The Approximability of Maximum Rooted Triplets Consistency with Fan Triplets and Forbidden Triplets

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  (Lund University, Sweden)

Introduction

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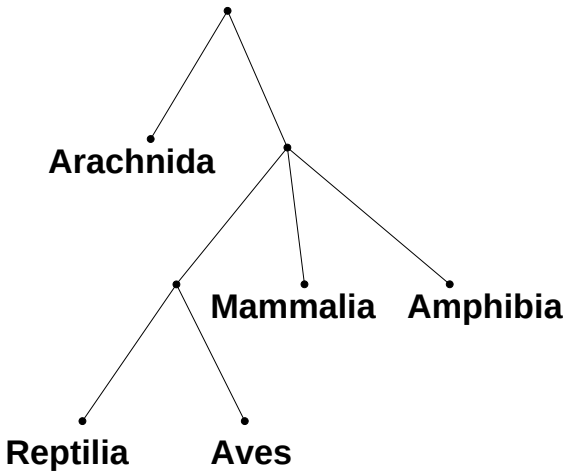
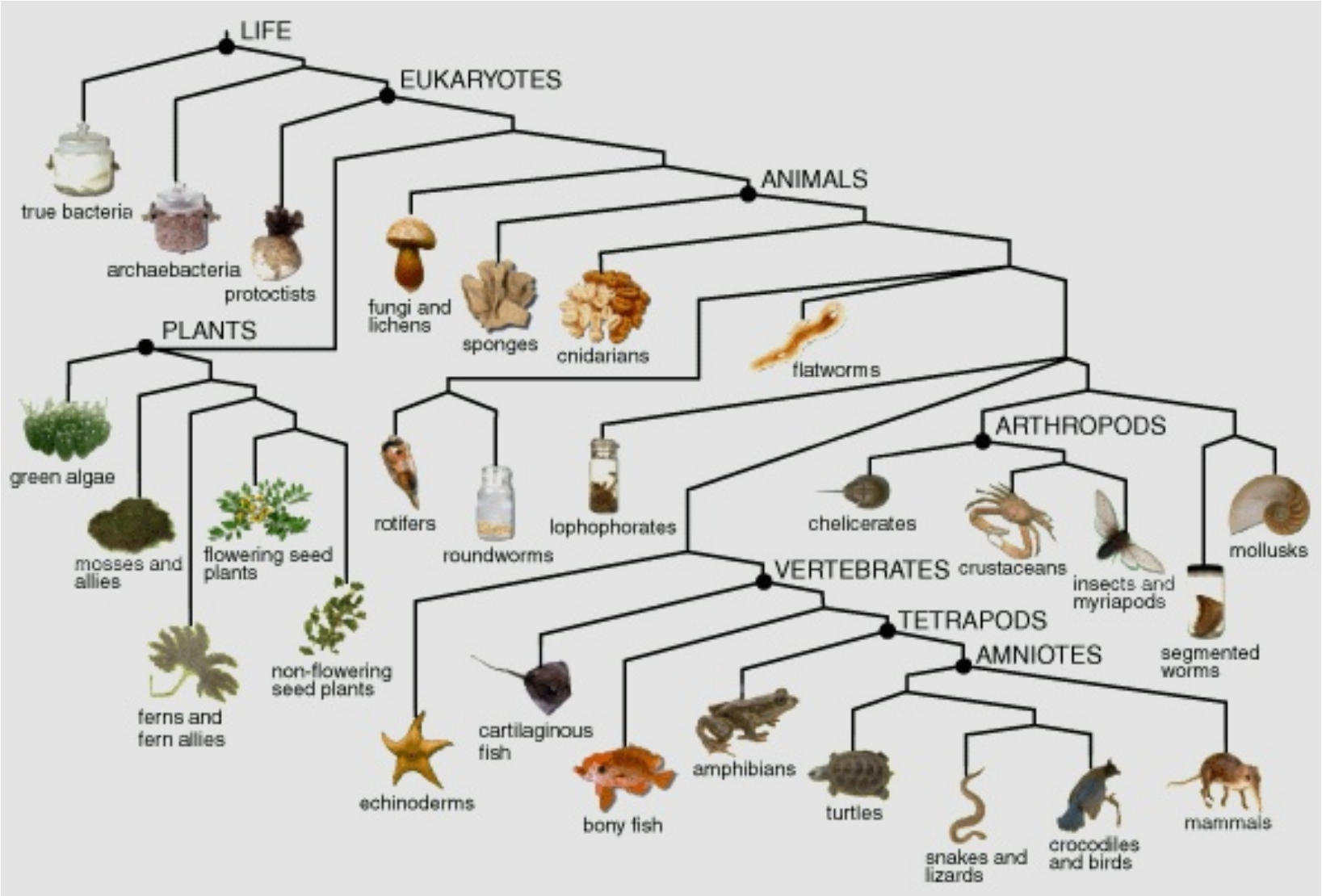


Main idea:

- Represent objects by *leaves* in the tree.
- Select branching structure so that *internal nodes* correspond to common ancestors.

Example



(Figure from `http://biology.unm.edu/ccouncil/Biology_203`)

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- For various reasons, inferring an accurate phylogenetic tree can be a difficult problem.
- For example, small changes in the input data may produce trees with very different structures.
- Furthermore, many of the underlying computational problems are $\mathcal{NP}$-hard optimization problems.

Inferring phylogenetic trees, cont.

Different types of data available. $\Rightarrow$ Different methods may be appropriate.

