

Nature 438, pp. 803-819 (2005)

Label Isomorphism: On the MAF Problems for Multiple Trees

Jianer Chen

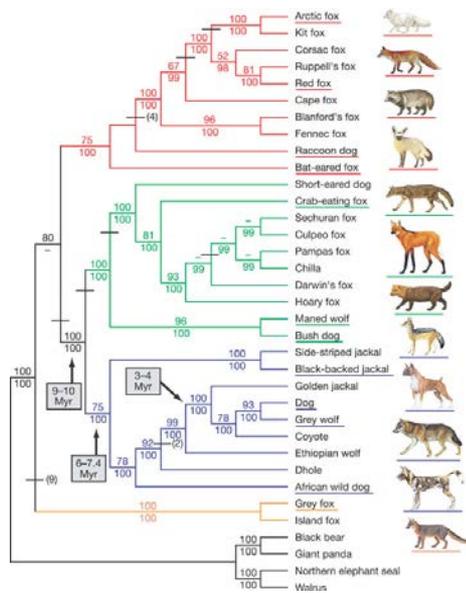
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IMS Singapore 2017



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A Quick Overview on MAF Algorithms and Label Isomorphism: On the MAF Problems for Multiple Trees

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Definitions

- **X-Tree (X-forest)**

A tree (forest) T for which there is a one-to-one mapping from the leaves of T to a symbol set X .

- **Agreement forest**

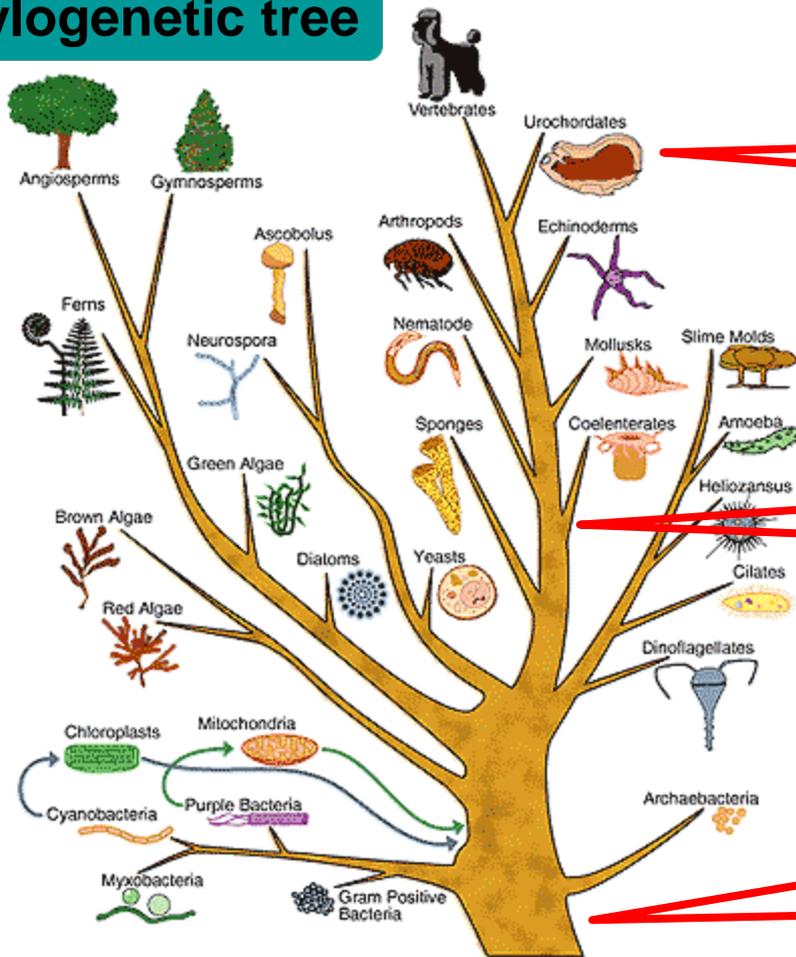
An agreement forest of two X -trees is an X -forest that is a subgraph of both the X -trees.

- **The Maximum Agreement Forest (MAF) Problem**

Find a maximum agreement forest (**maf**) for two given X -trees

Background

Phylogenetic tree



leaves are labeled with extant species

internal nodes correspond to speciation events

if rooted, the root represents the ancestor of all the species

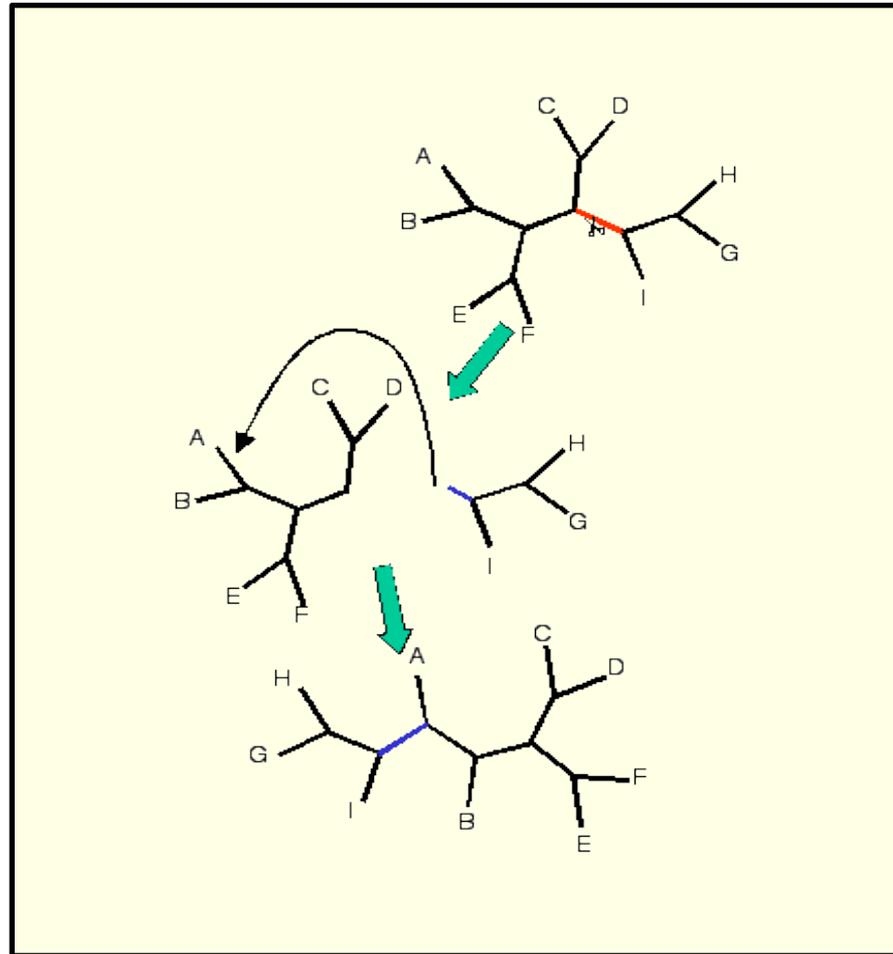
Background

- ❑ **Different experiments may result in different phylogenetic trees**
 - **Morphology**
 - **Molecular biology**
-

