

## RESEARCH

## A sample article title

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**Abstract****Keywords:****1 Introduction****2 The Maximum Bipartition Support Supertree Problem****2.1 Terminology and Preliminary**

Throughout the paper, we consider only unrooted trees. For any tree  $T$ , let  $V(T)$ ,  $E(T)$ , and  $L(T)$  denote the vertex set, the edge set, and the leaf set of  $T$ , respectively. For any  $v \in V(T)$ , let  $N_T(v)$  A tree is *fully resolved* if every non-leaf node has degree 3. Let  $\mathcal{T}_S$  denote the set of all fully resolved trees on leaf set  $S$ . In any tree  $T$ , each edge  $e$  induces a bipartition  $\pi_e := A|B$  of the leaf set, where  $A$  and  $B$  are the leaves in the two components of  $T - e$ , respectively. A bipartition  $A|B$  is non-trivial if both sides have size at least 2. For a tree  $T$ ,  $C(T) := \{\pi_e \mid e \in E(T)\}$  denotes the set of all bipartitions of  $T$ . For a fully resolved tree with  $n$  leaves,  $C(T)$  contains  $2n - 3$  bipartitions, exactly  $n - 3$  of which are non-trivial. A tree  $T'$  is a *refinement* of  $T$  if  $T$  can be obtained from  $T'$  by contracting a set of edges. Equivalently,  $T'$  is a refinement of  $T$  if and only if  $C(T) \subseteq C(T')$ .

Two bipartitions  $\pi_1$  and  $\pi_2$  of the same leaf set are *compatible* if and only if there exists a tree  $T$  such that  $\pi_1, \pi_2 \in C(T)$ . The following theorem and corollary give other categorizations of compatibility.

**Theorem 1** (Theorem 2.20 of [?]) *A pair of bipartitions  $A|B$  and  $A'|B'$  of the same set is compatible if and only if at least one of the four pairwise intersections  $A \cap A'$ ,  $A \cap B'$ ,  $B \cap A'$ ,  $B \cap B'$  is empty.*

**Corollary 1** *A pair of bipartitions  $A|B$  and  $A'|B'$  of the same set is compatible if and only if one side of  $A|B$  is a subset of one side of  $A'|B'$ .*

A tree  $T$  restricted to a subset  $R$  of its leaf set, denoted  $T|_R$ , is the minimal subtree of  $T$  spanning  $R$  with nodes of degree two suppressed. A bipartition  $\pi = A|B$  restricted to a subset  $R \subseteq A \cup B$  is  $\pi|_R = A \cap R|B \cap R$ . We have the following intuitive lemma with its proof in the appendix.

**Lemma 1** *Let  $T$  be a tree with leaf set  $S$  and let  $\pi = A|B \in C(T)$  be a bipartition induced by  $e \in E(T)$ . Let  $R \subseteq S$ .*

- 1 *If  $R \cap A = \emptyset$  or  $R \cap B = \emptyset$ , then  $e \notin E(T|_R)$ .*
- 2 *If  $R \cap A \neq \emptyset$  and  $R \cap B \neq \emptyset$ , then for any  $\pi' \in C(T|_R)$  induced by  $e' \in E(T|_R)$ ,  $\pi|_R = \pi'$  if and only if  $e \in P(e')$ .*

**Corollary 2** *Let  $T$  be a tree with leaf set  $S$  and let  $\pi = A|B \in C(T)$  be a bipartition induced by  $e \in E(T)$ . Let  $R \subseteq S$  such that  $R \cap A \neq \emptyset$  and  $R \cap B \neq \emptyset$ . Then  $\pi|_R \in C(T|_R)$ .*

**Definition 1** *For two trees  $T, T'$  with the same leaf set, the bipartition support of them is  $\text{bisup}(T, T') := |C(T) \cap C(T')|$ .*

Bipartition support measures the similarity between the topology of the trees.

## 2.2 Problem Statement

Let  $T_1$  and  $T_2$  be two fully resolved trees on leaf sets  $S_1$  and  $S_2$ , respectively, such that  $X := S_1 \cap S_2 \neq \emptyset$ . Let  $S := S_1 \cup S_2$ . The maximum bipartition support supertree problem on two input trees, abbreviated MAX-BISUP-SUPERTREE-2, finds a fully resolved supertree  $T^*$  on leaf set  $S$  that maximizes the sum of the bipartition support of  $T^*$  with respect to  $T_1$  and  $T_2$ . That is,

$$\begin{aligned} T^* &= \operatorname{argmax}_{T \in \mathcal{T}_S} \text{bisup}(T|_{S_1}, T_1) + \text{bisup}(T|_{S_2}, T_2) \\ &= \operatorname{argmax}_{T \in \mathcal{T}_S} |C(T|_{S_1}) \cap C(T_1)| + |C(T|_{S_2}) \cap C(T_2)|. \end{aligned}$$

We call  $\text{bisup}(T|_{S_1}, T_1) + \text{bisup}(T|_{S_2}, T_2)$  the support score of  $T$  when  $T_1$  and  $T_2$  are clear from context.

