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碩士論文

Department of Computer Science and Information Engineering College of Electrical Engineering and Computer Science National Taiwan University

**Master Thesis** 

一個相容超樹問題的改進演算法

An Improved Algorithm for Compatible Supertree Problem



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摘要

在演化生物學中,尋找超樹是個重要的主題。一棵半標籤樹T 是一個有以下特性的 樹:(1)每個T 的頂點可以有零到多個標籤;(2)每個標籤在T 裡只出現一次;(3)所有 的樹葉與無分叉的頂點都至少有一個標籤。如果滿足以下性質,則稱半標籤樹T 遠祖 顯示另一棵半標籤樹T':(1)如果x 在T'裡是y 的祖先,則x 在T 裡仍是y 的祖先;(2) 各自來說,如果在T'之中,x,y 不在從樹根到y,x 的路徑上,則各自來說x,y 在T 之 中不會在從樹根到y,x 的路徑上。一個排名半標籤樹T 是一棵在每個頂點上都有一個 排名值的半標籤樹。如果u 是v 的祖先,則u 的排名會比v 的排名小。如果滿足以下 條件,則稱排名半標籤樹T 保存一個相對分歧時刻div(L) < div(L'): lca(L) 的排名小 於lca(L') 的排名。其中L 及L' 是兩個標籤集合, lca(L) 則是那些標籤所在頂點的最接 近共同祖先。

我們提出一個在O(h log<sup>2</sup> h) 時間與O(h) 空間內找到一個排名半標籤樹的演算法, 此樹遠祖顯示輸入的一組半標籤樹P與一組相對分歧時刻D。其中h是P中每棵樹的標 籤數目總和加上D中每個相對分歧時刻中的標籤數目總和。

#### Abstract

Finding supertrees is critical in evolutionary biology. A semi-labeled tree T is a rooted tree satisfies the following: (1) each node in  $\mathcal{T}$  has zero to multiple labels, (2) each label in  $\mathcal{T}$  appears only once, and (3) all leaves and non-branching internal nodes have at least one label. A semi-labeled tree  $\mathcal{T}$  ancestrally displays another semilabeled tree  $\mathcal{T}'$  if the following are satisfied: (1) if x is an ancestor of y in  $\mathcal{T}'$ , then x is an ancestor of y in T; and (2) if x, y are not on the path from root to y, x in T', respectively, then x, y are not on the path from root to y, x, respectively. A ranked semi-labeled tree  $\mathcal{T}$  is a semi-labeled tree with one rank on each node, and if u is an ancestor of v, then the rank of u is smaller than the rank of v. A ranked semi-labeled tree  $\mathcal{T}$  preserves a relative divergence date div(L) < div(L') where L and L' are two set of labels, if the rank of lca(L) is smaller than the rank of lca(L') where lca(L) is the least common ancestor of the vertices which the labels  $l \in L$  is on. We show a  $O(m \log^2 m)$ -time and O(m)-space algorithm to find a ranked semi-labeled tree which ancestrally displays a set P of semi-labeled trees and preserves a set D of relative divergence dates, where mis the sum of the number of labels in each trees in P and of labels in L and L' in each relative divergence dates in D.

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## **Chapter 1**

# Introduction

Finding supertrees is critical in evolutionary biology [3]. This paper focuses on the following TREE COMPATIBILITY problem defined by Bordewich, Evans, and Semple [4] which integrates smaller evolutionary trees with additional labels on internal nodes and the relative orders of two divergence events into one evolutionary tree. A label on an internal node of a evolutionary tree may represent a taxon at higher taxonomic level than all its descendants [9]. The relative orders of divergence events can be collected from fossil data or molecular dating techniques [5].

Unless specified, all the trees are rooted and directed from root to leaves, and we use a vertex and the labels on the vertex interchangeably. The label set of a structure S, denoted L(S), is the set of all labels in it.

For any set S, let |S| denote the cardinality of S.

### **1.1 Problem definition**

Let *T* be a rooted tree. Each node *v* of *T* is associated with a set  $L_T(v)$  of labels, where  $L_T(v)$  is allowed to be empty. Let  $L_T$  denote the union of  $L_T(v)$  over all nodes *v* of *T*. We say that *T* is a *semi-labeled tree* if both of the following conditions hold.

- *Condition C1:*  $L_T(u) \cap L_T(v) = \emptyset$  holds for any two distinct nodes u and v of T.
- *Condition C2:*  $L_T(u)$  is not empty for each node u that has at most one child in T.

By Condition C1, we can specify a node u with nonempty  $L_T(u)$  by any label in  $L_T(u)$ . For any two distinct nodes u and v of T, we say that u is an *ancestor* of v if u belongs to the path of T between v and the root of T. For any semi-labeled tree T, define

$$D(T) = \{(a, b) \mid a, b \in L_T, a \text{ is an ancestor of } b \text{ in } T\};$$
  

$$N(T) = \{\{a, b\} \mid a, b \in L_T, a \text{ and } b \text{ are unrelated in } T\}.$$

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For any two semi-labeled trees T and T', we say that T ancestrally displays T' if  $D(T') \subseteq D(T)$  and  $N(T') \subseteq N(T)$  [8]. A function r from the nodes of T to non-negative integers is a rank of T if r(u) < r(v) holds for any nodes u and v such that u is an ancestor of v in T [5]. A relative divergence date on T is a constraint of in the form div(L) < div(L'), where L and L' are nonempty subsets of  $L_T$ .

A tree T with rank function r preserves a relative divergence date div(L) < div(L') if

$$r(lca_T(L)) < r(lca_T(L'))$$

Given a set P of rooted semi-labeled tree and a set D of relative divergence dates, the TREE COMPATIBILITY problem, defined in [4] seeks a ranked semi-labeled tree



Figure 1.1: A ranked semi-labeled tree in (b) ancestrally displays rooted semi-labeled trees and preserves relative divergence dates in (a).

which ancestrally displays *P* and preserves *D*, or reports "incompatible" if no such tree exists.