Background

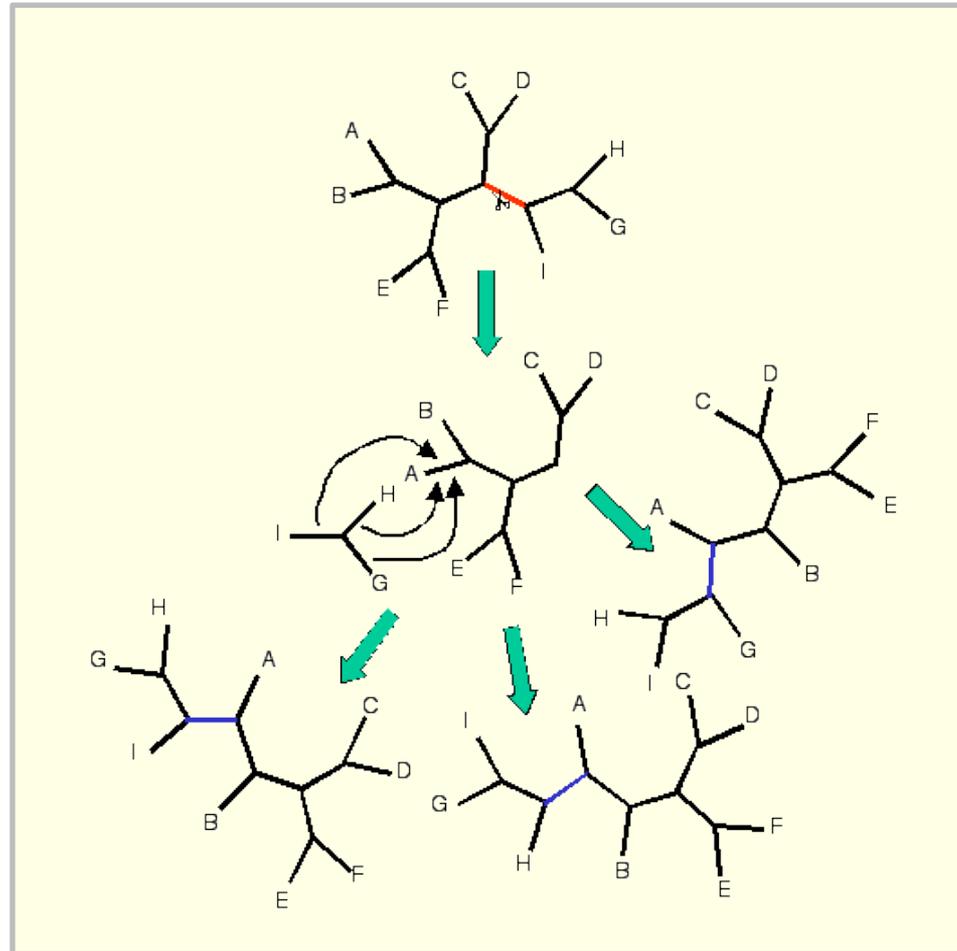
- ❑ **Different experiments may result in different phylogenetic trees**
 - **Morphology**
 - **Molecular biology**
- ❑ **Distance metrics have been proposed to facilitate the comparison of different phylogenetic trees for their similarity:**
 - Robinson-Foulds, Nearest Neighbor Interchange (NNI), TBR, SPR, ...

Subtree-Prune-and-Regraft (SPR)



<http://artedi.ebc.uu.se/course/X3-2004/Phylogeny/>

Tree-Bisection-and-Reconnection (TBR)



<http://artedi.ebc.uu.se/course/X3-2004/Phylogeny/>

Background

- **The Maximum Agreement Forest (MAF) Problem**
Find a maximum agreement forest (maf) for two given X-trees
 - **SPR distance corresponds to the order of an MAF in rooted trees [Bordewich 2005]**
 - **TBR distance corresponds to the order of an MAF in unrooted trees [Allen 2000]**
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Find a maximum agreement forest (maf) for two given X-trees

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- **TBR distance corresponds to the order of an MAF in unrooted trees [Allen 2000]**

- **The MAF problem can be equivalently defined as to remove the minimum number of edges to make the two X-trees isomorphic (thus, a minimization problem, instead of a maximization problem).**

Background

□ The Maximum Agreement Forest (MAF) Problem

Find a maximum agreement forest (maf) for two given X-trees

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➤ TBR distance corresponds to the order of an MAF in unrooted trees [Allen 2000]

□ The **MAF problem** can be equivalently defined as to remove the minimum number of edges to make the two X-trees isomorphic (thus, a minimization problem, instead of a maximization problem).

□ The problem of constructing an MAF for two binary X-trees is NP-hard [Allen and Steel 2001], and MAX SNP-hard [Bordewich et al. 2008]

Background

- Most existing algorithms work by progressively removing edges from the X -trees to eventually make the trees isomorphic. Thus, we are actually working on two X -forests, instead of two X -trees.
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- Most existing algorithms work by progressively removing edges from the X -trees to eventually make the trees isomorphic. Thus, we are actually working on two X -forests, instead of two X -trees.
 - **The MAF Problem Revised**
Remove the minimum number of edges from two given X -forests to make them isomorphic.
 - **The MAF Problem Further Revised (parameterized)**
For two given X -forests, can we remove k edges from one of the X -forests to make it a subgraph of the other X -forest.
-

Background

- Isomorphism of X-forests

The definition is up to a “**forced contraction**” operation that removes unlabeled leaves and contracts degree-2 vertices.

- Forest-structured set

An X-forest can be regarded as the set X plus a structure enforced by the forest. The structure restricts the ways of splitting the set X . This view is more formal and sometimes more convenient when discussing operations on X-forests.

Parameterized Algorithms

For two unrooted binary trees:

- ❑ Fixed parameter tractable [Allen-Steel 2001]
 - ❑ Time $O(4^k k^5 + n^{O(1)})$ [Hallett-McCartin 2007]
 - ❑ $O^*(4^k k)$ -time algorithm [Whidden-Zeh 2009]
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For two rooted binary trees:

- ❑ Time $O(4^k k^4 + n^3)$ [Bordewich et al. 2008]
- ❑ $O^*(2.42^k)$ -time algorithm [Whidden et al. 2013]
- ❑ $O^*(2.344^k)$ -time algorithm [Z. Chen-Fan-Wang 2013]

Call for work

- “We should also look at the case where T_1 and T_2 are not necessarily binary unrooted trees.”
[Hallett-McCartin, *Theory of Computing Systems* 41, pp. 539-550, 2007]
 - “The most important open problem is extending our approach to computing MAFs and MAAFs for multifurcating trees and for more than two trees.”
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Parameterized algorithms for

- two general X-trees
- Multiple binary X-trees
- Multiple general X-trees

Call for work

Remark. It makes perfect sense to consider MAF for non-binary trees and for more than two trees:

- ❑ Ambiguities in which the order of more than 2 branches cannot be reliably resolved by phylogenetic tree construction algorithms (soft multifurcations)
 - ❑ Truly multifurcations (hard multifurcations)
 - ❑ NCBI Taxonomy (an important source of species trees): more than half of its branches being multifurcating
 - ❑ MAF on multifurcating trees also corresponds to SPR and TBR distances on the trees
 - ❑ Phylogenetic tree for the same collection of species may be constructed using more than two methods, each producing a different tree.
-

Two General X-trees (quick overview)

Given a pair of general X-forests (F_1, F_2) , and an integer k , remove at most k edges in the larger-order X-forest so that it becomes a subgraph of F_1 and F_2 .

Two General X-trees (quick overview)

Given a pair of general X-forests (F_1, F_2) , and an integer k , remove at most k edges in the larger-order X-forest so that it becomes a subgraph of F_1 and F_2 .