The more general maximum bipartition support supertree problem on a set of  $N$  input trees, abbreviated MAX-BISUP-SUPERTREE- $N$ , takes in a set of input trees  $T_1, T_2, \dots, T_N$  with leaf sets  $S_1, S_2, \dots, S_N$ , respectively. MAX-BISUP-SUPERTREE- $N$  finds a fully resolved supertree  $T^*$  on leaf set  $S$  that maximizes the sum of the bipartition support of  $T^*$  with respect to every input tree. That is,

$$T^* = \operatorname{argmax}_{T \in \mathcal{T}_S} \sum_{i \in [N]} \text{bisup}(T|_{S_i}, T_i)$$

## 2.3 Algorithm

We present a polynomial time algorithm for MAX-BISUP-SUPERTREE-2 in this subsection. We first set up the notations for the algorithm and the analysis. Let  $T_1, T_2, S_1, S_2$ , and  $X$  be defined as from the problem statement. Let  $T_1|_X$  and  $T_2|_X$  be the backbone trees of  $T_1$  and  $T_2$ , respectively. Let  $\Pi$  be the set of bipartitions of  $X$ . Let Triv and NonTriv denotes the set of trivial and non-trivial bipartitions in  $C(T_1|_X) \cup C(T_2|_X)$ . For each  $e \in E(T_i|_X)$ ,  $i \in \{1, 2\}$ , let  $P(e)$  denote the path in

$T_i$  from which  $e$  is obtained by suppressing all degree-two nodes. Let  $w(e)$  be the number of edges on  $P(e)$ .

For any bipartition  $\pi$  of  $X$ , let  $e_i(\pi)$  denote the edge that induces  $\pi$  in  $T_i|_X$  for  $i \in \{1, 2\}$ . We define a weight function  $w : \Pi \rightarrow \mathbb{N}_{\geq 0}$  such that for any bipartition  $\pi$  of  $X$ ,  $w(\pi) = w(e_1(\pi)) + w(e_2(\pi))$ . If for any  $i \in \{1, 2\}$ , no  $e_i(\pi)$  induces  $\pi$  in  $T_i|_X$ , then we use  $w(e_i(\pi)) = 0$ . Therefore, for any  $\pi \notin C(T_1|_X) \cup C(T_2|_X)$ ,  $w(\pi) = 0$ . For any set  $F$  of bipartitions,  $w(F) = \sum_{\pi \in F} w(\pi)$ .

For each  $i \in \{1, 2\}$  and each  $e \in E(T_i|_X)$ , let  $\text{In}(e)$  be the set of internal nodes of  $P(e)$ . For each  $v \in \text{In}(e)$ , let  $L(v)$  be the set of leaves in  $S_i \setminus X$  whose connecting path to the backbone tree  $T_i|_X$  goes through  $v$  and let  $T(v)$  be the minimal subtree spanning  $L(v)$  in  $T_i$ . We say  $T(v)$  is an extra subtree attached to  $v$ . Consider  $T(v)$  rooted at the node  $u$  which is the neighbor of  $v$  in  $T(v)$ . Let  $\mathcal{T}(e) := \{T(v) \mid v \in \text{In}(e)\}$ . Then  $\mathcal{T}(e)$  is the set of extra subtrees attached to internal nodes of  $P(e)$  in  $T_i$ . We note that  $|\mathcal{T}(e)| = |\text{In}(e)| = w(e) - 1$ . For any bipartition  $\pi \in C(T_1|_X) \cup C(T_2|_X)$ , we denote  $\mathcal{T}(\pi) := \mathcal{T}(e_1(\pi)) \cup \mathcal{T}(e_2(\pi))$ . Let  $\text{Extra}(T_i) := \bigcup_{e \in E(T_i|_X)} \mathcal{T}(e)$ . Then  $\text{Extra} := \text{Extra}(T_1) \cup \text{Extra}(T_2)$  denotes the set of all extra subtrees in  $T_1$  and  $T_2$ .

[figure to help](#)

[add intuition/overview for algorithm](#)

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#### Algorithm 1 Max-BiSup Supertree

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**Input:** two fully resolved trees  $T_1, T_2$  with leaf sets  $S_1$  and  $S_2$  where  $S_1 \cap S_2 = X \neq \emptyset$   
**Output:** a fully resolved supertree  $T$  on leaf set  $S = S_1 \cup S_2$  that maximizes the support score

- 1: compute  $C(T_1|_X)$  and  $C(T_2|_X)$
- 2: **for** each  $\pi \in C(T_1|_X) \cup C(T_2|_X)$  **do**
- 3:   compute  $\mathcal{T}(e_1(\pi)), \mathcal{T}(e_2(\pi)), \mathcal{T}(\pi)$  and  $w(\pi)$
- 4: construct  $T$  by having a star of leaf set  $X$  with center vertex  $\hat{v}$  and connecting the root of each  $t \in \text{Extra}$  to  $\hat{v}$ , let  $\tilde{T} = T$
- 5: **for** each  $\pi \in \text{Triv}$  **do**
- 6:    $T \leftarrow \text{Refine-Triv}(T_1, T_2, T, \pi, \hat{v}, \mathcal{T})$
- 7: let  $\tilde{T} = T$
- 8: construct the incompatibility graph  $G = (V_1 \cup V_2, E)$ , where  $V_1 = C(T_1|_X) - C(T_2|_X)$  and  $V_2 = C(T_2|_X) - C(T_1|_X)$ , and  $E = \{(\pi, \pi') \mid \pi \in V_1, \pi' \in V_2, \pi \text{ is not compatible with } \pi'\}$
- 9: compute the maximum weight independent set  $I$  in  $G$  with weight  $w$
- 10: let  $H(\hat{v}) = \text{NonTriv} \cap (C(T_1|_X) \cup C(T_2|_X))$
- 11: **for** each  $\pi \in \text{NonTriv} \cap (C(T_1|_X) \cup C(T_2|_X))$  **do**
- 12:    $sv(\pi) = \hat{v}$
- 13: **for** each  $\pi \in \text{NonTriv} \cap (I \cup (C(T_1|_X) \cap C(T_2|_X)))$  **do**
- 14:    $T \leftarrow \text{Refine}(T_1, T_2, T, \pi, H, sv, \mathcal{T})$
- 15: let  $T^* = T$
- 16: refine  $T$  arbitrarily at polytomies until it is fully resolved
- 17: return  $T$

