two cases for such a triple:

(a) \( xy|z \in ab|b' \) (and w.l.o.g. \( x = a, y = b \)) such that
\[ \sigma(a) \neq \sigma(b) = \sigma(b'), (a, b) \notin E(G), \quad \text{and} \quad (a, b') \notin E(G), \]
and
(b) \( xy|z \in bb'|a \) (and w.l.o.g. \( x = b, y = b' \)) such that
\[ \sigma(a) \neq \sigma(b) = \sigma(b'), (a, b), (a, b') \notin E(G). \]

In Case (a), we have \( a, b \in L(T(v')) \), \( v' = z \in L(T(v'')) \) and \( (a, b) \in E(G) \). Assume, for contradiction, that there is a vertex \( b'' \) of color \( \sigma(b'') = \sigma(b) \) in \( L(T(v')) \). In this case, \( \text{lcary}(a, b) \preceq_T v \prec_T \rho = \text{lcary}(a, b') \) would imply that \( (a, b') \notin E(G) \). Hence, we obtain the informative triple \( ab|b'' \in \mathcal{R}(G, \sigma) \subseteq \mathcal{R}^B \) with \( b'' \in L(T(v')) \in L' \). By assumption, such a triple does not exist and thus we must have \( \sigma(b) \notin \sigma(L(T(v')))) \). Hence, every leaf \( c \in L(T(v')) \notin \emptyset \) satisfies \( \sigma(c) \neq \sigma(b) = \sigma(b') \).

Since the color \( \sigma(b) \) is not present in \( T(v') \) and \( \text{lcary}(c, b') = \text{lcary}(c, b) = \rho \), we can conclude that \( (c, b), (c, b') \in E(G) \). By Eq. 2, \( bb'|c \in \mathcal{R}^B \) and thus \( bb' \) is an edge in \( H \). However, as argued above, \( b \) and \( b' \) lie in distinct connected components \( C \) and \( C'' \) of \( H \); a contradiction.

In Case (b), we have \( b, b' \in L(T(v)) \), \( a = z \in L(T(v'')) \) and \( (a, b), (a, b') \in E(G) \). The latter implies that the color \( \sigma(b) \) is not present in the subtree \( T(v') \).

Now assume, for contradiction, that \( \sigma(b) \) is not present in \( T(v') \) either. Then, \( (c, b), (c, b') \in E(G) \) for any \( c \in L(T(v')) \notin \emptyset \), thus \( bb'|c \in \mathcal{R}^B \); a contradiction. Hence, there exists a vertex \( b'' \in L(T(v')) \) with \( \sigma(b'') = \sigma(b) \). Similarly, since \( \sigma(b) \notin \sigma(L(T(v')))) \), we can conclude that \( (a, b), (a, b'') \in E(G) \) and thus \( bb'|a \in \mathcal{R}^B \).

This implies that \( bb'' \) is an edge in \( H \). However, \( b \) and \( b'' \) lie in distinct connected components \( C \) and \( C'' \) of \( H \); a contradiction.

In summary, we conclude that for every edge \( H[L'] \) there is a triple \( xy|z \) with \( \{x, y, z\} \subseteq L' \), and hence \( xy \in E(H') \). Together with \( V(H[L']) = V(H') = L' \) and \( E(H') \subseteq E(H[L']) \), this implies \( H' = H[L'] \).

\[ \Box \]

**Lemma 4.6.** The BRT \( (T, \sigma) \) of a binary-explainable BMG \( (G, \sigma) \) satisfies \( r(T) = \text{cl}(\mathcal{R}^B(G, \sigma)) \).

**Proof.** First note that since \( (G, \sigma) \) is binary-explainable, Thm. 3.5 ensures the consistency of \( \mathcal{R}^B = \mathcal{R}^B(G, \sigma) \), and hence, the existence of the BRT \( (T, \sigma) \) and \( \text{cl}(\mathcal{R}^B) \). We proceed by induction on \( L := V(G) \).

The statement trivially holds for \( |L| \in \{1, 2\} \), since in this case, we clearly have \( r(T) = \text{cl}(\mathcal{R}^B) = \emptyset \). Moreover, we can assume w.l.g. that \( L = L_{2n} := \bigcup_{t \in \mathcal{R}^B} L(t) \) since otherwise Lemma 4.4 implies \( \mathcal{R}^B = \emptyset \). In this case, \( (T, \sigma) \) is the star tree on \( L \), and again \( r(T) = \text{cl}(\mathcal{R}^B) = \emptyset \).

For \( |L| > 2 \) and \( L = L_{2n} \) we assume that the statement is true for every binary-explainable BMG with less than \( |L| \) vertices. We write \( L_v := L(T(v)) \) for the set of leaves in the subtree of \( (T, \sigma) \) rooted at \( v \).

By construction of the BRT \( (T, \sigma) \) from \( \mathcal{R}^B \), there is a one-to-one correspondence between the connected components of the Aho graph \( [\mathcal{R}^B, L] \) and the children \( v \) of the root \( \rho \) of \( T \). For each such vertex \( v \in \text{child}_T(\rho) \), the graph \( G(T(v), \sigma_{|L_v}) \) is a BMG and, by Lemma 2.1, \( G(T(v), \sigma_{|L_v}) = (G[L_v], \sigma_{|L_v}) \).