General Idea (for most proposed algorithms):

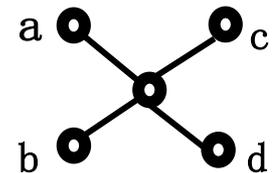
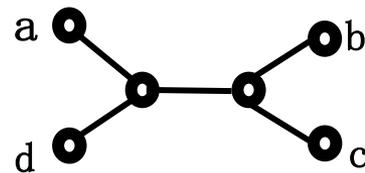
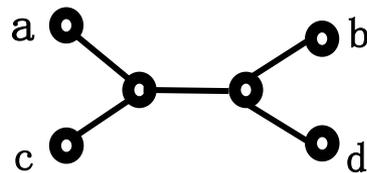
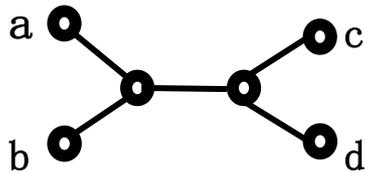
Repeat:

1. Identify structure inconsistency in F_1 and F_2 ;
2. Pick a collection B of edges in F_1 (and in F_2), and make sure one of the edges in B must be deleted in order to remove the inconsistency;
3. Branch on removing each of the edges in the collection B .

Two General X-trees (quick overview)

Branching based on global inconsistency

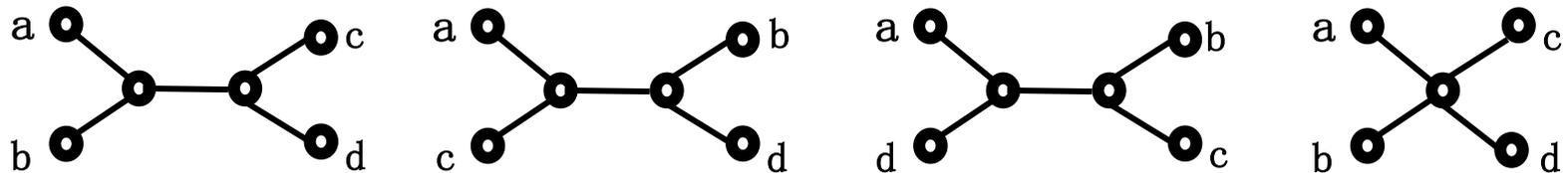
quartet on four labels a, b, c, d



Two General X-trees (quick overview)

Branching based on global inconsistency

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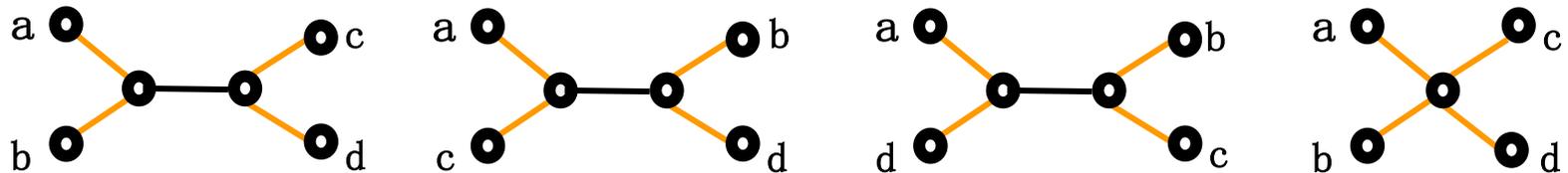
Observation.

If there are four labels a, b, c, d for which the quartets in F_1 and F_2 are different, then one of the edges in the quartet in F_1 is not in any MAF of F_1 and F_2 .

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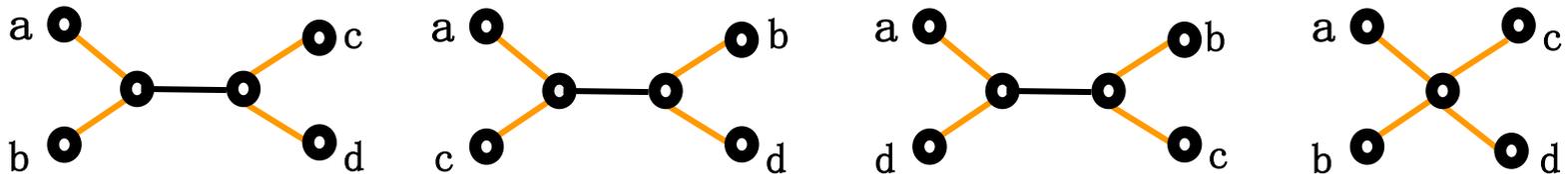
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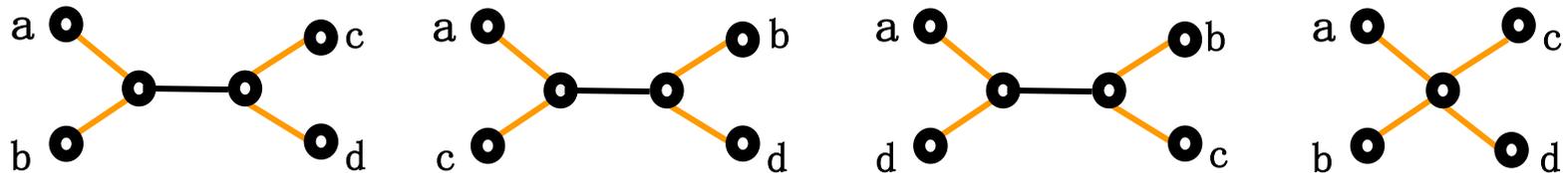
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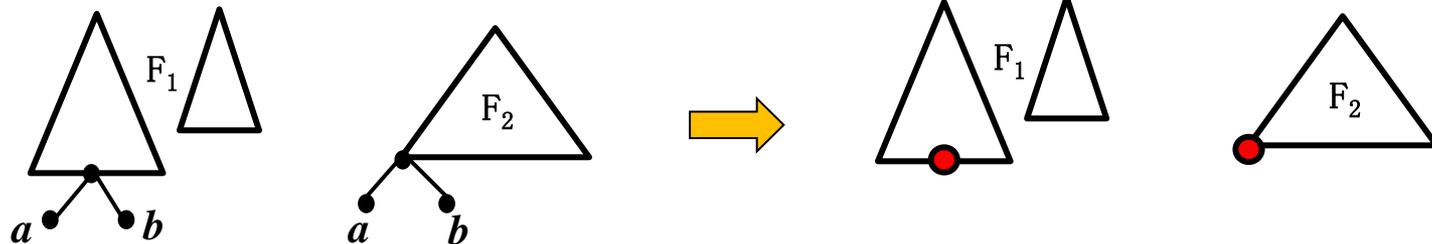
Remark. Hallett-McCartin initiated this method for MAF on two unrooted binary trees. **[Hallett-McCartin 2007]**

Two General X-trees (quick overview)