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#### Algorithm 2 Refine-Triv

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**Input:** two trees  $T_1, T_2$  with leaf sets  $S_1$  and  $S_2$  where  $S_1 \cap S_2 = X \neq \emptyset$ , an unrooted tree  $T$  on leaf set  $S = S_1 \cup S_2$ , a trivial bipartition  $\pi = A|B$  of  $X$ , a vertex  $\hat{v} \in V(T)$ , a dictionary  $\mathcal{T}$   
**Output:** an tree  $T'$  which is a refinement of  $T$  such that  $\pi \in C(T'|_X)$

- 1: detach all extra subtrees in  $\mathcal{T}(\pi)$  from  $\hat{v}$  and attach them onto  $(\hat{v}, a)$  such that the subtrees from  $\mathcal{T}(e_1(\pi))$  and subtrees from  $\mathcal{T}(e_2(\pi))$  are side by side and each group respects the ordering of subtrees in  $T_i$
- 2: return the resulting tree  $T'$

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For the analysis of the algorithm, we differentiate between two kinds of bipartitions in  $C(T_1) \cup C(T_2)$ . Let  $\Pi_Y = \{\pi = A|B \in C(T_1) \cup C(T_2) \mid \text{either } A \cap X =$

**Algorithm 3** Refine

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**Input:** two trees  $T_1, T_2$  with leaf sets  $S_1$  and  $S_2$  where  $S_1 \cap S_2 = X \neq \emptyset$ , an unrooted tree  $T$  on leaf set  $S = S_1 \cup S_2$ , a bipartition  $\pi = A|B$  of  $X$ , a dictionary  $H$ , a dictionary  $sv$ , a dictionary  $\mathcal{T}$

**Output:** an tree  $T'$  which is a refinement of  $T$  such that  $\pi \in C(T'|_X)$

- 1:  $v \leftarrow sv(\pi)$
- 2: compute  $N_A := \{u \in N_T(v) \mid \exists a \in A \text{ such that } u \text{ can reach } a \text{ in } T - v\}$  and  $N_B := \{u \in N_T(v) \mid \exists b \in B \text{ such that } u \text{ can reach } b \text{ in } T - v\}$ .
- 3:  $V(T) \leftarrow V(T) \cup \{v_a, v_b\}$ ,  $E(T) \leftarrow E(T) \cup \{(v_a, v_b)\}$
- 4:  $H(v_a) \leftarrow \emptyset, H(v_b) \leftarrow \emptyset$
- 5: **for** each  $u \in N_A \cup N_B$  **do**
- 6:   **if**  $u \in N_A$  **then** connect  $u$  to  $v_a$
- 7:   **else** connect  $u$  to  $v_b$
- 8: detach all extra subtrees in  $\mathcal{T}(\pi)$  from  $v$  and attach them onto  $(v_a, v_b)$  such that the subtrees from  $\mathcal{T}(e_1(\pi))$  and subtrees from  $\mathcal{T}(e_2(\pi))$  are side by side and each group respects the ordering of subtrees in  $T_i$
- 9: **for** each bipartition  $\pi' = A'|B' \in H(v)$  such that  $\pi' \neq \pi$  **do**
- 10:   detach all extra subtrees in  $\mathcal{T}(\pi')$  from  $v$
- 11:   **if**  $A' \subseteq A$  or  $B' \subseteq A$  **then**
- 12:      $sv(\pi') = v_a$  and  $H(v_a) \leftarrow H(v_a) + \pi'$
- 13:     attach all extra subtrees in  $\mathcal{T}(\pi')$  to  $v_a$
- 14:   **else if**  $A' \subseteq B$  or  $B' \subseteq B$  **then**
- 15:      $sv(\pi') = v_b$  and  $H(v_b) \leftarrow H(v_b) + \pi'$
- 16:     attach all extra subtrees in  $\mathcal{T}(\pi')$  to  $v_b$
- 17:   **else**
- 18:     discard  $\pi'$  and attach all extra subtrees in  $\mathcal{T}(\pi')$  to either  $v_a$  or  $v_b$
- 19: **for** each remaining extra subtree attached to  $v$  **do**
- 20:   detach it from  $v$  and attach it to either  $v_a$  or  $v_b$
- 21: delete  $v$  and incident edges from  $T$
- 22: return the resulting tree  $T'$

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$\emptyset$ , or  $B \cap X = \emptyset$ . Let  $\Pi_X = \{\pi = A|B \in C(T_1) \cup C(T_2) \mid A \cap X \neq \emptyset \text{ and } B \cap X \neq \emptyset\}$ . Intuitively,  $\Pi_X$  is the set of bipartitions in  $C(T_1) \cup C(T_2)$  that are induced by edges in the backbone trees  $T_1|_X$  and  $T_2|_X$  while  $\Pi_Y$  is the set of bipartitions in  $C(T_1) \cup C(T_2)$  that are induced by edges inside extra subtrees or connecting extra subtrees to the backbone trees.