This talk is focused on one particular method:
The phylogenetic supertree approach

Phylogenetic supertree

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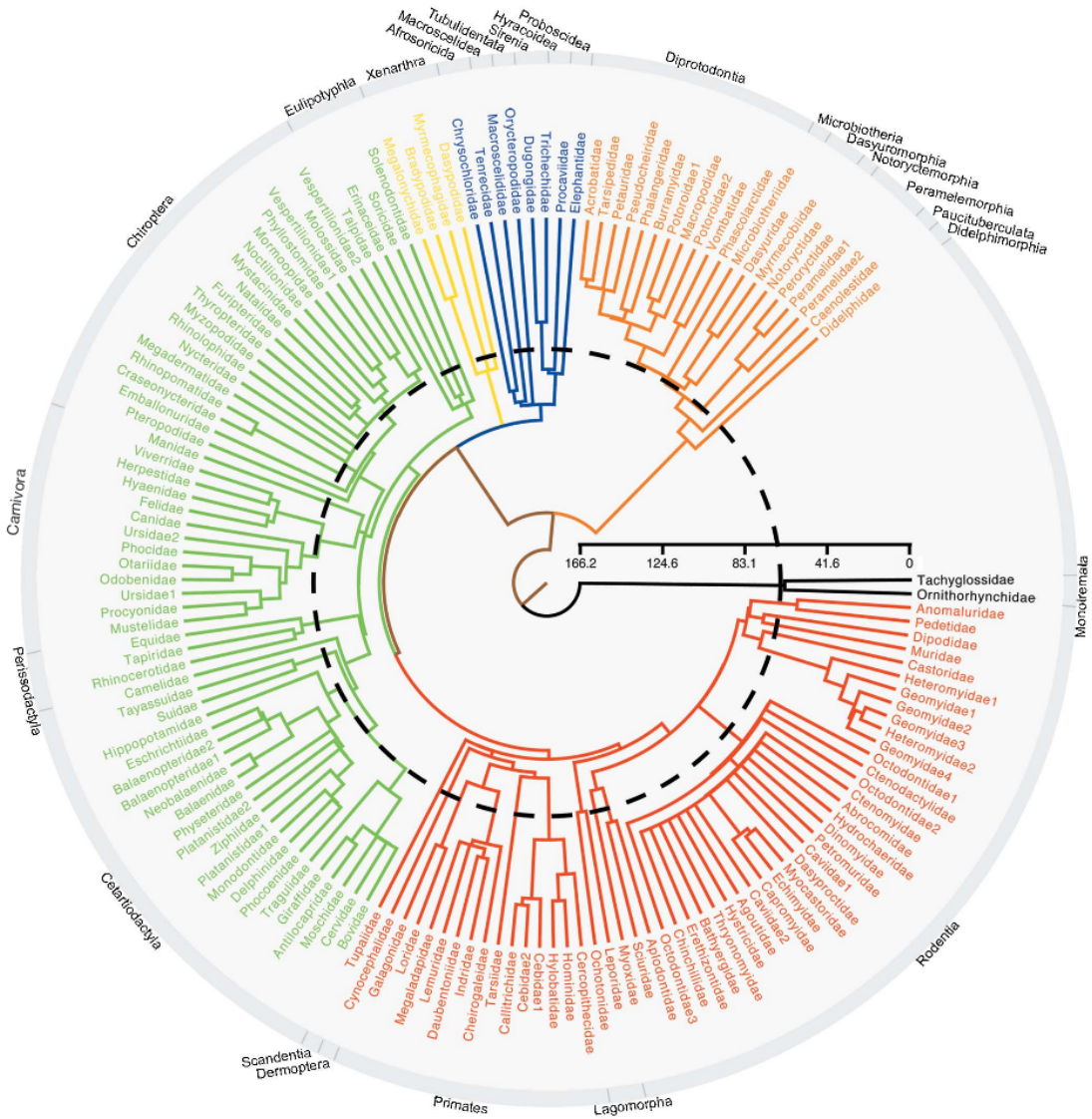
- Most individual studies investigate relatively few species.
  Supertrees allow us to deduce new, hypothetical evolutionary relationships.
- Computationally expensive methods can yield highly accurate phylogenetic trees for small, overlapping subsets of the objects.
  $\Rightarrow$ A "divide-and-conquer"-based technique for inferring large trees.
  Has become popular in recent years.

Phylogenetic supertree, example



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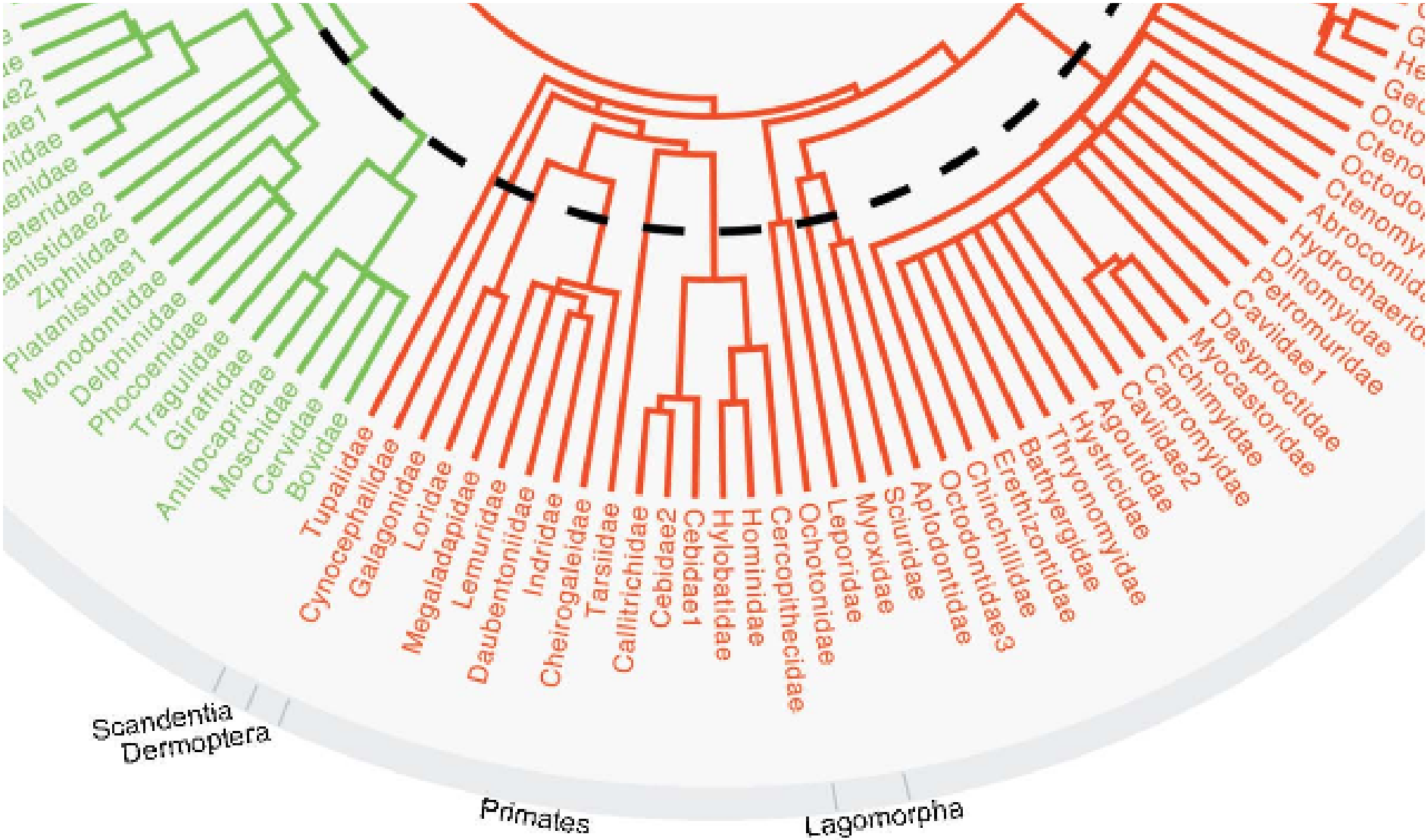