Branching based on local inconsistency

Review the process on binary trees

1. Pick a sibling pair a and b in F_2 ;
2. If a and b are also siblings in F_1 : shrink them;

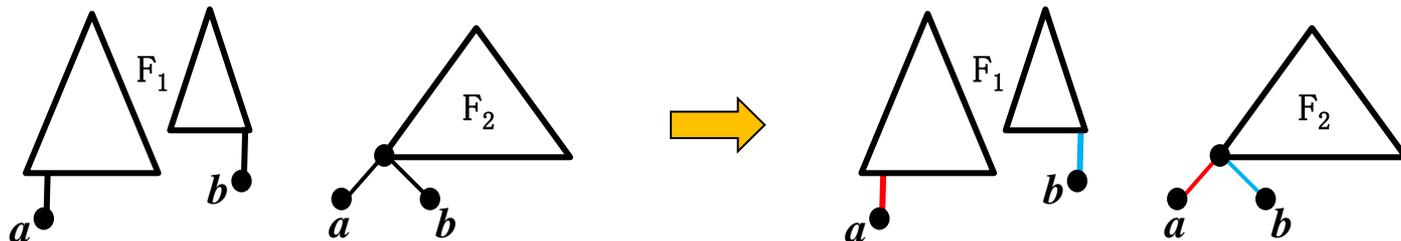


Two General X-trees (quick overview)

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Review the process on binary trees

1. Pick a sibling pair a and b in F_2 ;
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3. If a and b are in different trees in F_1 , branch on making either a or b as a single-vertex tree;

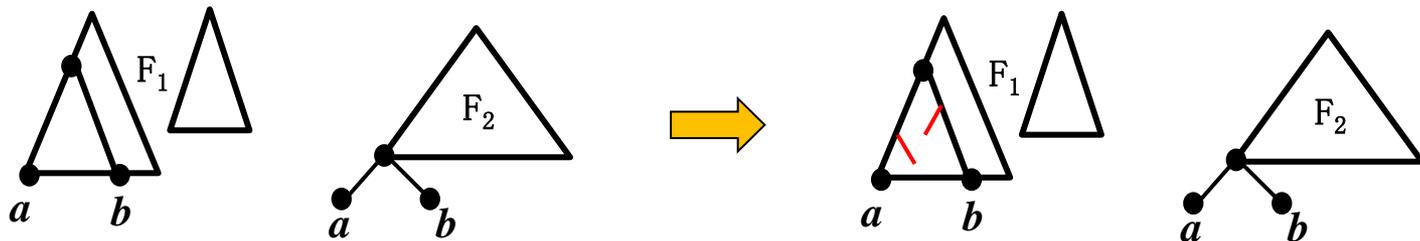


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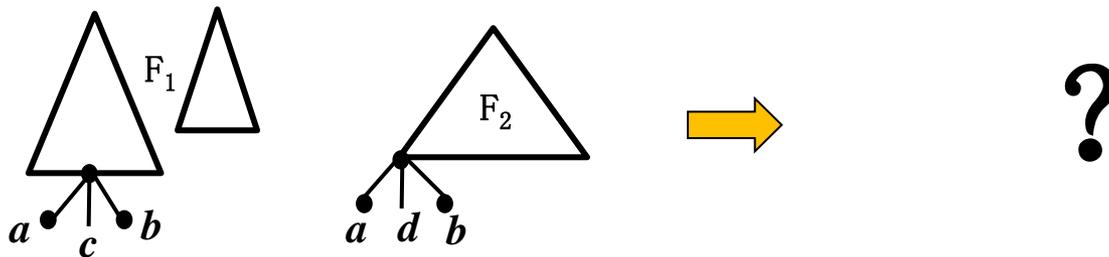


Two General X-trees (quick overview)

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On multifurcating trees

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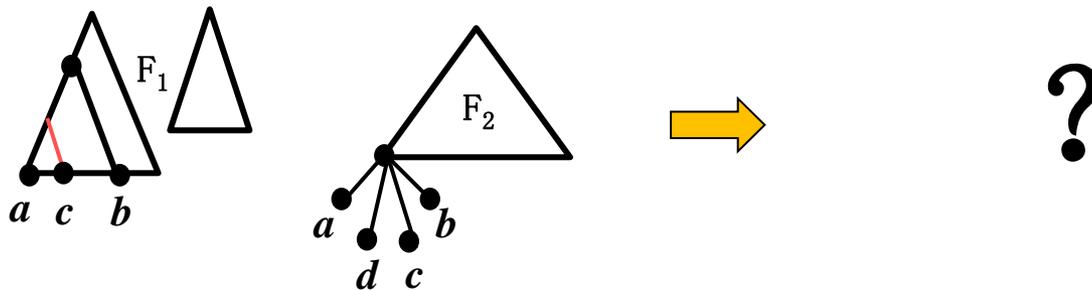


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Branching based on local inconsistency

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4. Otherwise, **branch on removing the edge incident to a , removing the edge incident to b , and removing all edges incident to the path connecting a and b .**



Two General X-trees (quick overview)

Branching based on local inconsistency

Thus, for general X-forest, we need new techniques to analyze the sibling structures.

We introduced a concept of BSS (**basic sibling set**), and apply branch-and-search based on BSS. For an inconsistency structure in BSS, we can identify at most 3 edges in an X-forest in which one must be removed.

Two General X-trees (quick overview)

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This gives an $O^*(3^k)$ -time parameterized algorithm for two unrooted multifurcating trees [JC-Fan-Sze 2013]:

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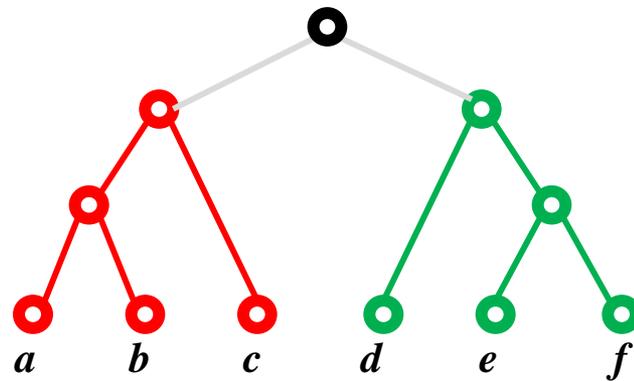
[Whidden-Beiko-Zeh 2016] developed an algorithm of time $O^*(2.42^k)$ for two rooted multifurcating trees, assuming soft multifurcations

Two General X-trees (quick overview)

This looks rather straightforward.

What is difficult/tricky?

Not all edges are essential



Therefore, we need a very careful formulation of the problem (forest-structured sets are useful), and operations are only on “essential” edges.

Multiple X-trees

MAF on Multiple Trees:

Given a collection $\mathbf{C} = \{T_1, T_2, \dots, T_h\}$ of X-trees over the same label-set X , and a parameter k , is there an agreement forest of order at most k for the collection?

Multiple X-trees

MAF on Multiple Forests:

Given a collection $\mathbf{C} = \{F_1, F_2, \dots, F_h\}$ of X-forests over the same label-set X , and a parameter k , is there an agreement forest whose order is at most k larger than the largest forest order in the collection?

Multiple X-trees

What is difficult on multiple trees?

Multiple X-trees

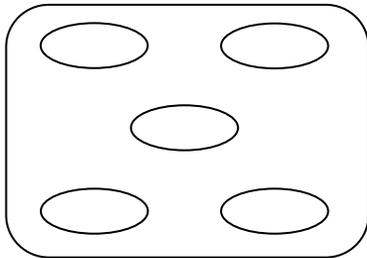
What is difficult on multiple trees?