Moreover, we have \( \mathcal{R}_{L_v} = \mathcal{R}^B(G[L_v], \sigma_{|L_v}) \) by Obs. 3.2. By the recursive construction of \( (T, \sigma) \) via BUILD, we therefore conclude that \( (T(v), \sigma_{|L_v}) \) is the BRT for the BMG \( (G[L_v], \sigma_{|L_v}) \). By induction hypothesis, we can therefore conclude \( r(T(v)) = \text{cl}(\mathcal{R}^B(G[L_v], \sigma_{|L_v})) \).

Let \( ab|c \in r(T) \) and suppose first \( lca_T((a, b, c)) \preceq_T v \prec_T \rho \) for some \( v \in \text{child}_T(\rho) \). In this case, we have \( ab|c \in r(T(v)) = \text{cl}(\mathcal{R}^B(G[L_v], \sigma_{|L_v})) \). Together with \( \mathcal{R}^B(G[L_v], \sigma_{|L_v}) = \mathcal{R}^B_{|L_v} \subseteq \mathcal{R}^B \) and monotonicity of the closure it follows \( ab|c \in \text{cl}(\mathcal{R}^B) \).

It remains to show that, for every triple \( ab|c \in r(T) \) with \( lca_T((a, b, c)) \preceq_T v \prec_T \rho \), it also holds \( ab|c \in \text{cl}(\mathcal{R}^B) \). In this case, we have \( a, b \in L_v \) and \( c \in L_{v'} \) for two distinct children \( v \) and \( v' \) of the root \( \rho \). As argued above, \( L_v \) and \( L_{v'} \) correspond to two distinct connected components \( C_v \) and \( C_{v'} \) of \( [\mathcal{R}^B, L] \). Consider the set \( L' := L_v \cup L_{v'} = V(C_v) \cup V(C_{v'}) \). By Lemma 4.5, the Aho graph \( [\mathcal{R}^B_{|L'}, L'] \) consists exactly of the two connected components \( C_v \) and \( C_{v'} \), where \( C_v \) contains \( a \) and \( b \), and \( C_{v'} \) contains \( c \). This and the fact that \( L = L_{2n} \) allows us to apply Prop. 4.3 and to conclude that \( ab|c \in \text{cl}(\mathcal{R}^B) \).

In summary, every triple in \( ab|c \in r(T) \) satisfies \( ab|c \in \text{cl}(\mathcal{R}^B) \), thus \( r(T) \subseteq \text{cl}(\mathcal{R}^B) \). On the other hand, the fact that \( T \) displays \( \mathcal{R}^B \) and that \( r(T) \) is closed implies \( \text{cl}(\mathcal{R}^B) \subseteq \text{cl}(r(T)) = r(T) \). Therefore, \( \text{cl}(\mathcal{R}^B) = r(T) \).

\[ \square \]
Figure 2: A least resolved tree \((T, \sigma)\) explaining the BMG \((G, \sigma)\) with informative triples \(\mathcal{R} := \mathcal{R}(G, \sigma) = \{a_2 b_1 | a_1, a_2 b_1 | a_3, a_2 b_1 | b_2, a_1 b_1 | b_2\}\) for which \(r(T) \neq \text{cl}(\mathcal{R})\). The tree \((T', \sigma)\) also displays \(\mathcal{R}\) but \(a_1 a_2 | a_3 \in r(T)\) and \(a_1 a_2 | a_3 \notin r(T')\). In particular, \((T', \sigma)\) explains a different BMG \((G', \sigma)\) in which the arc \((a_3, b_2)\) is missing.

Figure 3: The binary-refinable tree (BRT) of the binary-explainable BMG \((G, \sigma)\) (cf. Fig. 1C) is better resolved than its LRT (cf. Fig. 1C). The remaining polytomy in the BRT (red arrow) can be resolved arbitrarily. Out of the three possibilities, one results in the original binary tree (cf. Fig. 1B).

Proposition 4.7. [8, Lemma 2.1] Let \(T\) be a phylogenetic tree and \(\mathcal{R} \subseteq r(T)\). Then \(\text{cl}(\mathcal{R}) = r(T)\) if and only if \(\mathcal{R}\) identifies \(T\).

From Lemma 4.6 and Prop. 4.7 we immediately obtain the main result of this section:

Theorem 4.8. Let \((G, \sigma)\) be a binary-explainable BMG with vertex set \(L\) and BRT \((T, \sigma)\). Then every tree on \(L\) that displays \(\mathcal{R}^B(G, \sigma)\) is a refinement of \((T, \sigma)\). In particular, every binary tree that explains \((G, \sigma)\) is a refinement of \((T, \sigma)\).

Corollary 4.9. If \((G, \sigma)\) is binary-explainable with BRT \((T, \sigma)\), then a binary tree \((T', \sigma)\) explains \((G, \sigma)\) if and only if it is a refinement of \((T, \sigma)\).