Let  $p_X(T)$  and  $p_Y(T)$  (we omit the parameters  $T_1$  and  $T_2$  for brevity) be the contributions to the support score of  $T$  from bipartitions of  $\Pi_X$  and  $\Pi_Y$  for any  $T \in \mathcal{T}_S$ , respectively. Formally, we have

$$p_X(T) = |C(T|_{S_1}) \cap C(T_1) \cap \Pi_X| + |C(T|_{S_2}) \cap C(T_2) \cap \Pi_X|,$$

$$p_Y(T) = |C(T|_{S_1}) \cap C(T_1) \cap \Pi_Y| + |C(T|_{S_2}) \cap C(T_2) \cap \Pi_Y|.$$

**Claim 1** *If Algorithm 1 returns a tree  $T$  such that  $p_X(T) \geq p_X(T')$  and  $p_Y(T) \geq p_Y(T')$  for any tree  $T'$  with leaf set  $S$ , then Algorithm 1 solves MAX-BISUP-SUPERTREE-2 correctly.*

*Proof* By definition of support score, any bipartition can only contribute to the support score if it is in  $C(T_1) \cup C(T_2)$ . It follows by definition of  $\Pi_X$  and  $\Pi_Y$  that  $\Pi_X$  and  $\Pi_Y$  is a disjoint decomposition of  $C(T_1) \cup C(T_2)$ . Thus, the support score of  $T$  equals  $p_X(T) + p_Y(T)$  for any tree  $T$  on leaf set  $S$ . Then if  $p_X(T) \geq p_X(T')$  and  $p_Y(T) \geq p_Y(T')$  for any tree  $T'$  with leaf set  $S$ ,  $T$  achieves the maximum support score among all trees of leaf set  $S$ , in particular, it achieves the maximum support score among all trees in  $\mathcal{T}_S$ .  $\square$

Therefore, it is enough for us to show that Algorithm 1 finds a tree  $T$  that maximizes both  $p_X(T)$  and  $p_Y(T)$  at the same time.

**Lemma 2** *For any tree  $T$  of leaf set  $S$  and any refinement  $T'$  of  $T$ ,  $p_X(T') \geq p_X(T)$  and  $p_Y(T') \geq p_Y(T)$ .*

*Proof* Since  $T'$  is an refinement of  $T$ ,  $C(T|_{S_i}) \subseteq C(T'|_{S_i})$  for any  $i \in \{1, 2\}$ . Therefore,  $|C(T|_{S_i}) \cap C(T_i) \cap \Pi_X| \leq |C(T'|_{S_i}) \cap C(T_i) \cap \Pi_X|$  for any  $i \in \{1, 2\}$ , and thus  $p_X(T) \leq p_X(T')$ . Similarly,  $|C(T|_{S_i}) \cap C(T_i) \cap \Pi_Y| \leq |C(T'|_{S_i}) \cap C(T_i) \cap \Pi_Y|$  for any  $i \in \{1, 2\}$ , and thus  $p_Y(T) \leq p_Y(T')$ .  $\square$

**Lemma 3** *For any tree  $T$  of leaf set  $S$ ,  $p_Y(T) \leq |\Pi_Y|$ . In particular, let  $\hat{T}$  be the tree constructed in Algorithm 1. Then,  $p_Y(\hat{T}) = |\Pi_Y|$ .*

*Proof* Since  $T_1$  and  $T_2$  has different leaf sets,  $C(T_1)$  and  $C(T_2)$  are disjoint. Since  $\Pi_Y \subseteq C(T_1) \cup C(T_2)$ ,  $C(T_1) \cap \Pi_Y$  and  $C(T_2) \cap \Pi_Y$  forms a disjoint decomposition of  $\Pi_Y$ . By definition of  $p_Y(\cdot)$ , for any tree  $T$  of leaf set  $S$ ,

$$\begin{aligned} p_Y(T) &= |C(T|_{S_1}) \cap C(T_1) \cap \Pi_Y| + |C(T|_{S_2}) \cap C(T_2) \cap \Pi_Y| \\ &\leq |C(T_1) \cap \Pi_Y| + |C(T_2) \cap \Pi_Y| \\ &= |\Pi_Y|. \end{aligned}$$

Fix any  $\pi = A|B \in \Pi_Y$ . By definition of  $\Pi_Y$ , either  $A \cap X = \emptyset$  or  $B \cap X = \emptyset$ . Assume without loss of generality that  $A \cap X = \emptyset$ . If  $\pi \in C(T_1)$ , let  $e_1$  be the edge that induces  $\pi$  in  $T_1$ . Then  $A \subseteq S_1 \setminus X$ , which implies either  $e_1$  is an internal edge in an extra subtree in  $\text{Extra}(T_1)$ , or  $e_1$  connects one extra subtree in  $\text{Extra}(T_1)$  to the backbone  $T_1|_X$ . In either case, the construction of  $\hat{T}$  ensures that  $\pi \in C(\hat{T}|_{S_1})$ . Similarly if  $\pi \in C(T_2)$ , then  $\pi \in C(\hat{T}|_{S_2})$  by construction. Therefore, each bipartition  $\pi \in \Pi_Y$  contributes 1 to  $|C(\hat{T}|_{S_i}) \cap C(T_i) \cap \Pi_Y|$  for exactly one  $i \in \{1, 2\}$  and thus it contributes 1 to  $p_Y(\hat{T})$ . Hence,  $p_Y(\hat{T}) = |\Pi_Y|$ .  $\square$