- Consider an instance $C = \{F_1, F_2, \dots, F_h\}$
- Increase the order of an AF may require to delete many edges in C (thus many branches);

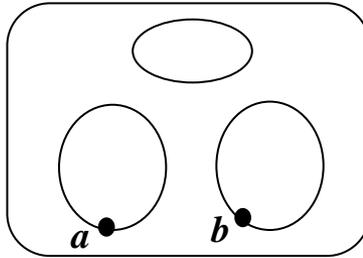
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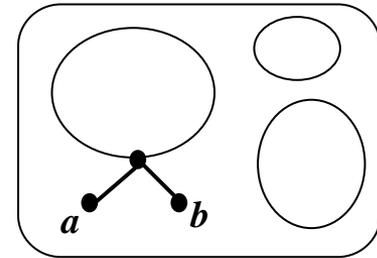
- Consider an instance $C = \{F_1, F_2, \dots, F_h\}$
- Increase the order of an AF may require to delete many edges in C (thus many branches);
- Branching on a forest of small order “wastes” time (without increase the order of an AF).



F_1



F_2

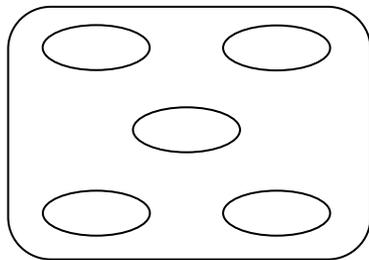


F_3

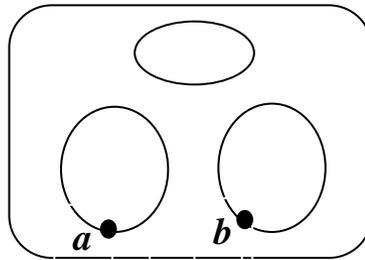
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What is difficult on multiple trees?

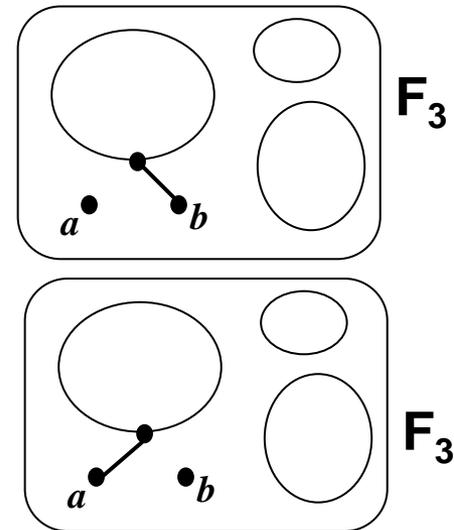
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F_1



F_2



F_3

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Multiple X-trees

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Observation. A MAF for the collection \mathbf{C} is an agreement forest for F_1 and F_2

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Observation. A MAF for the collection \mathbf{C} is an agreement forest for F_1 and F_2

Basic idea. Examine all agreement forests for F_1 and F_2 , and check if each of them is an MAF for the collection \mathbf{C}

Multiple X-trees

MAF on Multiple Forests:

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For a collection \mathbf{C} of rooted binary trees:

Using inconsistency in F_1 and F_2 , identify no more than 3 edges in F_1 , in which one of the edges must be removed.

An $O^*(3^k)$ -time algorithm for the problem [Shi-Wang-JC 2013]

Multiple X-trees

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For a collection \mathbf{C} of unrooted binary trees:

Using inconsistency in F_1 and F_2 , identify no more than 4 edges in F_1 , in which one of the edges must be removed.

An $O^*(4^k)$ -time algorithm for the problem [Shi-Wang-JC 2013]

Multiple X-trees

In principle, the above techniques can be used for developing parameterized algorithms for multiple general X-trees.

However, the multifurcating structures cause much more tedious case-by-case analysis, and also make the branch-and-search process much less efficient.

We would look for conceptually simpler and more efficient methods.

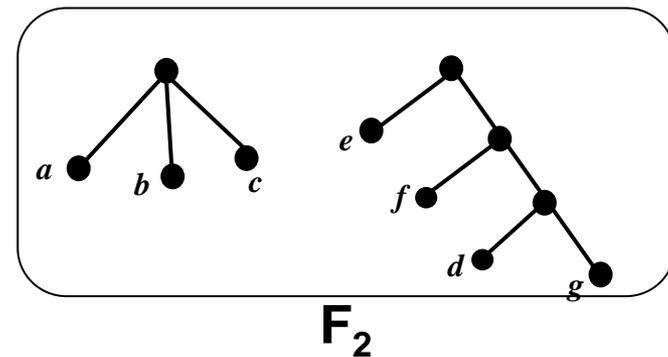
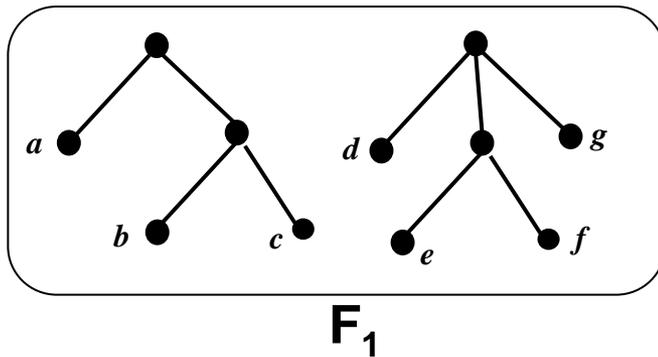
Multiple X-trees

Recall that one source that causes inefficiency is sometimes we have to branch on a forest of small order.

Thus, if we can maintain the condition that all forests in the collection are of the same order, then this undesired situation will be avoided.

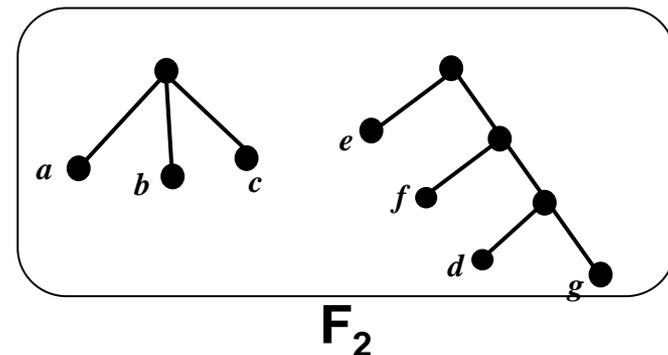
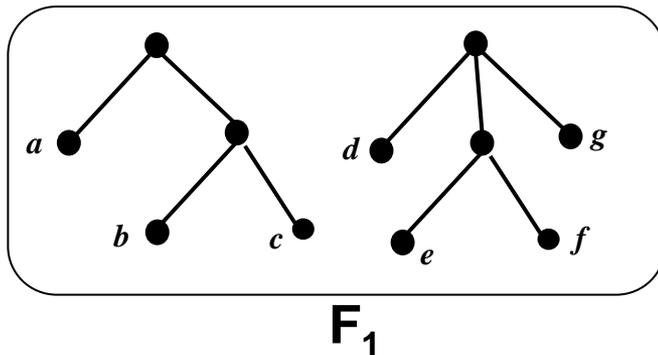
Multiple X-trees

- Two X-forests are **label isomorphic** if they have the same label partitions (the corresponding trees may not necessarily be isomorphic).
- A collection $C = \{F_1, F_2, \dots, F_h\}$ is **label isomorphic** if every pair of forests in the collection are label isomorphic.