The ranked semi-labeled tree in figure 1.1b ancestrally displays all rooted semilabeled trees and preserves all relative divergence dates in figure 1.1a.

The best result is  $O(n^3m^3)$  time and  $O(n^2m^2)$  space with  $n = |L(P) \cup L(D)|$ , and m = |P| + |D| by Bordewich, Evans, and Semple [4]. And for each relative divergence dates in the form div(S) < div(S'), the size of S and S' are limited to 2 in their algorithm. Moreover, all compatible trees can be enumerated in the same work. [4]

In this work, we reduce the time and space complexity of TREE COMPATIBILITY with a constraint graph based algorithm in the following time and space bound.

**Theorem 1.1.** Given a set P of rooted semi-labeled trees and a set D of relative divergence dates, a ranked semi-labeled tree  $(\mathcal{T}, r)$  which ancestrally displays P and preserves D can be built in  $O(h \log^2 h)$  time with O(h) space if such tree exists, or the incompatibility can be

detected in the same bound if not. And h = ||P|| + ||D|| where  $||P|| = \sum |L(\mathcal{T})|$  for  $\mathcal{T} \in P$ and  $||D|| = \sum |L(r)|$  for  $r \in D$ .

The previous best result is  $O(n^3m^3)$  time and  $O(n^2m^2)$  space, by applying the techniques in [2], it is not hard to acquire a  $O(n^2m^2\log^2 nm)$  time and  $O(n^2m^2)$  space algorithm with  $n = |L(P) \cup L(D)|$ , and m = |P| + |D|. Our work further reduce the time to  $O(nm\log^2 nm)$  and space to O(nm). While in our notations, the previous best result becomes  $O(h^2\log^2 h)$  time and  $O(h^2)$  space with h = ||P|| + ||D||.

Moreover, our result has the following additional features.

- 1. The ordering property. An algorithm satisfies *ordering property* if with the permutation of input trees as new input, the output tree will be the same one. [20]
- 2. The renaming property. An algorithm satisfies *renaming property* if with renamed labels as new input, the output tree will be the same one with labels renamed accordingly. [20]
- Optional compact form of relative divergence date. The relative divergence date in the form div(S, x) < div(S', x') with x, x' ∈ {0, 1} represents all relative divergence dates in the form div(s) < div(s') for any subset s ∈ S and s' ∈ S' with s = max{x|S|,1} and s' = max{x'|S'|,1}.</li>

### 1.2 Related work

**Descending from BUILD.** A stream of long developing supertree methods started from applying BUILD algorithm [1] in this domain [6, 7, 14, 18, 19]. The input rooted semi-labeled trees are labeled only on leaves and singularly-labeled. A tree is *singularly-labeled* if each node has at most one label. The BUILD algorithm uses O(Nn) time, and

Henzinger [12] cut its complexity down to  $min\{O(Nn^{1/2}), O(N + n^2 \log n)\}$  with N the number of vertices and n the number of distinct labels. The MINCUTSUPERTREE [17] algorithm and its modified versions [15] improved BUILD to solve incompatible data set with weights on each tree.

In successive works, the input was then expanded in two ways: one is the inclusion of non-tree constraints, and the other is allowing labels for internal vertices.

The inclusion of relative divergence dates. In RANKEDTREE algorithm [5], the input is a set D of relative divergence dates. It outputs a rooted semi-labeled tree with rank. The input rooted semi-labeled trees are labeled only on leaves and singularly-labeled. It runs in  $O(|D| + n^3)$  time where n = |L(D)|.

The inclusion of rooted semi-labeled trees. In ANCESTRALBUILD algorithm [8], the input is a set of rooted semi-labeled trees. And the output tree ancestrally displays all the trees in input. It runs in  $O(t^2n^3)$  where t is the number of trees and n is the number of taxa [2]. When the input trees are all singularly-labeled, the ANCESTRAL-BUILD\* algorithm [2] cut down the complexity to  $O(\log^2 n \cdot (\sum_{T_i \in P} \sum_{u \in I(T_i)} d(u)^2))$  for n = |L(P)| and I(T) is the set of all internal nodes in tree T. For other variants of ANCESTRALBUILD with singularly-labeled trees, NESTEDSUPERTREE [9] solves the rest types of incompatible inputs, after excluding pairwise inconsistent and ancestor-descendant contradiction. The input P is *pairwise inconsistent* if there exists two labels  $x, y \in L(P), x$  is a strict ancestor of y in a tree but x is not strict ancestor of y in some tree T with  $\{x, y\} \subseteq L(T)$ . P is *ancestor-descendant contradiction* if there is a directed loop in G where V(G) = L(P) and  $E(G) = \{(x, y) : x \in L(u), y \in L(v), (u, v) \in T, T \in P\}$ .

And MINEDGEWEIGHTTREE [9], a variant of NESTEDSUPERTREE, allows weighted

trees and can be modified easily to have flexible weighting functions on either edges or labels.

**The applications.** For applications, ANCESTRALBUILD, its variants, and RANKEDTREE are demonstrated on real data or used in [11, 16].

The approaches of RANKEDTREE and ANCESTRALBUILD are combined in the TREE COMPATIBILITY problem [4]. It takes a set P of ranked semi-labeled trees and a set D of relative divergence dates as input, and then rejects incompatible input, or output a ranked semi-labeled tree if input is compatible. The algorithms BUILDPLUS [4] solve this problem in cubic time  $O((nm)^3)$  where n is the number of labels in input and m is the number of trees plus the number of relative divergence dates [4]. ALLBUILDPLUS [4] in the same work output all compatible trees.