**Claim 2** *Let  $\hat{T}$  be the tree constructed in Algorithm 1, then  $p_X(\hat{T}) = 2|X|$ .*

*Proof* Let the center of the star from which  $\hat{T}$  is constructed be the center of  $\hat{T}$ . For each  $v \in X$ , consider the bipartition  $\pi_v = \{v\} \mid S \setminus \{v\}$  induced by the edge that connects the leaf  $v$  to the center. It is easy to see that  $\pi_v|_{S_i} = \{v\} \mid S_i \setminus \{v\} \in C(T_i) \cap C(\hat{T}|_{S_i})$  for any  $i \in \{1, 2\}$  as  $\pi_v|_{S_i}$  is a trivial bipartition of  $S_i$  and must be present in any tree on leaf set  $S_i$ . We also know  $\pi_v|_{S_i} \in \Pi_X$  as  $\pi_v \in C(T_1) \cup C(T_2)$  and both sides of  $\pi_v$  has non-empty intersection with  $X$ . Thus,  $\pi_v|_{S_i} \in C(\hat{T}|_{S_i}) \cap C(T_i) \cap \Pi_X$  for any  $i \in \{1, 2\}$ . So for each  $v \in X$ ,  $\pi_v|_{S_1}$  and  $\pi_v|_{S_2}$  each contributes 1 to  $p_X(\hat{T})$ . Therefore,  $p_X(\hat{T}) \geq 2|X|$ .

Fix any bipartition  $\pi = A|B$  induced by any other edge of  $\hat{T}$  such that  $\pi|_{S_i} \in C(\hat{T}|_{S_i})$  for some  $i \in \{1, 2\}$ . By construction of  $\hat{T}$ , the edge inducing  $\pi$  is either inside an extra subtree or connecting the root of an extra subtree to the center

Therefore, either  $A \subseteq S \setminus X$  or  $B \subseteq S \setminus X$ , which implies  $\pi|_{S_i} \notin \Pi_X$  for any  $i \in \{1, 2\}$ . Hence, there is no other bipartition of  $\hat{T}$  such that when restrict to  $S_i$  contributes to  $p_X(\hat{T})$ . Therefore,  $p_X(\hat{T}) = 2|X|$ .  $\square$

**Lemma 4** *Let  $\pi = A|B$  be a bipartition of  $X$ . Let  $T$  be a tree of leaf set  $S$  such that  $\pi \notin C(T|_X)$  and all bipartitions in  $C(T|_X)$  are compatible with  $\pi$ . Let  $T'$  be a refinement of  $T$  such that for all  $\pi' \in C(T'|_{S_i}) \setminus C(T|_{S_i})$  for some  $i \in \{1, 2\}$ ,  $\pi'|_X = \pi$ . Then,  $p_X(T') - p_X(T) \leq w(\pi)$ .*

*Proof* By definition of  $p_X(\cdot)$ ,

$$\begin{aligned} & p_X(T') - p_X(T) \\ &= |C(T'|_{S_1}) \cap C(T_1) \cap \Pi_X| + |C(T'|_{S_2}) \cap C(T_2) \cap \Pi_X| \\ &\quad - (|C(T|_{S_1}) \cap C(T_1) \cap \Pi_X| + |C(T|_{S_2}) \cap C(T_2) \cap \Pi_X|) \\ &= |(C(T'|_{S_1}) \setminus C(T|_{S_1})) \cap C(T_1) \cap \Pi_X| + |(C(T'|_{S_2}) \setminus C(T|_{S_2})) \cap C(T_2) \cap \Pi_X| \\ &= \sum_{i=1,2} |(C(T'|_{S_i}) \setminus C(T|_{S_i})) \cap C(T_i) \cap \Pi_X|. \end{aligned}$$

Therefore, we only need to prove that  $\sum_{i=1,2} |(C(T'|_{S_i}) \setminus C(T|_{S_i})) \cap C(T_i) \cap \Pi_X| \leq w(\pi)$ . For any  $\pi' \in (C(T'|_{S_i}) \setminus C(T|_{S_i})) \cap C(T_i) \cap \Pi_X$  for any  $i \in \{1, 2\}$ , we have  $\pi'|_X = \pi$ .

We differentiate three different cases for the proof of the above statement: 1)  $\pi \notin C(T_1|_X) \cup C(T_2|_X)$ , 2)  $\pi \in C(T_1|_X) \Delta C(T_2|_X)$ , 3)  $\pi \in C(T_1|_X) \cap C(T_2|_X)$ .