Multiple X-trees

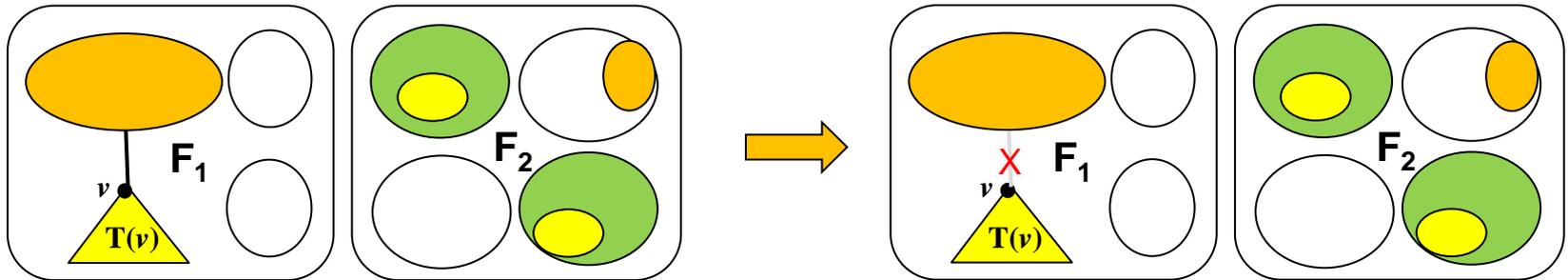
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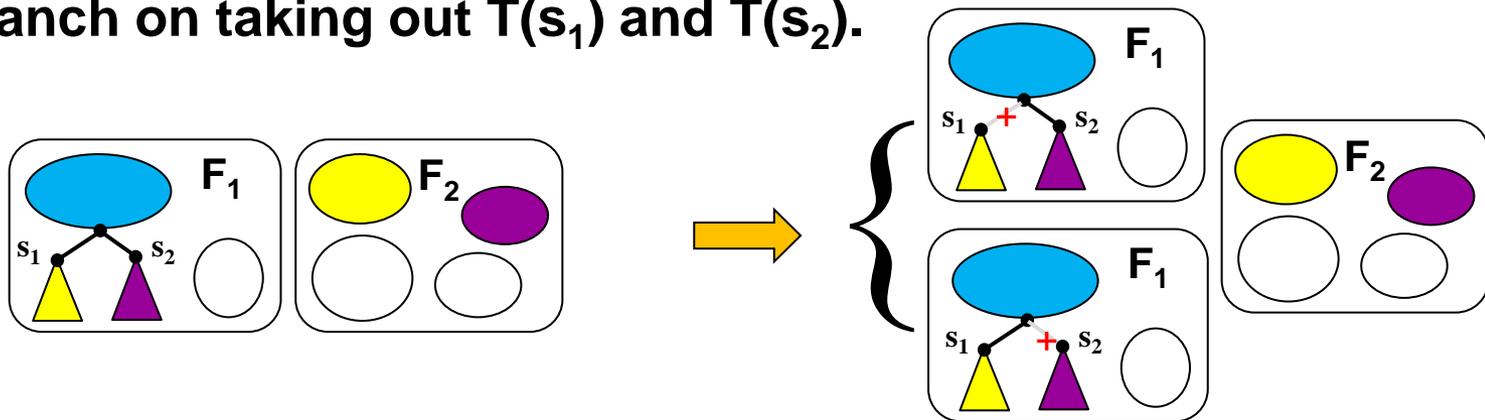
How expensive is it to achieve label isomorphism?

Achieving Label Isomorphism

Reduction Rule 1. If F_1 has a vertex v and F_2 has trees T_1, \dots, T_d such that $L(v) = T \cap (T_1 \cup \dots \cup T_d)$, then take $T(v)$ out of T .



Branching Rule 1. If F_1 has two siblings s_1 and s_2 and F_2 has trees T_1, T_2 such that $L(s_1) \subseteq L(T_1)$ and $L(s_2) \subseteq L(T_2)$, then branch on taking out $T(s_1)$ and $T(s_2)$.



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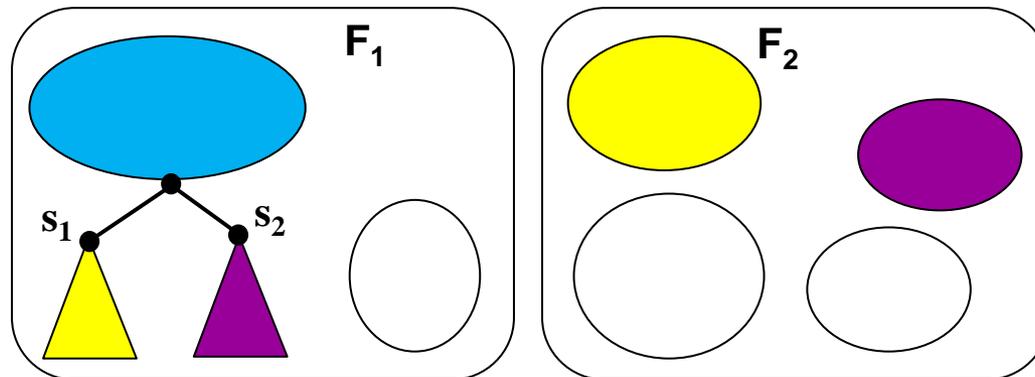
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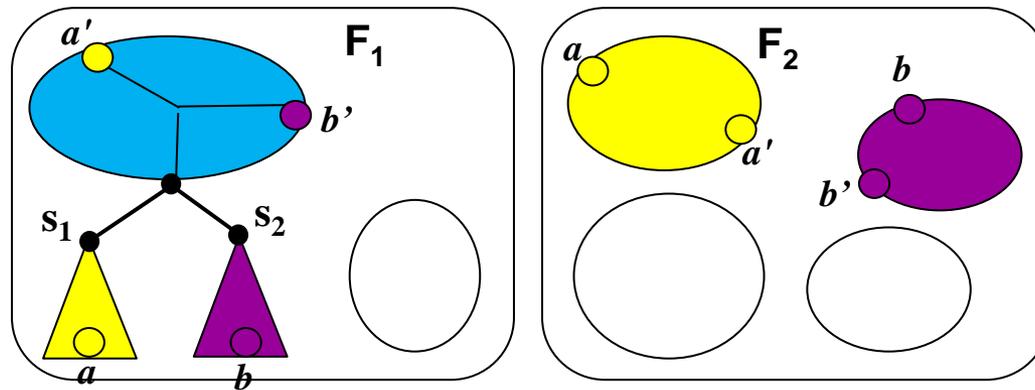