## 1.3 Roadmap

The TREE COMPATIBILITY problem is reduced to the CONSTRAINT GRAPH COMPAT-IBILITY problem in Section 2, the CONSTRAINT GRAPH COMPATIBILITY problem is solved in Section 3, and our result is proved in Section 4.

## **Chapter 2**

# **Preliminary**

The TREE COMPATIBILITY and CONSTRAINT GRAPH COMPATIBILITY problem are abbreviated to TC and GC, respectively.

For a graph G, let C(G) be the connected components of G. For a connected component  $C \in C(G)$ , if, after the removal of a set of vertices in C, C becomes a set of connected components C, let C be the *children* of C, denoted *child*(C). And let the *main* connected component, denoted M(C), be an arbitrarily chosen connected component  $C' \in C$  with  $|E(C')| \ge |E(C'')|$  for  $C'' \in C$  and the *new* connected component, denoted N(C), be  $C \setminus M(C)$  where C = child(C).

## 2.1 Generalization of input tree

A ranked semi-labeled tree is *fully-labeled* if each node has at least one label. A fully-labeled semi-labeled tree is called *fully-labeled* tree.

**Lemma 2.1.** Let *P* and *D* be the input of *TC*. Without loss of generality, *P* can be assumed as fully-labeled and with a common root  $\rho \notin L(D)$ .

### 2.2 Decremental connectivity problem

Let G = (V, E) be an undirected graph. The DECREMENTAL CONNECTIVITY PROB-LEM maintains G with the operation of edge removal, and the query of whether two vertices are connected.

**Lemma 2.2** (Holm et al. [13], Thorup [21]). The DECREMENTAL CONNECTIVITY PROB-LEM can be solved in  $O(m \log^2 n + p \log n / \log \log n)$  and O(m) space with p queries, where n = |V|, m = |E|.

## 2.3 The batch deletion problem

For a graph *G* supporting the operation of vertex set removal with all vertices removed are in the same component, let *W* be a *component graph* data structure, if *W* is a data structure with respect to *G* maintaining a property of *G*, and after the removal of a vertex set, *G* becomes *G'*. the property of *G* remains maintained if the update function U(x) of *W* are called for each  $x \in C$ , some  $C \in C(G)$ .

W has partial update property if

- 1. *W* is initially maintained.
- 2. *W* is maintained, if, after a connected component  $C \in C(G)$  becomes its children C by removal of some vertices S in V(C), the following is satisfied,
- For each connected component C' ∈ C ∪ S except an arbitrary one C'' ∈ C, C' is updated by the following:
- 4. The update function provided by W is called for all vertices in C'.

**Lemma 2.3** (Even et al. [10], Henzinger et al. [12], and Berry et al. [2]). For a component graph data structure W with respect to G and update function U(x), and W has the partial update property, if the DECREMENTAL CONNECTIVITY PROBLEM can be solved in T(n,m,p) time and S(n,m,p) space with G and p queries, then W is maintained by calling U(x) at most  $O(\log n)$  times for each  $x \in V(G)$  with total  $O(m \log n + T(n,m,m))$  time and O(m + S(n,m,m)) space where n,m are the number of vertices and edges in G, respectively.



## **Chapter 3**

# **The BUILDPLUS Algorithm**

Since our improvement is based on the BUILDPLUS algorithm [4], we describe it first.

## 3.1 Terms

For a vertex x and a structure G, let  $indegree_G(x)$  and  $outdegree_G(x)$ , denote the indegree and outdegree of x in G, respectively.

## 3.2 A Reduction

#### 3.2.1 Constraint Graph

A constraint graph  $\mathcal{G} = (G, \phi, Q, R)$  consists of

- 1. a directed graph *G*,
- 2. a coloring function  $\phi: V(G) \rightarrow \{blue, aqua\},\$
- 3. a directed graph *Q*, and

4. a directed graph R,

where  $L(G), V_a(G)$  are the set of blue and aqua vertices in G, respectively.

Let  $L(Q) = L(G) \cap V(Q)$ ,  $L(R) = L(G) \cap V(R)$ , and  $V_a(R) = V_a(G) \cap V(R)$ .

In G, for an aqua vertex  $a \in V_a(G)$ ,  $indegree_G(a) = 0$ .

In Q, V(Q) = L(Q) = L(G), and E(Q) are called *red edges*.

In R,  $V(R) = L(G) \cup V_a(G)$ . For a blue vertex  $b \in L(R)$ ,  $indegree_R(b) = 0$ . For  $a \in V_a(R)$ ,  $outdegree_R(a) = 0$ .

*Remark* 3.1. The edges in graphs G,Q, and R are constraints. A vertex with indegree 0 in all graphs can be removed in the iteration of BUILDPLUS, and the removed vertices becomes node in output tree.

### 3.2.2 The constraint graph compatibility problem

A ranked semi-labeled tree  $\mathcal{T}$  *displays* a constraint graph  $\mathcal{G} = (G, \phi, Q, R)$ , if

- 1. L(T) = L(G).
- 2. For two labels x, y with a directed path from x to y in G, x is an ancestor of y in  $\mathcal{T}$ .
- For an edge (x, y) ∈ L(Q), x, y are not on the path from root to y, x in T, respectively.
- 4. For an aqua vertex a, let  $L = \{x \in L(R) : (x, a) \in E(R)\}$ , and  $L' = \{y \in G : (a, y) \in E(G)\}$ . We have rank(lca(L)) < rank(lca(L')) in  $\mathcal{T}$ .

The CONSTRAINT GRAPH COMPATIBILITY problem,  $\mathcal{GC}$  for short, try to find a ranked semi-labeled tree  $\mathcal{T}$  displays the input constraint graph  $\mathcal{G} = (G, \phi, Q, R)$ , or

output "incompatible" if not, where all  $v \in V(G)$  are all in the same core.