Assuming that evolution of a gene family only progresses by bifurcations and that the correct BMG \((G, \sigma)\) is known, Cor. 4.9 implies that the true (binary) gene tree displays the BRT of \((G, \sigma)\). Fig. 3 shows the LRT and BRT for the BMG \((G, \sigma)\) in Fig. 1C. The BRT is more finely resolved than the LRT, see also Fig. 1D. The difference arises from the triple \(a_2 a_3 | c_2 \in \mathcal{R}^B(G, \sigma) \setminus \mathcal{R}(G, \sigma)\). The true gene tree in Fig. 1(A,B) is a binary refinement of the BRT (and thus also of the LRT).

5 Simulation Results

Best match graphs contain valuable information on the (rooted) gene tree topology since both their LRTs and BRTs are displayed by the latter (cf. [6] and Cor. 4.9). Hence, they are of interest for the reconstruction of gene family histories. In order to illustrate the potential benefit of using the better resolved BRT instead of the LRT, we simulated realistic evolutionary scenarios using the library AsymmeTree [22]. In brief, species trees are generated using the Innovation Model [11]. A so-called planted edge above the root is added to account for the ancestral line, in which gene duplications may already occur. This planted tree \(S\) is then equipped with a dating function that assigns time stamps to its vertices. Binary gene trees \(\tilde{T}\) are simulated along the edges of the species tree by means of a constant-rate birth-death process extended by additional branchings at the speciations. For HGT events, the recipient branches are assigned at random. An extant gene \(x\) corresponds to a branch of \(\tilde{T}\) that reaches present time and thus a leaf \(s\) of \(S\), determining \(\sigma(x) = s\). All other
leaves of $\tilde{T}$ correspond to losses. To avoid trivial cases, losses are constrained in such a way that every branch (and in particular every leaf) of $S$ has at least one surviving gene. The observable part $T$ of $\tilde{T}$ is obtained by removing all branches that lead to losses only and suppressing inner vertices with a single child. From $(T, \sigma)$, the BMG and its LRT and BRT are constructed.

We consider single leaves and the full set $L$ as trivial clades since they appear in any phylogenetic tree $T = (V, E)$ with leaf set $L$. We can quantify the resolution $\text{res}(T)$ as the fraction of non-trivial clades of $T$ retained in the LRT or BRT, respectively, which is the same as the fraction of inner edges that remain uncontracted. To see this, we note that $T$ has between 0 and $|L| - 2$ edges that are not incident with leaves, with the maximum attained if and only if $T$ is binary. Thus $T$ has $|E| - |L|$ edges that have remained uncontracted. On the other hand, each vertex of $T$ that is not a leaf or the root defines a non-trivial clade. Thus $T$ contains $|V| - 1 - |L|$ non-trivial clades. Since $|E| = |V| - 1$ we have

$$\text{res}(T) := \frac{|E| - |L|}{|L| - 2} = \frac{|V| - 1 - |L|}{|L| - 2}. \quad (4)$$

The parameter $\text{res}(T)$ is well-defined for $|L| > 2$, which is always the case in the simulated scenarios. It satisfies $\text{res}(T) = 0$ for a tree consisting only of the root and leaves, and $\text{res}(T) = 1$ for binary trees. Since the true gene tree $(T, \sigma)$ is binary, it displays both the LRT and BRT of its BMG. Thus we have $0 \leq \text{res(LRT)} \leq \text{res(BRT)} \leq \text{res}(T) = 1$.

The results for the simulated scenarios with different rates for duplications, losses, and horizontal transfers are summarized in Fig. 4. In general, the BRT is much better resolved than the LRT with the median values of $\text{res(BRT)}$ exceeding $\text{res(LRT)}$ by about a factor of two (cf. lower panel).

6 Concluding Remarks

We have shown here that binary-explainable BMGs are explained by a unique binary-resolvable tree (BRT), which displays the also unique least resolved tree (LRT). In general, the BRT differs from the LRT. All binary explanations are obtained by resolving the multifurcations in the BRT in an arbitrary manner. The constructive characterization of binary-explainable BMGs given here can be computed in near-cubic time, improving the quartic-time non-constructive characterization in [15], which is based on the hourglass being a forbidden induced subgraph. We note that binarizing a leaf-colored tree $(T, \sigma)$ does not affect its “biological feasibility”, i.e., the existence of a reconciliation map $\mu : T \to S$ to a given or unknown species tree $S$, since every gene tree $(T, \sigma)$ can be reconciled
with any species tree on the set $\sigma(L(T))$, see e.g. [7]. We can therefore safely use the additional information contained in the BRT compared to the LRT. As discussed in [15], poor resolution of the LRT is often the consequence of consecutive speciations without intervening gene duplications. The same argumentation applies to the BRT, which we have seen in Sec. 5 to be much better resolved than the LRT. Still BRTs usually are not binary. We can expect that the combination of the BRT with \textit{a priori} knowledge on the species tree $S$ can be used to unambiguously resolve most of the remaining multifurcations in the BRT. The efficient computation of BRTs is therefore of practical relevance whenever evolutionary scenarios are essentially free from multifurcations, an assumption that is commonly made in phylogenetics but may not always reflect the reality [21].

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