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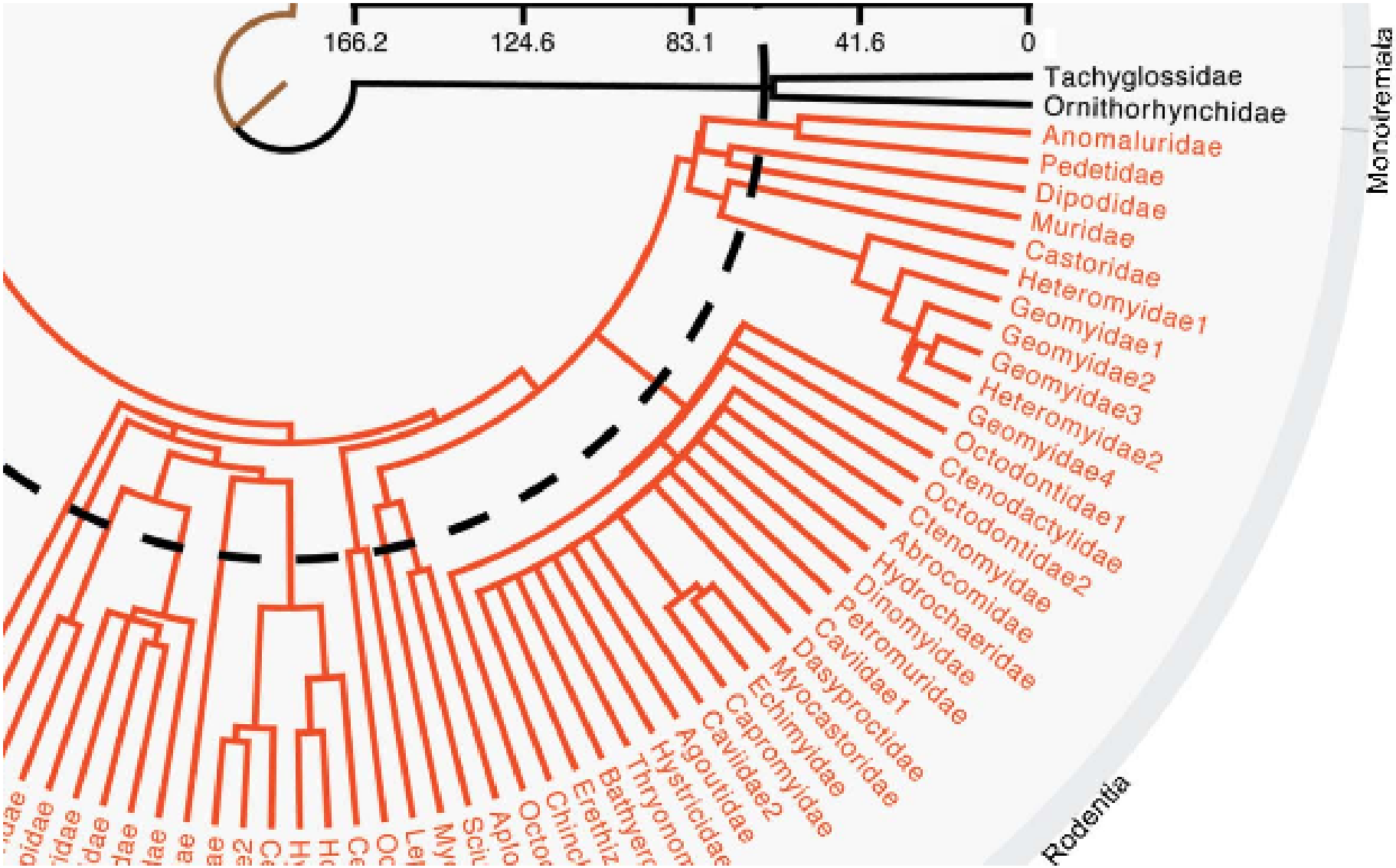

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- Also, every leaf is identified with its label.