Case 1): Let  $\pi \notin C(T_1|_X) \cup C(T_2|_X)$ . Since no edge induces  $\pi$  in  $T_1|_X$  or  $T_2|_X$ , we have  $w(\pi) = 0$ . Assume for contradiction that there exists a bipartition  $\pi' \in (C(T'|_{S_i}) \setminus C(T|_{S_i})) \cap C(T_i) \cap \Pi_X$  for some  $i \in \{1, 2\}$ . Since  $\pi \notin C(T_1|_X) \cup C(T_2|_X)$  and  $\pi'|_X = \pi$ , by Corollary 2,  $\pi' \notin C(T_i)$  for any  $i \in \{1, 2\}$ . This contradicts with the fact that  $\pi' \in C(T_i)$  for some  $i \in \{1, 2\}$ . Therefore, the assumption that there exists such a bipartition  $\pi'$  is wrong and  $\sum_{i=1,2} |(C(T'|_{S_i}) \setminus C(T|_{S_i})) \cap C(T_i) \cap \Pi_X| = 0 \leq w(\pi)$ .

Case 2): Let  $\pi \in C(T_1|_X) \Delta C(T_2|_X)$ . Assume without loss of generality that  $\pi \in C(T_1|_X) \setminus C(T_2|_X)$ . Then, we have  $w(\pi) = w(e_1)$ . Let  $\pi' \in (C(T'|_{S_i}) \setminus C(T|_{S_i})) \cap C(T_i) \cap \Pi_X$  for some  $i \in \{1, 2\}$ . Since  $\pi'|_X = \pi$  and  $\pi \notin C(T_2|_X)$ , by Corollary 2, we have  $\pi' \notin C(T_2)$ . Since  $\pi' \in C(T_i)$  for some  $i \in \{1, 2\}$ , it must be that  $\pi' \in C(T_1)$ . By Lemma 1, the edge which induces  $\pi'$  in  $T_1$  is an edge on  $P_1(e_1)$ . Since there are  $w(e_1)$  edges on  $P_1(e_1)$ , there are at most  $w(e_1)$  distinct such bipartitions  $\pi'$ s, and thus the statement is proved.

Case 3): Let  $\pi \in C(T_1|_X) \cap C(T_2|_X)$ . Then we have  $w(\pi) = w(e_1) + w(e_2)$ . Fix any  $\pi' \in (C(T'|_{S_1}) \setminus C(T|_{S_1})) \cap C(T_1) \cap \Pi_X$ . Since  $\pi' \in C(T_1)$  and  $\pi'|_X = \pi \in C(T_1|_X)$ , by Lemma 1, the edge  $e'$  that induces  $\pi'$  is an edge on  $P_1(e_1)$ . Recall that  $w(e_1) = |P_1(e_1)|$ , then we have  $|(C(T'|_{S_1}) \setminus C(T|_{S_1})) \cap C(T_1) \cap \Pi_X| \leq |P_1(e_1)| = w(e_1)$ . Similarly,  $|(C(T'|_{S_2}) \setminus C(T|_{S_2})) \cap C(T_2) \cap \Pi_X| \leq |P_2(e_2)| = w(e_2)$ . Therefore,  $\sum_{i=1,2} |(C(T'|_{S_i}) \setminus C(T|_{S_i})) \cap C(T_i) \cap \Pi_X| \leq w(\pi)$ .  $\square$

**Lemma 5** For any compatible set  $F$  of bipartitions of  $X$ , let  $T$  be a tree of leaf set  $S$  such that  $C(T|_X) = F$ . Then  $p_X(T) \leq \sum_{\pi \in F} w(\pi)$ .

*Proof* Fix an arbitrary ordering of bipartitions in  $F$  and let them be  $\pi_1, \pi_2, \dots, \pi_k$ , where  $k = |F|$ . Let  $F_i = \{\pi_1, \dots, \pi_i\}$  for any  $i \in \{0, 1, \dots, k\}$ . In particular,  $F_0 = \emptyset$  and  $F_k = F$ . Let  $T^i$  be obtained by contracting any edge  $e$  in  $T$  such that  $\pi_e \in \Pi_X$  and  $\pi_e|_X \notin F_i$ . Then  $C(T^i|_X) = F_i$ . In particular, we know  $C(T^0|_X) = \emptyset$ . By construction,  $T^i$  is a refinement of  $T^{i-1}$  for any  $i \in \{1, 2, \dots, k\}$  such that for any  $\pi' \in C(T^i) \setminus C(T^{i-1})$ ,  $\pi'|_X = \pi_i$ . Then by Lemma 4,  $p_X(T^i) - p_X(T^{i-1}) \leq w(\pi_i)$ . Therefore,

$$p_X(T) - p_X(T^0) = \sum_{i=1}^k p_X(T^i) - p_X(T^{i-1}) \leq \sum_{i=1}^k w(\pi_i).$$

We also know that  $p_X(T^0) = 0$  (expand on this) and thus  $p_X(T) \leq \sum_{\pi_i \in F} w(\pi_i)$  as desired.  $\square$

**Claim 3** Let  $\tilde{T}$  be the tree constructed in Algorithm 1, then  $p_X(\tilde{T}) = \sum_{\pi \in \text{Triv}} w(\pi)$ .