#### 3.2.3 The Reduction

**Lemma 3.2.** [Bordewich et al. [4]] The TREE COMPATIBILITY problem can be reduced to CONSTRAINT GRAPH COMPATIBILITY problem. Given an instance of CONSTRAINT GRAPH COMPATIBILITY problem, a constraint graph  $\mathcal{G}$  which is reduced from P and D, the instance of TREE COMPATIBILITY, if CONSTRAINT GRAPH COMPATIBILITY returns a ranked hierarchy  $\mathcal{H}$ , then  $\mathcal{H}$  ancestrally displays P and preserves D.

The reduction is described as following:

- 1. Let  $L(G) = L(Q) = L(R) = L(P) \cup L(D)$ .
- 2. For an internal node u in T and all its children  $v \in child(u)$ , add arcs  $\{(x, y) : x \in L(u), y \in L(v)\}$  in G, where  $T \in P$ .
- 3. For each pair of siblings  $N \in T$ , add arcs  $E = \{(x, y) : x \in u, y \in v, u \neq v, u, v \in N\}$  in Q.
- 4. For each relative divergence date div(L) < div(L'), an aqua vertex a are built in G and R, arcs  $\{(a, y) : y \in L'\}$  are built in G, and arcs  $\{(x, a) : x \in L\}$  are built in R.
- 5. For each relative divergence date div(L, x) < div(L', x) in the compact form, it is expressed by corresponding relative divergence dates  $D_i$ , and then  $D_i$  is built by the previous step.

The above version of constraint graph applies the method of restricted descendancy graph shown in [2], and by Proposition 4 in [2], it can replace the original version of constraint graph in [4].

To prove Lemma 3.2, it is sufficient to show if there exists a ranked semi-labeled tree  $\mathcal{T}$  which ancestrally displays P and preserves D, then CONSTRAINT GRAPH COM-PATIBILITY returns  $\mathcal{T}$  displaying  $\mathcal{G}$ . The sufficiency is shown in [4].

Furthermore, if there exists no tree which ancestrally displays P and preserves D, then the CONSTRAINT GRAPH COMPATIBILITY returns "incompatible."

## 3.3 The Algorithm

#### 3.3.1 Terms

Let  $\mathcal{G} = (G, \phi, Q, R)$  be a constraint graph. A *core* of  $\mathcal{G}$  is a connected component in G, and let  $C(\mathcal{G})$  denote the cores in G. A *source* of  $\mathcal{G}$  is a blue vertex with indegree 0 in G, Q. Let  $x \leq_{\mathcal{T}} y$  if x is an ancestor of y. Let  $||\mathcal{G}||$  be |V(G)| + |E(G)| + |V(Q)| + |E(Q)| + |V(R)| + |E(R)|.

#### 3.3.2 Ranked Hierarchy

In [4], the ranked hierarchy is used as a data structure for recording the output tree in the main iteration. A ranked hierarchy  $H_T$  can be transformed into a unique ranked semi-labeled tree T.

A *cluster* is a set of labels. In the corresponding tree  $\mathcal{T}$  and a vertex u, the cluster  $C_{\mathcal{T}}(u)$  is

$$\bigcup_{v:u\leq_T v} L(v)$$

A ranked hierarchy is set of clusters and a rank on each cluster, for each pair of clusters  $C_{\mathcal{T}}(u)$  and  $C_{\mathcal{T}}(v)$  with  $C_{\mathcal{T}}(v) \subseteq C_{\mathcal{T}}(u)$ , we have  $rank(C_{\mathcal{T}}(u)) < rank(C_{\mathcal{T}}(v))$ .

#### 3.3.3 GraphBuild Algorithm

The GRAPHBUILD algorithm to solve CONSTRAINT GRAPH COMPATIBILITY problem. It can be derived from the BUILDPLUS in [4].

Algorithm 1 GraphBuild(G) 1: Create  $\mathcal{G}_0$  from  $\mathcal{G}$ . 2: repeat Iteration *k*, starting from 0. 3: // Phase 2 4: Let  $S_a = \{a : a \in V(G_{2k}), a \notin V(Q_{2k})\}$ 5:  $\mathcal{G}_{2k+1} \leftarrow \mathcal{G}_{2k} \setminus S_a.$ 6: // Phase 1 7: Let  $S = \{s : indegree(s) = 0 \text{ in } G_{2k+1}, Q_{2k+1}\} \setminus \{s : indegree(s) \neq 0 \text{ in } Q_{2k}\}.$ 8:  $\mathcal{G}_{2k+2} \leftarrow \mathcal{G}_{2k+1} \setminus S$ 9: Let  $\pi_{k+1}$  be the partition of the vertex set of  $G_{2k+2}$  induced by the cores of 10:  $G_{2k+2}$ .  $\mathcal{H}_{k+1} \leftarrow \mathcal{H}_k \cup \pi_{k+1}$ 11: for all cluster  $B \in \pi_k \setminus \pi_{k+1}$  do 12:  $r'(B) \leftarrow k.$ 13: end for 14: 15: **until** (a) All vertices in  $G_{2k+2}$  are removed, or (b) it is impossible to do so. 16: Incompatible. The input is incompatible in condition (b) 17: **Compatible.** In condition (a),  $H_k$  is a ranked semi-labeled tree which ancestrally displays P' and P and preserves D.

18: **Restriction.** Restrict  $\mathcal{H}_k$  to  $L(P) \cup L(D)$  and get  $\mathcal{H}$ .

#### **3.3.4** The creation of $\mathcal{G}_m$

If  $|C(\mathcal{G})| = 1$ , Let  $\mathcal{G}_0 = \mathcal{G}$ . Otherwise, create a blue vertex  $\rho$  in G, Q, R, and arcs  $(\rho, x) \in E(G)$  for each blue vertex  $x \in L(G)$ .