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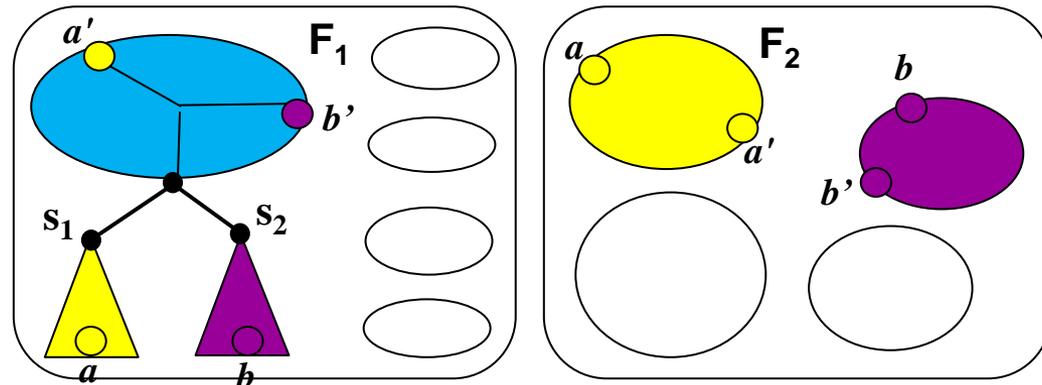
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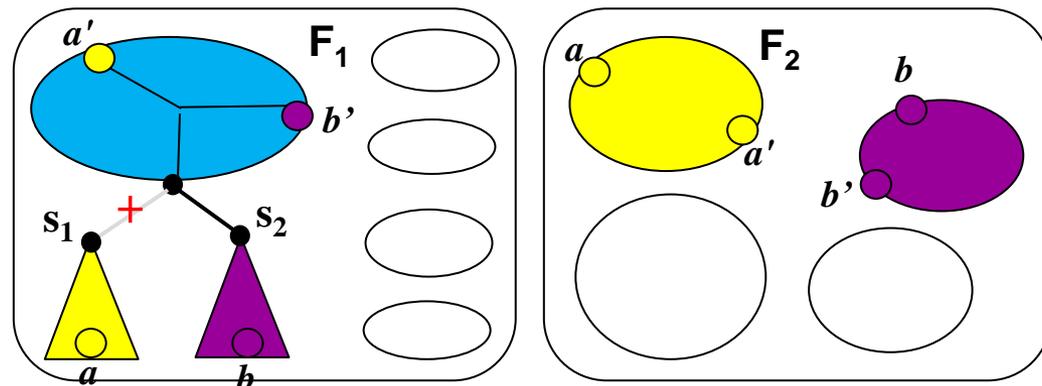


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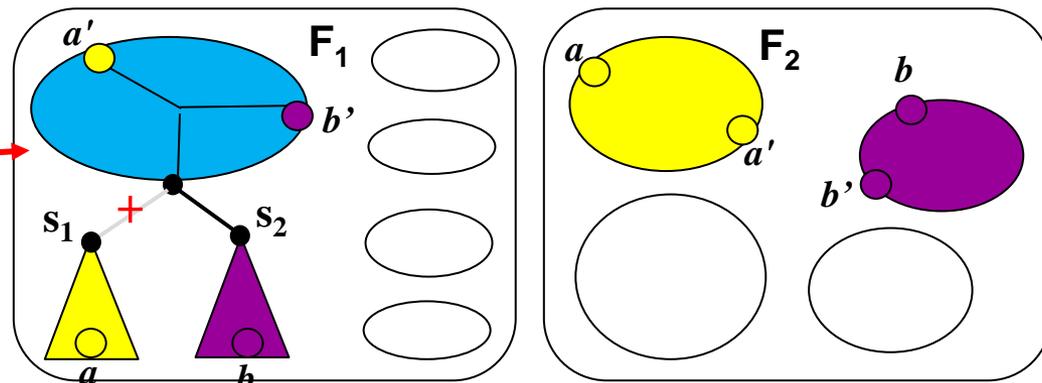
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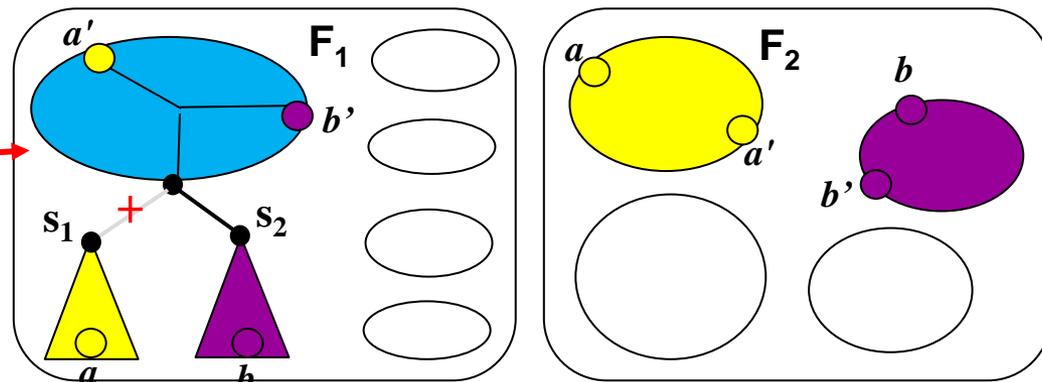
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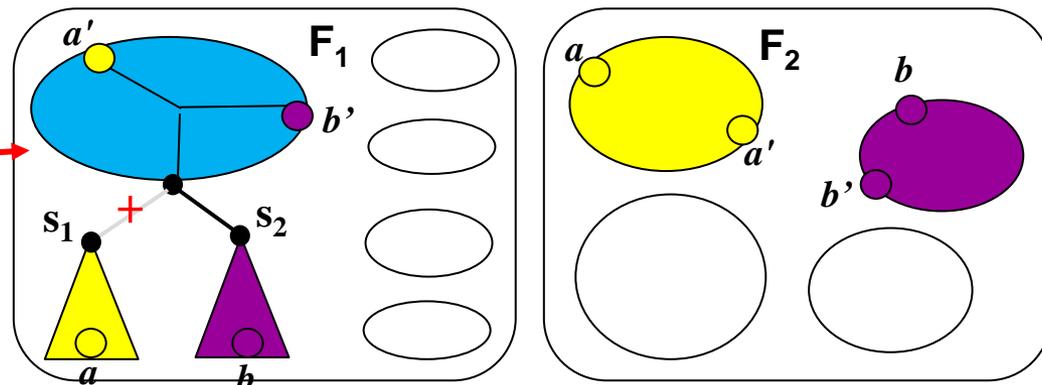
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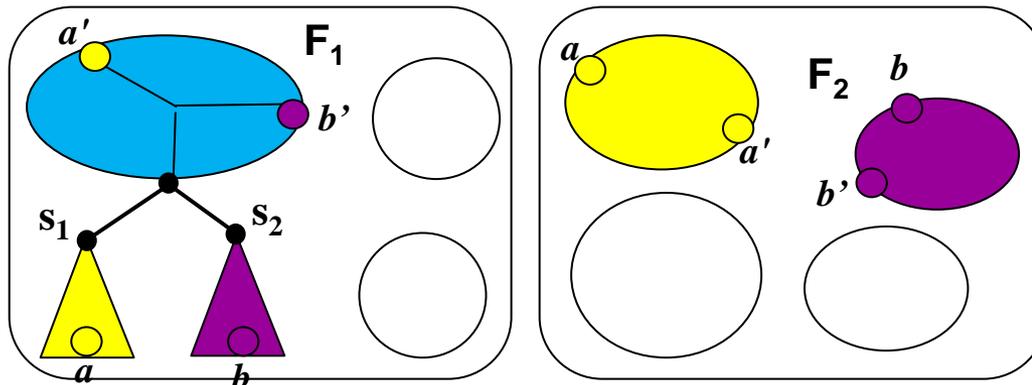
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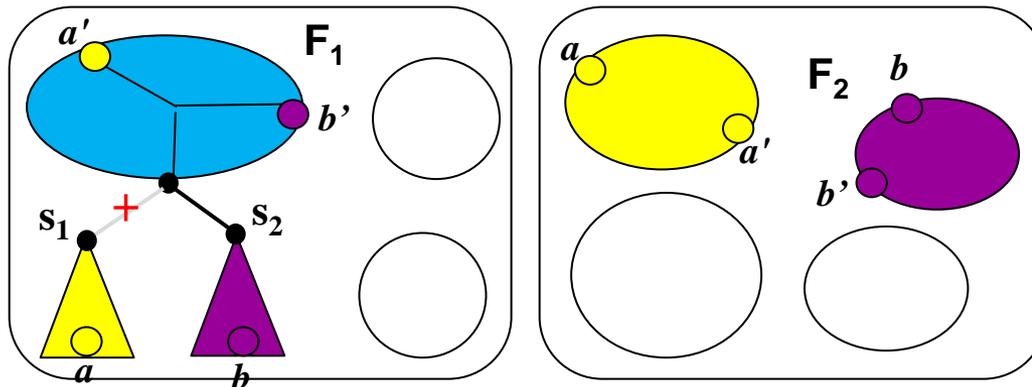
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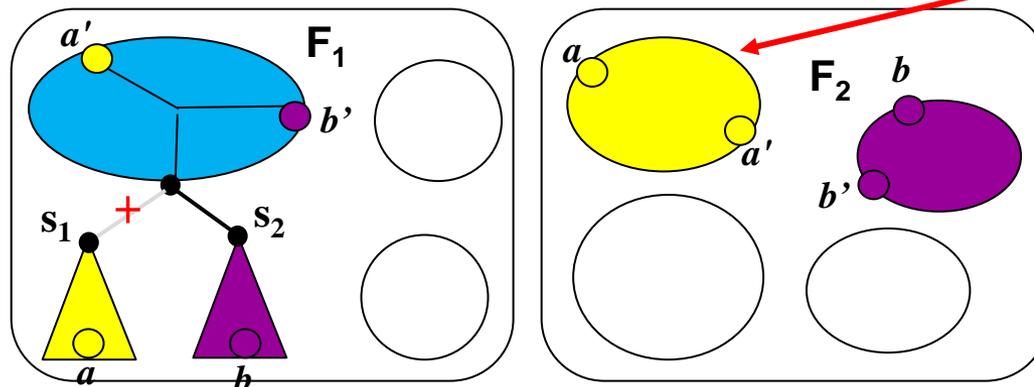
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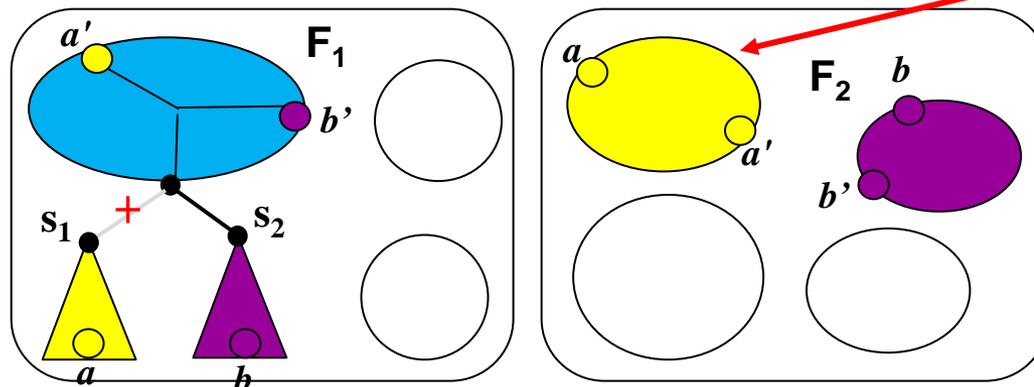
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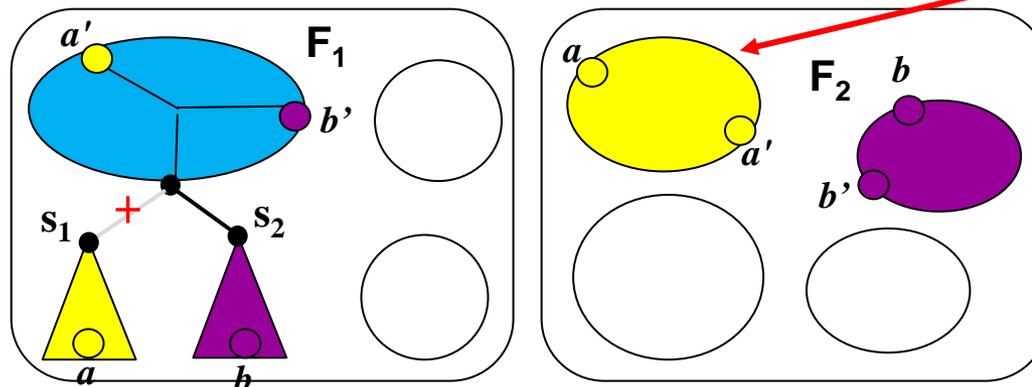
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Theorem. Let Φ_1 and Φ_2 be label-isomorphic X -forests, obtained by h applications of Branching Rule 1 on X -forests F_1 and F_2 . Then