*Proof* Let  $\pi = a|B$  be a trivial bipartition of  $X$ . We know both  $e_1(\pi)$  and  $e_2(\pi)$  exist and abbreviate them by  $e_1$  and  $e_2$ . Consider all extra subtrees in  $\mathcal{T}(e_1)$  and index the extra subtrees as  $t_1, t_2, \dots, t_p$  such that  $t_1$  is the closest  $a$  in  $T_1$  and  $p = |\mathcal{T}(e_1)| = w(e_1) - 1$ . Similarly, index the extra subtrees in  $\mathcal{T}(e_2)$  to be  $t'_1, t'_2, \dots, t'_q$  such that  $t'_1$  is closest to  $a$  in  $T_2$  and  $q = |\mathcal{T}(e_2)| = w(e_2) - 1$ . For each  $k \in [w(e_1)]$ , we define

$$A_k := \bigcup_{i=1}^{k-1} L(t_i) \cup a, \quad \pi_k := A_k|S_1 \setminus A_k,$$

and for each  $k \in [w(e_2)]$ , we define

$$A'_k := \bigcup_{i=1}^{k-1} L(t'_i) \cup a, \quad \pi'_k := A'_k|S_2 \setminus A'_k.$$

It follows by definition that  $\pi_k$  for any  $k \in [w(e_1)]$  is the bipartition induced by the  $k$ th edge on  $P(e_1)$  in  $T_1$  numbered from the side of  $a$ , which implies  $\pi_k \in C(T_1)$  for any  $k \in [w(e_1)]$ . Similarly,  $\pi'_k \in C(T_2)$  for any  $k \in [w(e_2)]$ . In particular, we notice that  $\pi_1 = \pi'_1 = \pi$ . Clearly, all these bipartitions are also in  $\Pi_X$  because both sides have none empty intersection with  $X$ .

Since Algorithm 2 moves all extra subtrees in  $\mathcal{T}(\pi)$  onto the edge  $(\hat{v}, a)$  and orders them such that extra subtrees in  $\mathcal{T}(e_1)$  (and  $\mathcal{T}(e_2)$ , respectively) follows the order of trees within the group on  $T_1$  ( $T_2$ ), i.e.,  $t_1$  ( $t'_1$ ) is closest to  $a$  and  $t_p$  ( $t'_q$ ) is furthest away, it is easy to see that we also have  $\pi_k \in C(T|_{S_1})$  for any  $k \in [w(e_1)]$  and  $\pi'_k \in C(T|_{S_2})$  for any  $k \in [w(e_2)]$ , where  $T$  is the tree obtained after add  $\pi$  to the backbone through Algorithm 2. Therefore,  $|C(T|_{S_1}) \cap C(T_1|_X) \cap \Pi_X|$  is increased by  $w(e_1) - 1$  by the algorithm as  $\pi_k \notin C(T|_{S_1})$  before the algorithm for all  $k \in [w(e_1)]$  except

$k = 1$ . Similarly,  $|C(T|_{S_1}) \cap C(T_2|_X) \cap \Pi_X|$  is increased by  $w(e_2) - 1$ , so  $p_X(T)$  is increased by  $w(e_1) + w(e_2) - 2 = w(\pi) - 2$  by running Algorithm 2 on  $T$  and  $\pi$ . Since running Algorithm 2 to add other trivial bipartitions of  $X$  never destroys the bipartitions of  $S_1$  or  $S_2$  already in  $T$ , we have  $p_X(\hat{T}) = p_X(T) + \sum_{\pi \in \text{Triv}} (w(\pi) - 2) = 2|X| + \sum_{\pi \in \text{Triv}} (w(\pi) - 2) = \sum_{\pi \in \text{Triv}} w(\pi)$ .  $\square$

**Lemma 6** *Let  $T$  be a tree from Algorithm 1 before a refinement step. Let  $\pi = A|B \in \text{NonTriv} \cap (I \cup (C(T_1|_X) \cap C(T_2|_X)))$ . Let  $T'$  be a refinement of  $T$  obtained from running Algorithm 3 on  $T$  and  $\pi$ , with the auxiliary data structures  $H$ ,  $sv$ , and  $\mathcal{T}$ . Then,  $p_X(T') - p_X(T) = w(\pi)$ .*

*Proof* The algorithm makes sure that  $\pi \notin C(T|_X)$  and all bipartitions in  $C(T|_X)$  are compatible with  $\pi$   $\square$

Let  $G$  be the incompatibility graph defined in Algorithm 1 and  $I$  be the maximum weight independent set in  $G$  with weight function  $w$ . Let  $G' = (V'_1 \cup V'_2, E')$  be another incompatibility graph such that  $V'_1 = C(T_1|_X)$  and  $V'_2 = C(T_2|_X)$ , and  $E' = \{(\pi, \pi') \mid \pi \in V'_1, \pi' \in V'_2, \pi \text{ is not compatible with } \pi'\}$ . Let  $I' := I \cup (C(T_1|_X) \cap C(T_2|_X))$ .

**Claim 4**  *$I'$  is a maximum weight compatible subset of  $C(T_1|_X) \cup C(T_2|_X)$  with weight function  $w$ .*

*Proof* Since all bipartitions in  $C(T_1|_X)$  are compatible with each other and all bipartitions in  $C(T_2|_X)$  are compatible with each other, all bipartitions in  $C(T_1|_X) \cap C(T_2|_X)$  are compatible with all bipartitions in  $C(T_1|_X) \cup C(T_2|_X)$ . Therefore,  $C(T_1|_X) \cap C(T_2|_X)$  is a set of isolated vertices in  $G'$ . Since  $V \setminus V' = C(T_1|_X) \cap C(T_2|_X)$ , we know that  $G'$  is just  $G$  with extra isolated vertices. Therefore, it is easy to see that  $I'$  is a maximum weight independent set in  $G'$ . Since  $G'$  is the full incompatibility graph on  $V' = C(T_1|_X) \cup C(T_2|_X)$ ,  $I'$  corresponds to a maximum weight compatible subset of  $C(T_1|_X) \cup C(T_2|_X)$ .  $\square$