When the constraint graph  $\mathcal{G}_{m-1}$  becomes  $\mathcal{G}_m$ , the following maintenance in  $Q_m$  is done:

1. The arcs (x, y) with x, y are in different cores are removed.

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2. For an aqua vertex a, let  $L(a) = \{u : (u, a) \in E(R)\}$ . If not all L(a) are in the same core in G, if some vertices in L(a) are not in G, or if  $|L(a)| = \emptyset$ , a is removed from R.

### 3.3.5 The BuildPlus algorithm

The BUILDPLUS algorithm reduces the input P and D to the input G of GC. G then be solved by GRAPHBUILD. By Lemma 3.2, the output of GC is the output of TC.

## **Chapter 4**

## **Restricted constraint graph**

We replace the constraint graph with a restricted constraint graph. A *restricted con*straint graph is a constraint graph, with the modification of intermediate vertices, red bundles, and aqua bundles. A restricted constraint graph  $G'_k$  is associated with a constraint graph  $G_k$  if  $G_0$  and  $G'_0$  are reduced from the same input P and D of  $\mathcal{TC}$ , and  $G_k, G'_k$  are derived from  $G_{k-1}, G'_{k-1}$ , respectively, with the same vertices set removed.

## 4.1 Intermediate vertices

**Lemma 4.1.** Let P and D be the input of TC, and  $\mathcal{G}_0 = (G_0, \phi, Q_0, R_0)$  be the input of  $\mathcal{GC}$ reduced from P and D. Let  $\mathcal{G}'_k = (G'_k, \phi, Q'_k, R'_k)$  be a restricted constraint graph associated with  $\mathcal{G}_k$ . Then (1)  $L(G_k) = L(G'_k)$ ; (2) for each  $x \in L(G_k)$ , outdegree<sub> $G_k$ </sub>(x) = 0 if and only if  $outdegree_{G'_k}(x) = 0$ ; (3) for each two  $x, y \in L(G_k)$ , x, y are connected in  $G_k$  if and only if x, y are connected in  $G'_k$ .

Furthermore,  $|V(G''_k)| + |E(G''_k)| = O(||P||)$ , where  $G''_k = G \setminus V_a(G)$  and the reduction of  $G''_k$  can be done in O(||P||).

*Proof.* For each internal node  $u \in T$ , if |L(u)| > 1 and |L(child(u))| > 1, an intermediate vertex t and edges  $\{(x,t) : x \in L(u)\} \cup \{(t,y) : y \in L(child(u))\}$  is built in G' for each  $T \in P$ . Let  $\phi(t) = indigo$ , a new color in  $\phi$ .

After the removal of sources S,  $\mathcal{G}_{k-1}$  becomes  $\mathcal{G}_k$ ,  $\mathcal{G}'_{k-1}$  becomes  $\mathcal{G}'_k$ . If after the removal of S, the indegree of t will become 0, t is add to S. Note that the vertices in S are still in the same core.

For each  $y \in \{y \in L(G_{k-1}) : (t, y) \in E(G_{k-1})\}$ , y has indegree 0 in  $G_k$  For each two  $y, z \in \{y, z \in L(G_{k-1}) : (t, y), (t, z) \in E(G_{k-1})\}$ , y, z are connected in  $G_k$ , if and only if y, z are connected in  $G'_k$ .

### 4.2 Bundles

**Lemma 4.2.** For the restricted constraint graph  $\mathcal{G} = (G, \phi, Q, R)$  reduced from P and D, the total update time for red edge removal step and of aqua label removal step can be done in  $O(h \log^2 h)$  time and O(h) space, where h = ||P|| + ||D|| + |V(G')| + |E(G')|, and G' be the subgraph of G induced by L(G).

#### 4.2.1 Red bundles

A red bundle tree T is a non-empty three-layered rooted tree in Q. If  $v \in V(T)$  has no outdegree, v has exactly two ancestors.

**Terms.** Let L(T) be the leaves of T,  $\rho(T)$  be the root of T, I(T) be the internal nodes of T,  $P_T(x)$  be the parent of x in T. For a subset  $L' \subseteq L(T)$ , let  $\Psi_T(L')$  be the red bundle tree induced by L' and all the ancestors of L' in T. For a vertex  $v \in I(T)$ ,  $v \notin V(G) \cup L(Q) \cup V(R)$ . For a leaf  $x \in L(T)$ ,  $x \in L(Q)$ . A red bundle tree T is removed if I(T) is removed from Q. For a set of blue vertices S, let RT(S) be the red bundle trees T with  $L(T) \cap S \neq \emptyset$ , and for a graph G, let RT(G) be RT(L(G)).

**Lemma 4.3.** For a constraint graph  $\mathcal{G} = (G, \phi, Q, R)$ , An blue vertex x has no red edge if and only if x has no edges from red bundle trees.

For a constraint graph  $\mathcal{G}_k = (G_k, \phi, Q_k, R_k)$  and a blue vertex  $x \in L(G_k)$ , Let

$$\Lambda_k(x) = \{ y : (x, y) \in E(Q_k) \}.$$

**Lemma 4.4.** Let  $\mathcal{G}_0$  be the input constraint graph, and  $\mathcal{G}_k = (G_k, \phi, Q_k, R_k)$  be a constraint graph with k > 0 from  $\mathcal{G}_{k-1}$  by removal of a vertex set. If a data structure W keeps  $\Upsilon_0(x) = \Lambda_0(x)$ , and  $\Upsilon_k(x) = \Lambda_k(x)$ , and the vertex set  $\{x : |\Upsilon_k(x)| = 0, |\Upsilon_{k-1}(x)| \neq 0\}$  can be known, for each blue vertex  $x \in L(G_k)$ , then W can replace the red edges.