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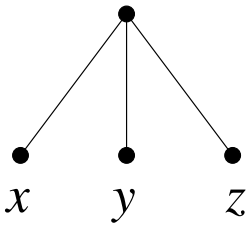
There are four different possible trees leaf-labeled by $\{x, y, z\}$:



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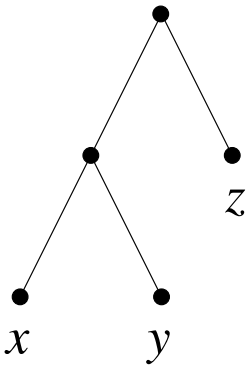

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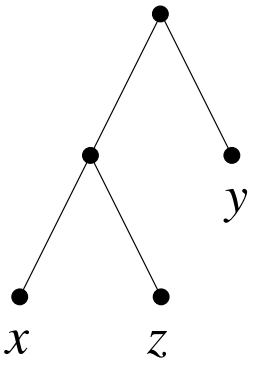

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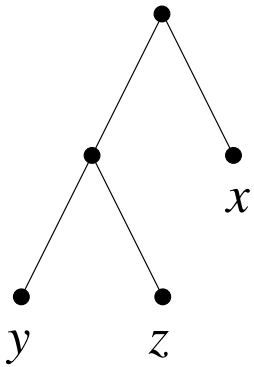

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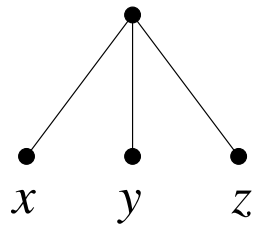

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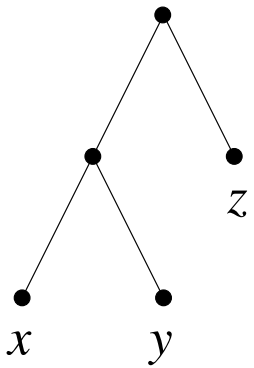

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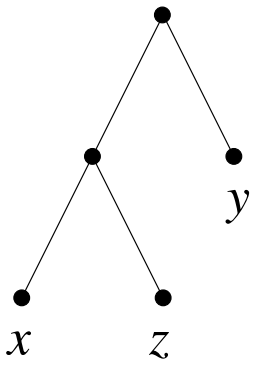

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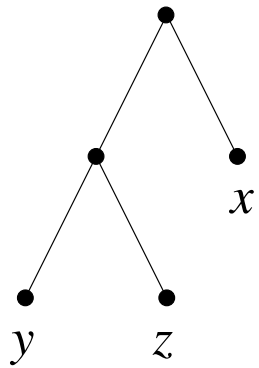

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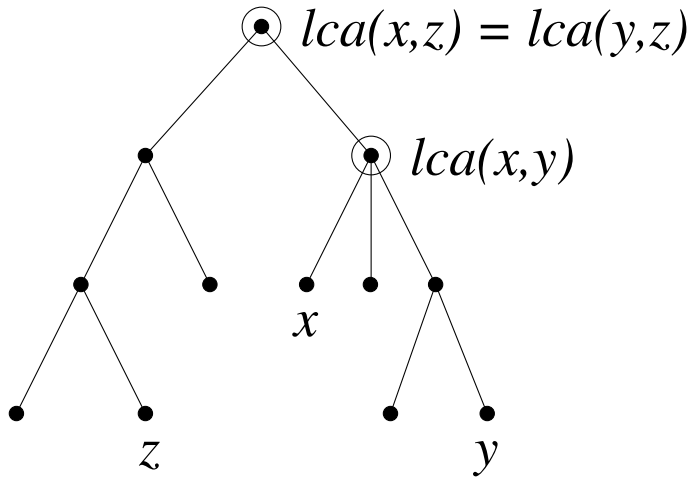
Two types of rooted triplets:

- *Fan triplet* = One internal node $(x|y|z)$
- *Resolved triplet* = Two internal nodes $(xy|z,\ xz|y,$ and $yz|x)$

Notation, cont.

Let x, y, z be three leaves in a tree T.

- If $lca(x, y)$ is a proper descendant of $lca(x, z) = lca(y, z)$ in T then we say that T and the resolved triplet $xy|z$ are *consistent*.



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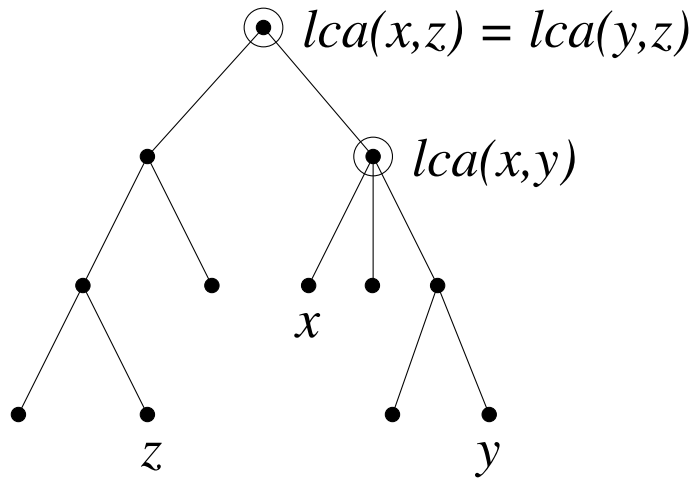

- On the other hand, if $lca(x, y) = lca(x, z) = lca(y, z)$ in T then T and the fan triplet $x|y|z$ are *consistent*.