$$\text{Ord}(\Phi_1) = \text{Ord}(\Phi_2) \geq h + \max\{\text{Ord}(F_1), \text{Ord}(F_2)\}$$

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For a given instance $\{F_1, F_2, \dots, F_h\}$, we always pick an F_p of the largest order and an F_q that is not label-isomorphic to F_p , and make them label-isomorphic. This process decreases the parameter k at least as good as $T(k) = 2 T(k-1)$

Multiple X-trees

Observation. Any MAF algorithm of running time $O^*(c^k)$ with $c \geq 2$ on two X-forests, based on exhaustive search can be translated into an $O^*(c^k)$ -time MAF algorithm on multiple X-forests.

Remark. This seems to provide a rather general tool to reduce the MAF problem on multiple trees to the problem with two trees.

Corollary. The MAF problem on multiple rooted general X-trees can be solved in time $O^*(2.42^k)$.

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- ❑ Ratio-(d+1) for two rooted general trees [Rodrigues et al. 2007]
- ❑ Ratio-8 for multiple rooted binary trees [Chataigner 2005]

Approximation Algorithms

More recent work on two binary trees

For two rooted binary trees

- 3-approximation in linear time [Whidden-Zeh 2009]
 - 2.5-approximation [Shi et al. 2016]
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For two unrooted binary trees

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Approximation Algorithms

Our Approach

- **Basic idea:**

In the study of parameterized algorithms for the MAF problem, our basic operation is to find a collection B of essential edges in which one must be removed, and branch on removing each of the edges in B

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In the study of parameterized algorithms for the MAF problem, our basic operation is to find a collection B of essential edges in which one must be removed, and branch on removing each of the edges in B

- **Thus:**

If we remove **all** edges in B , then we get an approximation algorithm of ratio $|B|$ for the MAF problem.

Approximation Algorithms

- **3-approximation for MAF on 2 unrooted general X-trees** [JC-Fan-Sze 2013]

Approximations on 2 rooted (soft) general X-trees with ratio 4 [van Iersel et al. 2014] and 3 [Whidden et al. 2016]

- **3-approximation for MAF on multiple rooted binary trees** [JC-Shi-Feng-Wang 2014]

3-approximation for the problem was independently developed by [Mukhopadhyay-Bhabak 2016]

- **4-approximation for MAF on multiple unrooted binary trees** [JC-Shi-Feng-Wang 2014]
-

Conclusions and Final Remarks

- ❑ **MAF and related problems from evolutionary biology offer nice combinatorial structures for algorithmic research;**
 - ❑ **The research is still in a fairly preliminary stage;**
 - ❑ **Most developed techniques are elementary based on straightforward combinatorial structural analysis;**
 - ❑ **Deeper insight and new techniques for more efficient algorithms?**
 - ❑ **Lower bounds?**
 - ❑ **Problem kernelizations?**
-