*Proof.* In BUILDPLUS, a vertex has no red edges if  $|\Lambda_k(x)| = 0$ .

**Property.** When a core *C* becomes its children *C*, the following property is maintained:

**Property 4.5.** for each red bundle tree  $T \in BT(C)$ , T becomes the forest  $child(T) = {\Psi_T(L') : L' = L(T) \cap L(C'), C' \in C}$ , where the I(T) could be duplicated or moved in the induction while L' stays the same vertices set.

**The reduction** In the reduction from  $\mathcal{TC}$  to  $\mathcal{GC}$ , for each node p with outdegree greater than 1, a red bundle tree T with root r is built. For each child v of p, a vertex k is created as a child of r. And for each label  $x \in L(v)$ , a leaf x is created as a child of k.

The removal of red bundle tree For a red bundle tree T, if  $\rho(T)$  has only one child, remove T.

Let

$$\Upsilon_k(x) = \bigcup_{T \in RT(x)} \Upsilon_k(x, T).$$

We prove that  $\Upsilon_k(x) = \Lambda_k(x)$ , and the vertex set  $S = \{x : |\Upsilon_k(x)| = 0, |\Upsilon_{k-1}(x)| \neq 0\}$ 

*Proof.* Let  $\mathcal{G}_k = (G_k, Q_k, R_k)$  with  $k \ge 0$  be a constraint graph, and after the removal of some vertices  $S \in \mathcal{G}_k$  with  $S \in V(C)$ ,  $C \in G_k$ , let the resulting constraint graph be  $\mathcal{G}_{k+1}$ .

**Terms.** Let  $T \in RT(Q_k)$  be a red bundle tree and  $x \in L(Q_k)$  be a blue vertex.

Let 
$$\Upsilon_k(x,T)$$
 be  

$$\begin{cases} \{y \in L(T) : P_T(x) \neq P_T(y)\}, & \text{if } x \in T, \\ \emptyset, & \text{if } x \notin T. \end{cases}$$
And  $\Upsilon_k(x) = \bigcup_{T \in RT(Q_k)} \Upsilon_k(x,T)$  with  $k \ge 0$ .  
Let  $\Lambda_0(x) = \{y : (x,y) \in Q_0\}, \text{ and } \Lambda_0(x,T) = \Upsilon_0(x) \cap L(T).$  Let  $\Lambda_k(x) = \{y : (x,y) \in E(Q_k)\}$  and  $\Lambda_k(x,T) = \Lambda_{k-1}(x,T) \setminus \{y : (x,y) \in Q_{k-1}, (x,y) \notin Q_k\}$  with  $k > 0$ .

**Initialization.** When the constraint graph  $\mathcal{G}_{\ell}$  is built, for each  $x \in L(Q_0)$  and each  $T \in RT(Q_0)$ ,  $\Lambda_0(x) = \Upsilon_0(x)$  and  $\Lambda_0(x, T) = \Upsilon_0(x, T)$ .

For each  $x \in L(Q_k)$  and each  $T \in RT(Q_k)$ ,  $\Lambda_k(x) = \bigcup_{T \in RT(Q_k)} \Lambda_k(x, T)$ .

**Induction step.** When  $\mathcal{G}_k$  becomes  $\mathcal{G}_{k+1}$ , let  $C \in C(G_k)$  be the core with vertex set removed,  $\mathcal{C} = child(C)$ . Let x be a blue vertex,  $x \in L(C)$  before removal, and  $x \in L(C')$  after removal for  $C' \in \mathcal{C}$ . And Let  $T \in RT(Q_k)$  and  $T \in RT(x)$ , T becomes  $\mathcal{T} = child(T)$  in  $Q_{k+1}$ .

Let  $T' = \Psi_T(L')$  with  $L' = L(T) \cap L(C')$ . Since T' is the subtree of T induced by

L' and its ancestors,  $\Upsilon_{k+1}(x, T') = \Upsilon_k(x, T) \cap L(C')$ . Since all the red edges (x, y) with  $y \notin L(C')$  are removed,  $\Lambda_{k+1}(x, T') = \Lambda_k(x, T) \cap L(C')$ . With  $\Upsilon_k(x, T) = \Lambda_k(x, T)$ , we have  $\Upsilon_{k+1}(x, T') = \Lambda_{k+1}(x, T')$ .

An edge  $(P_{T'}(x), x)$  in T' is removed if and only if  $\rho(T') = \emptyset$ . And  $\rho(T') = \emptyset$  if and only if  $\Upsilon_{k+1}(x, T') = \emptyset$ . So,  $RT(x) = \emptyset$  if and only if x has no red edges.

For a constraint graph  $\mathcal{G} = (G, \phi, Q, R)$ , let  $||RT(Q)|| = \sum_{T \in RT(Q)} |V(T)|$ .

**Lemma 4.6.** For the constraint graph build by the reduction, ||RT(Q)|| = O(r). And the the reduction for the red bundles cost O(r) time and space where r = ||P||.

*Proof.* For each internal node u in each tree  $T \in P$ , a bundle tree with  $\bigcup_{v \in child(u)} |L(v)|$ leaves are created. So, ||RT(Q)|| = O(r). And it is a linear time reduction, so the time and space for the reduction are both O(r).

**Lemma 4.7.** The red bundle trees has the partial update property. And if each blue vertex updates red bundle trees at most O(t) times, the red bundles can be maintained in O(rt) time with O(r) space where r = ||RT(Q)|| for the input constraint graph  $\mathcal{G} = (G, \phi, Q, R)$ .

When a core *C* becomes its children C, let each blue vertex  $x \in C'$  updates each red bundle tree  $T \in RT(x)$  by the following steps, where  $C' \in C \setminus \{C''\}$  and  $C'' \in C$  is an arbitrary core.