Combining a set of rooted triplets

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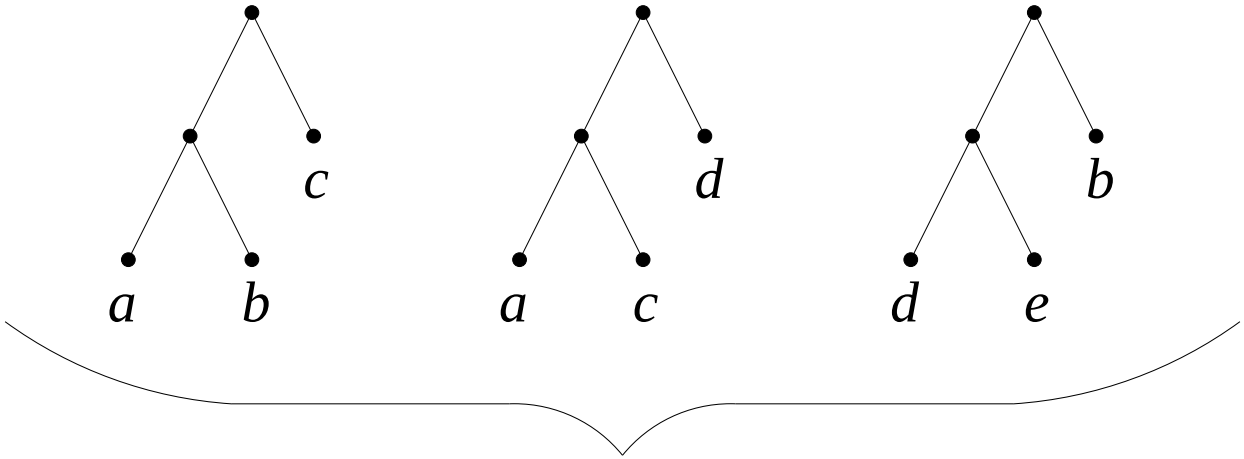

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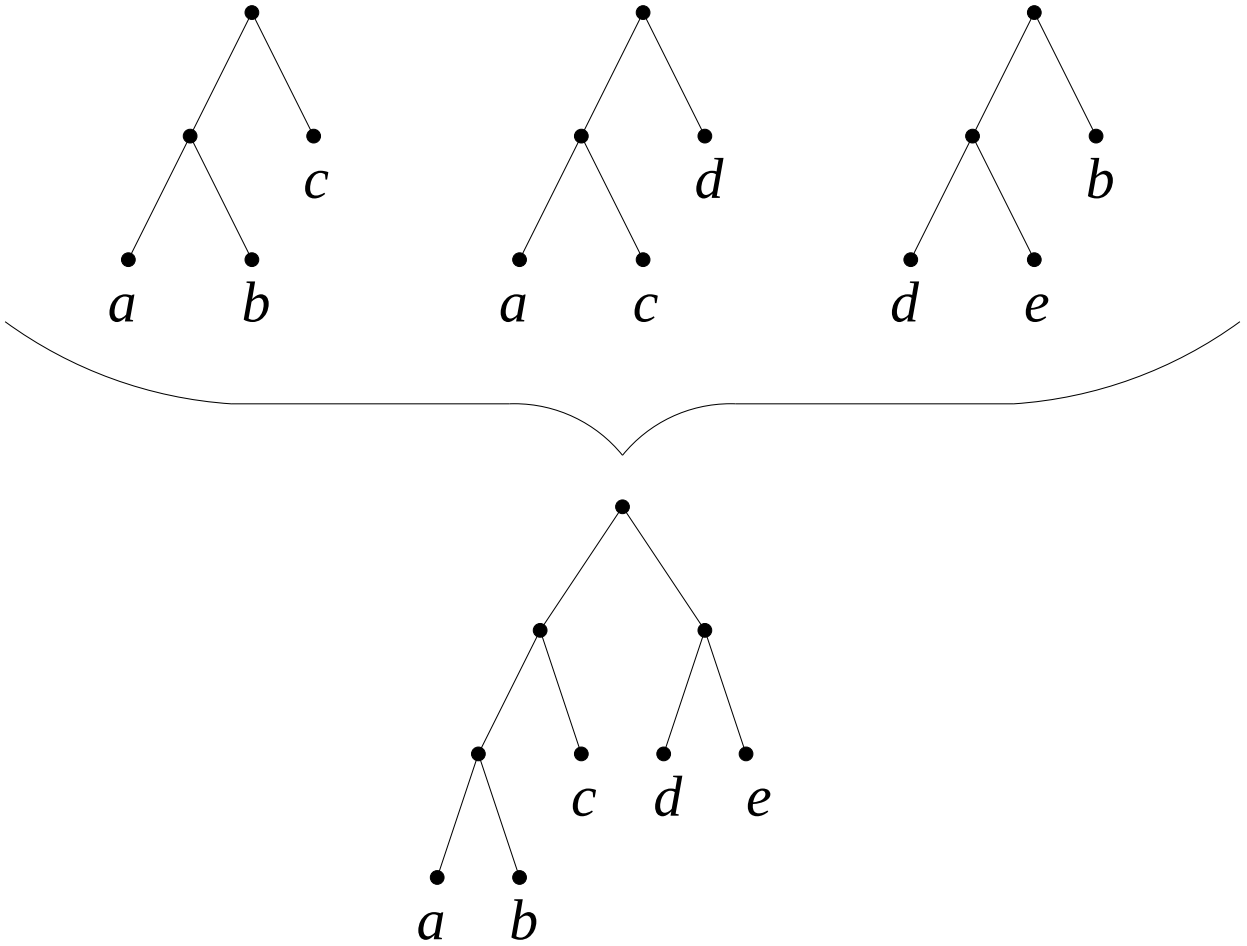