**Claim 5** *Let  $T^*$  be the tree defined in Algorithm 1,  $p_X(T^*) \geq p_X(T)$  for any tree  $T$  of leafset  $S$ .*

*Proof* Let  $T$  be any tree of leaf set  $S$ . Let  $F = C(T|_X)$ . Then by Lemma 5,  $p_X(T) \leq \sum_{\pi \in F} w(\pi) = \sum_{F \cap (C(T_1|_X) \cup C(T_2|_X))} w(\pi)$ . The equality follows from that  $w(\pi) = 0$  for any  $\pi \notin C(T_1|_X) \cup C(T_2|_X)$ . Since  $F \cap (C(T_1|_X) \cup C(T_2|_X))$  is a compatible subset of  $C(T_1|_X) \cup C(T_2|_X)$ ,  $w(F \cap (C(T_1|_X) \cup C(T_2|_X))) \leq w(I')$  by Claim 4. We also know by Claim 3 and Lemma 6,  $p_X(T^*) = \sum_{\pi \in I} w(\pi) + \sum_{\pi \in (C(T_1|_X) \cap C(T_2|_X))} w(\pi) = w(I')$ . Therefore,  $p_X(T) \leq w(I') = p_X(T^*)$ .  $\square$

**Theorem 2** *Algorithm 1 correctly solves MAX-BISUP-SUPERTREE-2 in  $O(n^3)$  (Checking this) time.*

*Proof* From Lemma 3 and Claim 5 and Lemma 2, we know that  $T^*$  defined in Algorithm 1 satisfy that  $p_X(T^*) \geq p_X(T)$  and  $p_Y(T^*) \geq p_Y(T)$  for any tree with leaf set  $S$ . Then by Claim 1, Algorithm 1 correctly solves MAX-BISUP-SUPERTREE-2. Next we analyze the running time of Algorithm 1.  $\square$



## 2.4 Hardness for MAX-BISUP-SUPERTREE-3

In this subsection, we show that MAX-BISUP-SUPERTREE- $N$  is NP-hard even when  $N = 3$ . We reduce the maximum weight independent set problem on tripartite graphs to MAX-BISUP-SUPERTREE-3. We first reproduce the theorem that proves the maximum weight independent set problem on tripartite graphs to be NP-hard.

**Theorem 3** MAX-BISUP-SUPERTREE-3 is NP-hard.

## Appendix A: Proofs from Section 2

Proof of Lemma 1

*Proof* Let  $T_R$  be the minimal subtree of  $T$  that spans  $R$ . It follows that the leaf set of  $T_R$  is  $R$  and  $T|_R$  is obtained from  $T_R$  by suppressing all degree-two nodes. Let  $\pi' = A'|B'$ . By definition of  $e$  inducing  $\pi = A|B$ , the vertices of  $A$  are all disconnected from vertices of  $B$  in  $T - e$ . If  $R \cap A \neq \emptyset$  and  $R \cap B \neq \emptyset$ , then  $e$  is necessary to connect  $R \cap A$  with  $R \cap B$ , and thus  $e$  must be in any tree spanning  $R$  and in particular  $e \in E(T_R)$ . Since  $T_R$  is a subgraph of  $T$ , the two components in  $T_R - e$  are subgraphs of the two components in  $T - e$ . Thus, the leaves of the two components in  $T_R - e$  are exactly  $R \cap A$  and  $R \cap B$ . We also know that suppressing degree-two nodes does not change the connectivity between any leaves so the leaves of the two components in  $T_R - P(e')$  (with vertices on the path also deleted) are the same as the leaves of the two components in  $T|_R - e'$ , which are  $A'$  and  $B'$ . If  $e \in P(e')$ , since all internal nodes of  $P(e')$  have degree two with both incident edges on  $P(e')$ , there is no leaf which exists in any of the two components in  $T_R - e$  but does not exist in the corresponding component in  $T_R - P(e')$ . Therefore,  $\pi|_R = R \cap A|R \cap B = A'|B' = \pi'$ . If  $e \notin P(e')$ , then since  $e \in E(T_R)$ , there must exist  $e'' \in E(T|_R)$  such that  $e'' \neq e'$  and  $e \in P(e'')$ . By the argument above,  $\pi|_R = \pi''$  where  $\pi''$  is the bipartition induced by  $e''$  in  $T|_R$ . Since  $e'' \neq e'$ , we know  $\pi' \neq \pi''$  and thus  $\pi|_R \neq \pi'$ . This concludes our proof that  $\pi|_R = \pi'$  if and only if  $e \in P(e')$ .  $\square$

### Competing interests

The authors declare that they have no competing interests.

### Author's contributions

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### Acknowledgements

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### Figures

**Figure 1** Sample figure title. A short description of the figure content should go here.

**Figure 2** Sample figure title. Figure legend text.

**Table 1** Sample table title. This is where the description of the table should go.

	B1	B2	B3
A1	0.1	0.2	0.3
A2	...	..	.
A3	..	.	.

**Tables**

**Additional Files**

Additional file 1 — Sample additional file title

Additional file descriptions text (including details of how to view the file, if it is in a non-standard format or the file extension). This might refer to a multi-page table or a figure.

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