For a red bundle tree *T*, let each node  $u \in I(T)$  has a pointer, which is null when created, and reset to null after each child core updated.

```
Algorithm 2 update(x,T)1: k \leftarrow P_T(x), r \leftarrow P_T(k).
 2: Let q be the pointer of k.
 3: if q is null then
          A node k' is created.
 4:
 5: else
          Let k' be the node q points to.
 6:
 7: end if
 8: Create edge (k', x).
 9: Let p be the pointer of r.
10: if p is null then
          A root r' is created.
11:
12: else
          Let r' be the node p points to
13:
14: end if
15: Create edge (r', k').
16: Remove (k, x).
17: Remove k if k has no child.
18: Remove r if r has no child.
```

After all vertices in C' updated, reset all visited pointers to null.

We then prove Lemma 4.7.

First, the bundles are initially maintained,  $T = \Psi_T(L)$ ,  $L = L(T) \cap L(C_0)$ , since all blue vertices are initially in the single core  $C_0$  of  $G_0$ .

**Correctness** After the removal of a set of vertices in C, each C' is updated.

For each C' and  $L' = L(T) \cap L(C')$ , we show that  $\Psi_T(L')$  is created. For  $w \in I(T) \setminus I(\Psi_T(L'))$ , w will not be visited in the update of C'. For  $u \in I(\Psi_T(L'))$  and the child v which visits u, in the first visit of u, the pointer of u is null, and a new node u' and the edge (u', v) are created as the duplication of u and (u, v). And in the subsequent visit of u, the same u' is used and (u', v) is created. So, after all leaves in L' update,  $\Psi_T(L')$  is created.

For the rest part of T, all leaves of  $L(T) \cap L(C'')$  are removed from T since all  $C' \in C \setminus C''$  are updated. And all internal nodes with outdegree 0 is removed. Also, no new edges are created to the  $V(\Psi_T(L''))$ . So, the tree  $\Psi_T(L'')$  is induced, where  $L'' = L(T) \cap L(C')$ . So the red bundles are maintained.

So, the red bundles has the partial update property.

**Complexity** For each x, constant space for each T is kept, since the number of ancestors, the edges and the pointers of x and its ancestors is O(1) though each update. And after C' is visited, the list of visited pointers can be released, the time and space of the list is constant for each pointer. Each update of x and T costs constant time. Since each x is updated at most t times, the total time for the update is  $\sum_{x \in L(Q_0)} RT(x)$ .

For each bundle tree with the outdegree of root 0, it is removed only once. So, the time for the removal is linear to the size of the red bundles in addition to the time above.

So, if each blue vertex updates red bundle trees at most O(t) times, the red bundles can be maintained in O(rt) time with O(r) space.

#### 4.2.2 Aqua bundles

An aqua bundle tree  $T \in R$  is a non-empty two-layered rooted tree consists of a root  $\rho(T)$  and two sets of leaves  $L(T) \subseteq L(R)$  and  $V_r(T) \subseteq V_r(R)$ . For T, |L(T)| > 0 and  $|V_r(T)| > 0$ . For a set of blue vertices S, let AT(S) be the red bundle tree T with  $L(T) \cap S \neq \emptyset$ , and for a graph G, let AT(G) be AT(L(G)). And a function  $x = \alpha(T)$  from AT(R) to  $N \cup \{0\}$ .

**Property.** When a core *C* becomes its children C, the following properties is maintained:

**Property 4.8.** For each  $u \in L(T)$  is removed form the constraint graph, remove u from T, too. For each  $T \in AT(C)$ , if  $|L(T) \cap L(C)| < |\alpha(T)|$ , T is removed.

## 4.2.3 Replacing the aqua edges with aqua bundles

Without the loss of generality, a relative divergence date div(L) < div(L') can be described as the compact form div(L, x) < div(L', x') with x = x' = 1.

Let indegree(a) be the indegree of the aqua vertex a in R.

**Lemma 4.9.** For a constraint graph  $\mathcal{G} = (G, \phi, Q, R)$  and each relative divergence date d in the form div(L, x) < div(L', x'), let the created set of aqua vertices be A. And let T be the corresponding aqua bundle.

*T* can replace *A* and the edges created in the reduction form div(L, x) < div(L', x').

**Lemma 4.10.** For a constraint graph  $\mathcal{G} = (G, \phi, Q, R)$  and each relative divergence date d in the form div(L, x) < div(L', x'), let the created set of aqua vertices be A.

At least one  $l \in L'$  is not connected to the aqua vertices  $a \in A$  with all  $a \in A$  with indegree(a) = 0 removed in the version of aqua vertices, if and only if all  $l \in L'$  is not

#### connected.

*Proof.* For div(L, x) < div(L', 1), it is true, since all aqua vertices connect to the same set of L'. For div(L, 1) < div(L', 0), it is true, since all aqua vertices a with (a, y) and  $y \in L'$  has same set of edges  $\{(b, a) : b \in L\}$  in R.

For div(L, 0) < div(L', 0), it is transformed into the set  $Div = \{div(L, 0) < div(\{v\}, 1),$ for  $v \in L'$ . For each  $d \in Div$ , d has the property. Since all are not connected if at least one is is not connected. We only need to show for an v and each  $u \in L$ ,  $\{div(u) < div(v, 1)\}$  has the property. And it is div(L, 0) < div(z), and shown in above case. That finishes the proof.

#### We then prove Lemma 4.9.

**Proof.** We prove T can replace A and the edges, by showing if each  $a \in A$  with indegree(a) = 0 removed, then a blue vertex  $b \in L'$  is connected to no aqua vertices  $a \in A$  in the version of aqua vertices, if and only if T is removed.