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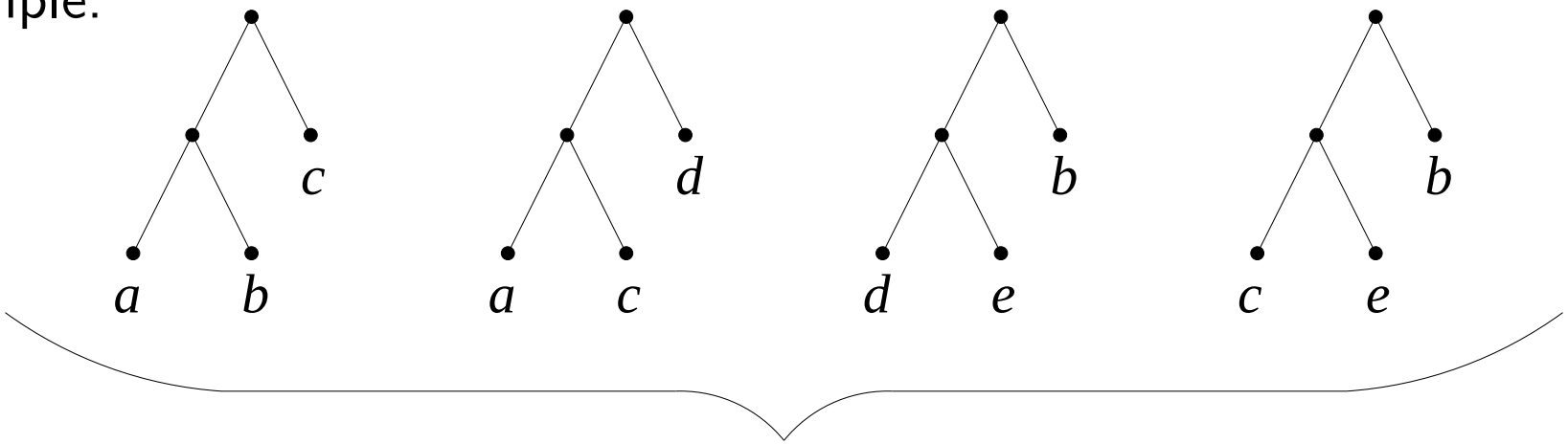

CONFLICT!!!

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Input: Two sets $\mathcal{G}$ and $\mathcal{B}$ of rooted triplets.

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The input rooted triplets can be interpreted as *constraints*:

- Resolved triplets in $\mathcal{G}$ = "constraints of type 1"
- Fan triplets in $\mathcal{G}$ = "constraints of type 2"
- Resolved triplets in $\mathcal{B}$ = "constraints of type 3" = "forbidden resolved triplets"
- Fan triplets in $\mathcal{B}$ = "constraints of type 4" = "forbidden fan triplets"

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  Polynomial-time algorithm to determine if there is a tree consistent with all of the resolved triplets in a set, and if so, to output such a tree.

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- Wu (2004):
  Exact $O(3^n(m+n^2))$-time algorithm for MTC restricted to resolved triplets, where n = number of leaf labels and m = number of input triplets.

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4. Polynomial-time approximation scheme (PTAS) for dense MTC, where an instance is called dense if it contains $\Omega(n^3)$ constraints:

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Proof: Let T be the output of the algorithm. There are two cases.

- $|\mathcal{R}_2| + |\mathcal{R}_3| \geq \frac{m}{4}$: Then T satisfies at least $\frac{m}{4}$ input constraints.
- $|\mathcal{R}_1| + |\mathcal{R}_4| > \frac{3m}{4}$: The output of [Gąsieniec *et al.* (1999)] is a binary tree consistent with at least $\frac{1}{3}$ of the input resolved triplets.
  $\Rightarrow$ T satisfies $\geq \frac{1}{3}|\mathcal{R}_1| + |\mathcal{R}_4| \geq \frac{1}{3}(|\mathcal{R}_1| + |\mathcal{R}_4|) > \frac{1}{3} \cdot \frac{3m}{4} = \frac{m}{4}$ constraints. □

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- Traceback to recover an optimal tree.
- $\Rightarrow O(3^n(m + n^2))$ time, where $n = |S|$ and $m =$ number of input triplets.

2. An exact algorithm for MTC, cont.

The new algorithm:

- **Notation:** For any $U \subseteq S$ and any partition P of U with $|P| \geq 2$, let
  - $w_2(P)$ = the number of input resolved triplets $ab|c$ such that a and b belong to two different parts in P and $c \notin U$.
  - $w_3(P)$ = the number of input fan triplets $a|b|c$ such that a, b, c belong to three different parts in P.
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  - $w_{f3}(P)$ = the number of input forbidden fan triplets $\neg(a|b|c)$ such that two elements in $\{a, b, c\}$ belong to two different parts in P and the remaining one does not belong to U.

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- Let $I(T)$ be the set of internal nodes in a tree T. For $v \in I(T)$, denote: T_v = the subtree of T rooted at v, $\{v_1, \ldots, v_l\}$ = the set of children of v, and π_v = the partition of $\Lambda(T_v)$ into $\Lambda(T_{v_1}), \ldots, \Lambda(T_{v_l})$.

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Lemma: For any T with $\Lambda(T) = S$, the # of input constraints satisfied by T is: $\sum_{v \in I(T)}(w_2(\pi_v) + w_3(\pi_v) + w_{f2}(\pi_v) + w_{f3}(\pi_v))$.

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- Let $k \geq 2$ be a parameter.

  The new algorithm forces the output to be a k-ary tree, i.e., a tree in which every internal node has at most k children.

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  $\Rightarrow$ $\boxed{O((k+1)^{n+1}(m+n))}$ time to solve MTC exactly over all k-ary trees.

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Exponential-time approximation scheme (ETAS) for MTC:
For any constant $\epsilon > 0$, we can build a tree consistent with $\geq (1 - \epsilon)$ of the maximum number of input constraints consistent with any tree in $O((\lceil \frac{12}{\epsilon} \rceil + 1)^{n+1}(m + n))$ time.

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- Suppose $\deg(v) = \ell > k$. For any fan triplet $a|b|c$ contributing to $w_3(\pi_v)$, if a, b, c are distributed among k groups uniformly at random then $Pr[$any two elements in $\{a, b, c\}$ end up in the same group$] \leq 1/k + 2/k = 3/k$.

  $\Rightarrow$ There exists some partition of $v_1, \ldots, v_\ell$ into k subtrees that satisfies $\geq 1 - 3/k$ of the fan triplets contributing to $w_3(\pi_v)$.

  etc. □

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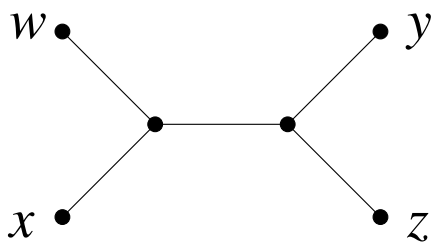
Relies on the technique introduced by [Jiang, Kearney, Li (2001)] for maximizing *unrooted quartet consistency* (MQC).

Unrooted quartet:



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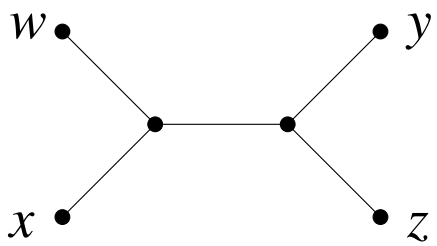

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We cannot apply their PTAS directly to our problem because of the fan triplets and the forbidden rooted triplets, but we can adapt their technique to our setting.

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The resulting algorithm:

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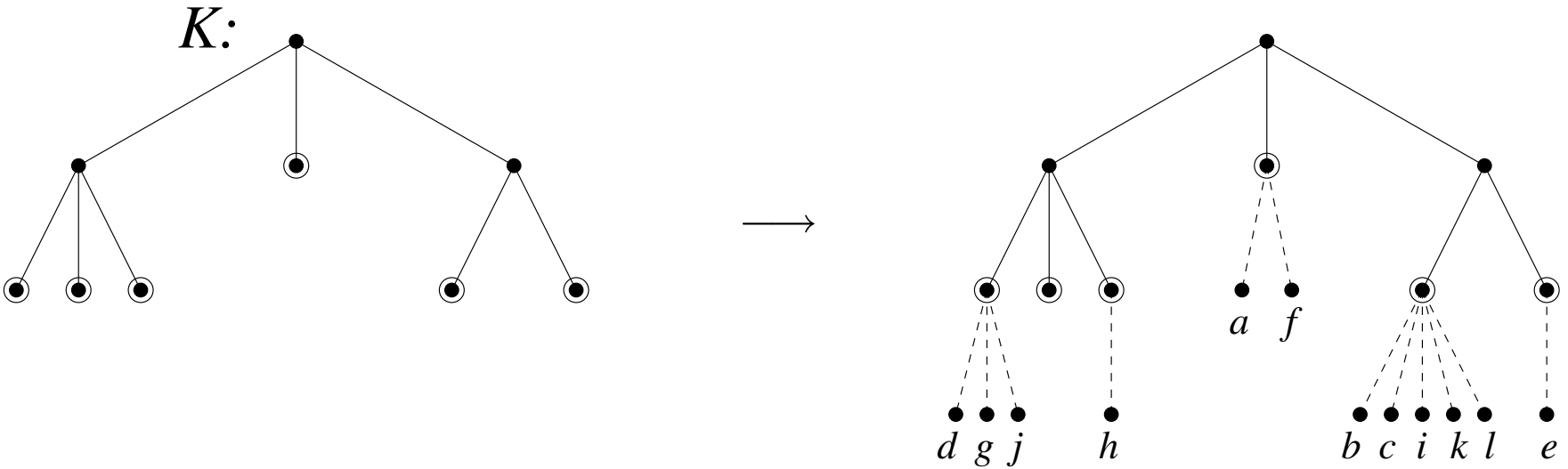
- For each such tree K: Every leaf of K is called a bin.
  Approximately solve the *Label-to-Bin Assignment Problem* (LBA) on K:
  Attach the n leaf labels to the k bins of K so that each bin gets $\leq \frac{6n}{k}$ leaves and the resulting tree is consistent with the maximum # of input constraints.



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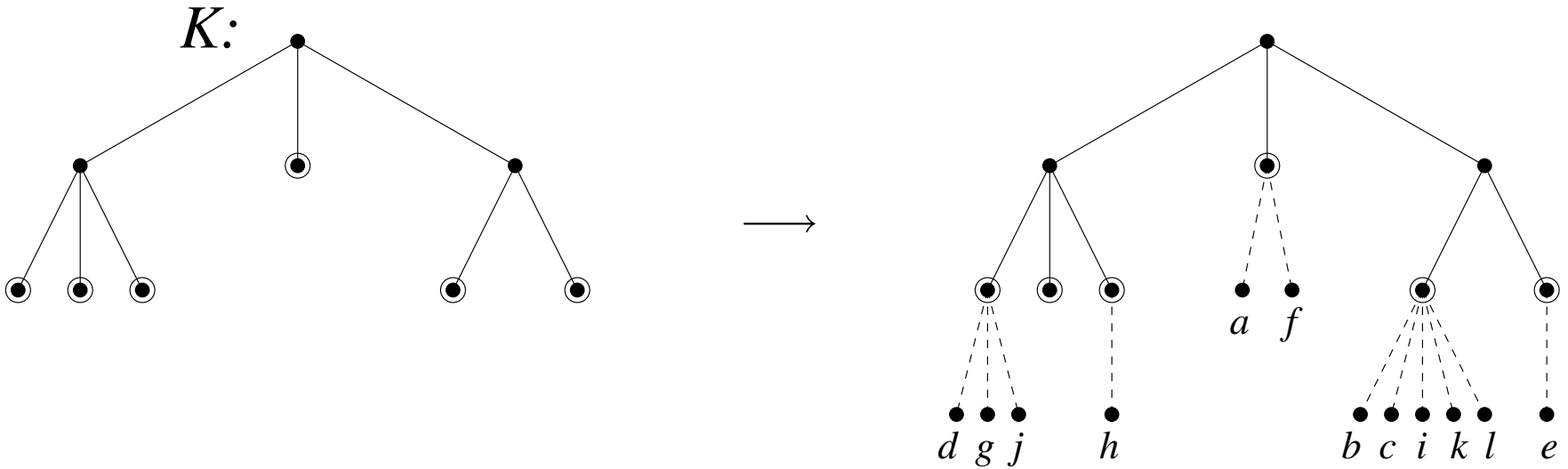

- Output the best solution to MTC found.