By Lemma 4.10, we only need to show that no blue vertex  $b \in L'$  is connected to any aqua vertices  $a \in A$  in the version of aqua vertices, if and only if *T* is removed.

For div(L, x) < div(L', x'), if all aqua vertex  $a \in A$  created by each  $d \in Div$  has indegree(a) = 0, then T can be removed, where Div is the expanded relative divergence dates  $\{div(l) < div(l'')\}$ .

If *T* can be removed, then all  $a \in A$  created by each  $d \in Div$  has indegree(a) = 0.

For div(L, x) < div(L', 1), in both version, an aqua vertex or aqua vertices are created and connected to  $l \in L'$  which keep l in the same core. And for div(L, x) < div(L', 0), an aqua vertex or a set of vertices are created for each  $l \in L'$ . In the both cases they keep the  $A' \subseteq L'$  with |A'| = max(1, x'|L'|) in the same core and prevent all  $l' \in A'$  becomes sources.

That finishes the proof.

**The reduction** The creation of aqua vertices and the edges for relative divergence dates is replaced by the steps here.

Let div(L, x) < div(L', x') be a relative divergence date. If x' = 0, an aqua vertex  $a_i$  is created for each  $z_i \in L'$ . If x' = 1, an aqua vertex a is created. Let the set of created aqua vertices be A. And an aqua bundle T is built with a root  $\rho$  and the leaves L(T) = L, f(T) = max(x|L|, 1), and  $V_a(T) = A$  where A is the set of aqua vertices created for this relative divergence date.

We then prove Lemma 4.9.

*Proof.* For x = 1, T is removed if some blue vertices in L are removed, or two blue vertices in L are in different cores. It is the same condition of removing edges on the aqua vertices in the version of aqua edges. So, all blue vertices created by  $\{div(L) < div(\{z\})\}$  with  $z \in L'$  are free to be removed.

For x = 0, *T* is removed if and only if all blue vertices in *L* are removed. In the version of aqua edges, for  $d \in \{div(y, 1) < div(L', x')\}$  with  $y \in L'$ , all sets of aqua edges for *d* have edge removed in *R* if and only if all *L'* have no edge from aqua vertex created from *d*.

For a constraint graph  $\mathcal{G} = (G, \phi, Q, R)$ , let  $||AT(Q)|| = \sum_{T \in AT(Q)} |V(T)|$ .

**Lemma 4.11.** For the constraint graph build by the reduction, ||AT(Q)|| = O(s). And the the reduction for the red bundles cost O(s) time and space where s = ||D||.

*Proof.* For each relative divergence date div(L, x) < div(L', x'), an aqua bundle is built with |L| + |L'| leaves. And the aqua vertices and edges created in G and R are at most O(|L'|). So, ||AT(Q)|| = O(s). It is a linear time reduction, so the time and space is O(s).

**Lemma 4.12.** The aqua bundle trees has the partial update property. And if each blue vertex updates aqua bundle trees at most O(t) times, the aqua bundles can be maintained in O(st) time with O(s) space where s = ||AT(Q)|| for the input constraint graph  $\mathcal{G} = (G, \phi, Q, R)$ .

*Proof.* The removed blue vertex can be identified, and when the removed blue vertex a updates the each  $T \in AT(a)$ , the removal of  $(a, \rho(T))$  can be done.

For each  $C' \in C \setminus C''$ , and each  $T \in AT(C')$ , since each blue vertex  $a \in L(C')$ updates, the total number of  $L(T) \cap L(C')$  can be known after C' is updated, and Tcan be removed if  $|L(T) \cap L(C')| < \alpha(T)$ .

For the core C'' not updated, since each  $T \in AT(C'')$  but  $T \notin AT(C')$  are not affected, the total number of  $L(T) \cap L(C'')$  will not be changed.

### 4.3 Proof

We now prove Lemma 4.2.

*Proof.* By Lemma 4.3 and Lemma 4.9, the red edge removal step and aqua label removal can be done by red bundles and aqua bundles.

With Lemma 4.6 and Lemma 4.11, if the update of a blue vertex is at most O(t) time, then this can be done in O(ht) time and O(h) space.

And with Lemma 2.3, since red bundles and aqua bundles has partial update prop-

erty, the times of update for each blue vertex is  $O(\log h)$  times, and if the framework in Lemma 2.3 can be done in T(n,m) time and S(n,m) space with graph G = (V, E), where n = |V|, m = |E|, then the total update time for red edge removal step and of aqua label removal step can be done in  $O(h \log h + T(h,h))$  time and O(h + S(h,h))space, where h = ||G|| with G the input constraint graph.



## **Chapter 5**

## **Proof of Theorem 1.1**

**Proof.** Let  $\mathcal{G} = (G, \phi, Q, R)$  be a restricted constraint graph reduced from the input Pand D of TREE COMPATIBILITY. Let G' be the subgraph of G induced by L(G).

By Lemma 4.1, |V(G')| + |E(G')| = O(||P||) and the reduction can be done in O(||P||) time and space. Let h = ||P|| + ||D||, we have ||P|| + ||D|| + |V(G')| + |E(G')| = O(h). By Lemma 4.2, the red edge removal step and of aqua label removal step can be done in  $O(h' \log^2 h')$  time and O(h) space, where h' = ||P|| + ||D|| + |V(G')| + |E(G')| = O(h).

And the time and space complexity of BUILDPLUS is O(h+T(h)) and O(h+S(h)), where h is the size of restricted constraint graph, T(h) is the time for creating  $\mathcal{G}_k$  from  $\mathcal{G}_{k-1}$  with  $\mathcal{G}_0 = \mathcal{G}$ .  $T(h) = O(h \log^2 h)$  and S(h) = O(h).

So, the TREE COMPATIBILITY can be solved in  $O(h \log^2 h)$  time and O(h) space, where h = ||P|| + ||D||.

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