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- Finally, define:

$$p(x) = \sum_{ab|c \in I} p_{ab|c}(x) + \sum_{a|b|c \in I} p_{a|b|c}(x) + \sum_{\neg(ab|c) \in I} p_{\neg(ab|c)}(x) + \sum_{\neg(a|b|c) \in I} p_{\neg(a|b|c)}(x)$$

- LBA becomes:

Maximize $p(x)$ subject to

$\sum_{i=1}^{k} x_{\ell i} = 1$ for each leaf label ℓ, $\sum_{\ell=1}^{n} x_{\ell i} \leq \frac{6n}{k}$ for each bin i,

and $x_{\ell i} \in \{0, 1\}$ for all ℓ, i.

4. A PTAS for dense MTC, cont.

- Finally, define:

$$p(x) = \sum_{ab|c \in I} p_{ab|c}(x) + \sum_{a|b|c \in I} p_{a|b|c}(x) + \sum_{\neg(ab|c) \in I} p_{\neg(ab|c)}(x) + \sum_{\neg(a|b|c) \in I} p_{\neg(a|b|c)}(x)$$

- LBA becomes:

Maximize $p(x)$ subject to

$\sum_{i=1}^{k} x_{\ell i} = 1$ for each leaf label ℓ, $\sum_{\ell=1}^{n} x_{\ell i} \leq \frac{6n}{k}$ for each bin i,

and $x_{\ell i} \in \{0, 1\}$ for all ℓ, i.

Arora, Karger, Karpinski (1999):
A degree-d polynomial integer program is c-smooth if the absolute value of each coefficient of each degree-i term is $\leq c \cdot n^{d-i}$.

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As in Jiang *et al.* (2001), apply the general-purpose PTAS of Arora *et al.* (1999) for c-smooth integer programs to get a PTAS for our variant of LBA.

4. A PTAS for dense MTC, cont.

Time complexity analysis:

- k is a constant, so the number of unlabeled, unordered rooted trees with k leaves and no degree-1 nodes is a constant.

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$\Rightarrow$ The time complexity is polynomial. □

4. A PTAS for dense MTC, cont.

Approximation ratio analysis:

Lemma: Let T be a tree consistent with the maximum number of constraints in I. There exists a tree T' obtained by attaching the n leaf labels to an unlabeled tree with k bins such that $|\mathcal{R}_{T'} \cap I| \geq |\mathcal{R}_T \cap I| - \frac{96}{k} \cdot n^3$.

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The PTAS of Arora *et al.* finds an $(1 - \epsilon'')$ approximation T'' of such a T', so:

$$|\mathcal{R}_{T''} \cap I| \;\geq\; (1 - \epsilon'') \cdot |\mathcal{R}_{T'} \cap I| \;\geq\; (1 - \epsilon'') \cdot (|\mathcal{R}_T \cap I| - \frac{96}{k} \cdot n^3)$$

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Next, note that $|I| \geq \gamma \cdot n^3$ for some constant γ by the definition of dense.
The $\frac{1}{4}$-approximation algorithm from before $\Rightarrow |\mathcal{R}_T \cap I| \geq \frac{|I|}{4} \Rightarrow n^3 \leq \frac{4 \cdot |\mathcal{R}_T \cap I|}{\gamma}$

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Combine the inequalities:

$$|\mathcal{R}_{T''} \cap I| \;\geq\; (1 - \epsilon'') \cdot |\mathcal{R}_T \cap I| \cdot (1 - \frac{96}{k} \cdot \frac{4}{\gamma})$$

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Combine the inequalities:

$$|\mathcal{R}_{T''} \cap I| \;\geq\; (1-\epsilon'') \cdot |\mathcal{R}_T \cap I| \cdot (1 - \frac{96}{k} \cdot \frac{4}{\gamma})$$

Finally, for any specified $\epsilon > 0$, choosing $k \geq \frac{96 \cdot 4 \cdot 2}{\gamma \cdot \epsilon}$ and $\epsilon'' \leq \frac{\epsilon}{2}$ gives:

$$|\mathcal{R}_{T''} \cap I| \;\geq\; |\mathcal{R}_T \cap I| \cdot (1 - \frac{\epsilon}{2}) \cdot (1 - \frac{\epsilon}{2}) \;\geq\; |\mathcal{R}_T \cap I| \cdot (1-\epsilon) \qquad \square$$

Summary

1. Polynomial-time $\frac{1}{4}$-approximation algorithm for MTC.

2. Extension of Wu's exact exponential-time algorithm for MTC restricted to resolved triplets to also allow fan triplets, forbidden resolved triplets, and forbidden fan triplets.

   It takes an additional parameter $k \geq 2$ as input and forces the output to be a tree in which every internal node has at most k children.

   $\Rightarrow$ Running time: $\boxed{O((k+1)^{n+1}(m+n))}$

3. Exponential-time approximation scheme (ETAS) for MTC:

   For any constant $\epsilon > 0$, we can build a tree consistent with $\geq (1-\epsilon)$ of the maximum number of input constraints consistent with any tree in $\boxed{O((\lceil \frac{12}{\epsilon} \rceil + 1)^{n+1}(m+n))}$ time.

4. Polynomial-time approximation scheme (PTAS) for dense MTC, where an instance is called dense if it contains $\Omega(n^3)$ constraints:

   For any constant $\epsilon > 0$, we can build a tree consistent with $\geq (1-\epsilon)$ of the maximum number of input constraints consistent with any tree in polyn. time.