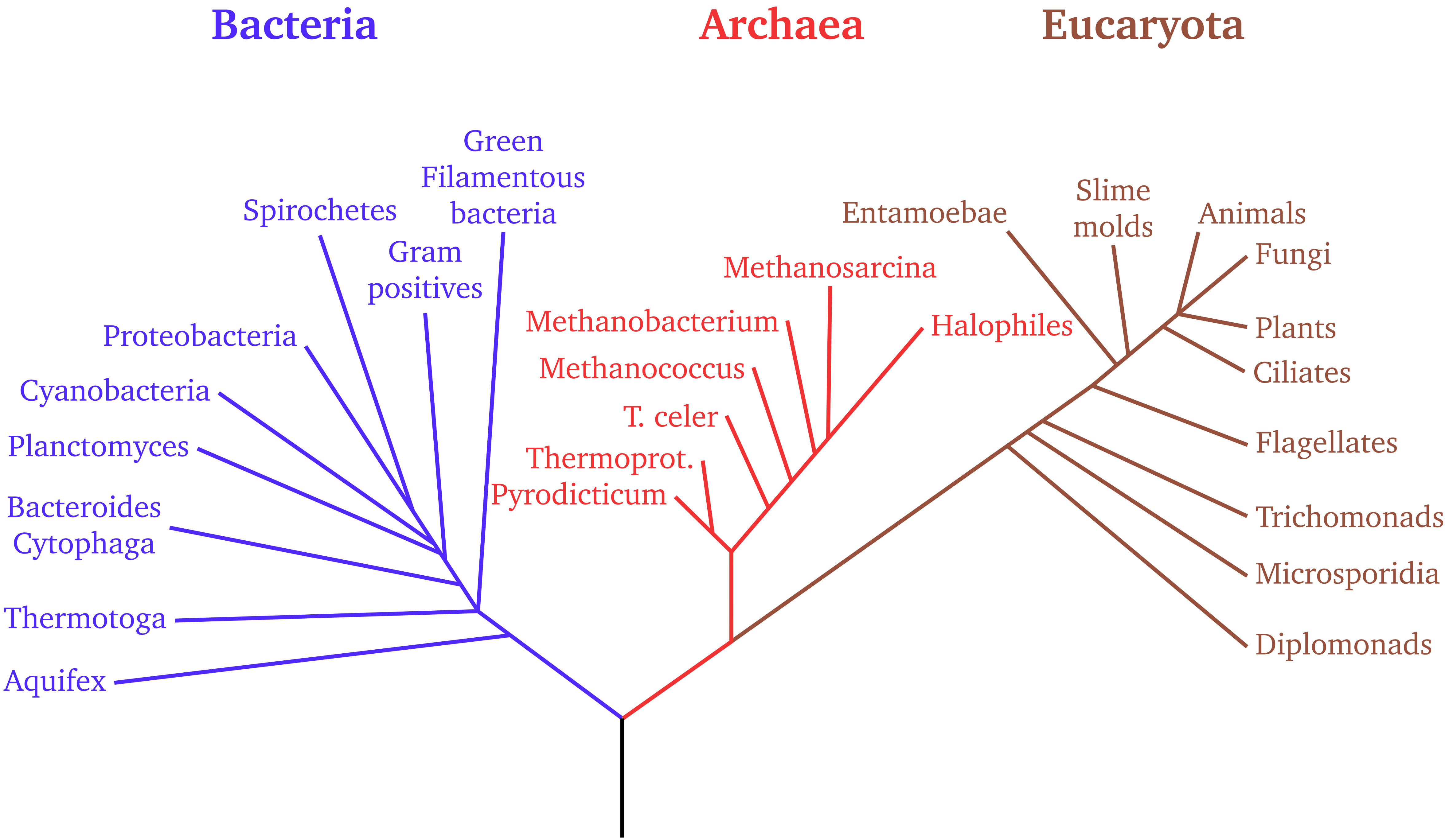
Comparing Phylogenies

Kernelization, Depth-Bounded Search and Beyond

Norbert Zeh

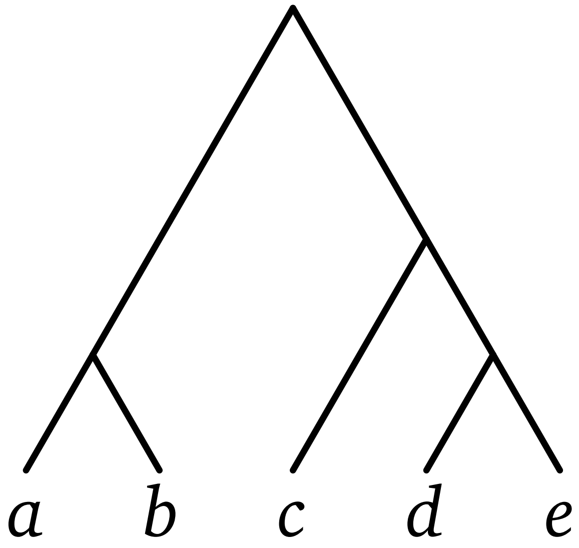
Dalhousie University

Phylogenetic Trees



Reticulation Events

Lateral gene transfer (subtree prune-and-regraft)



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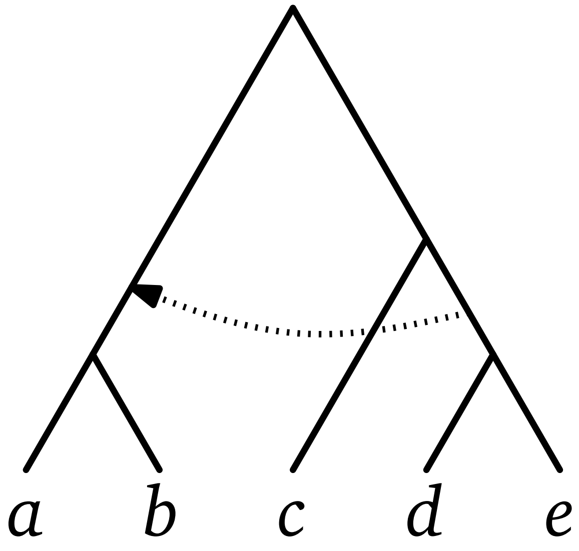

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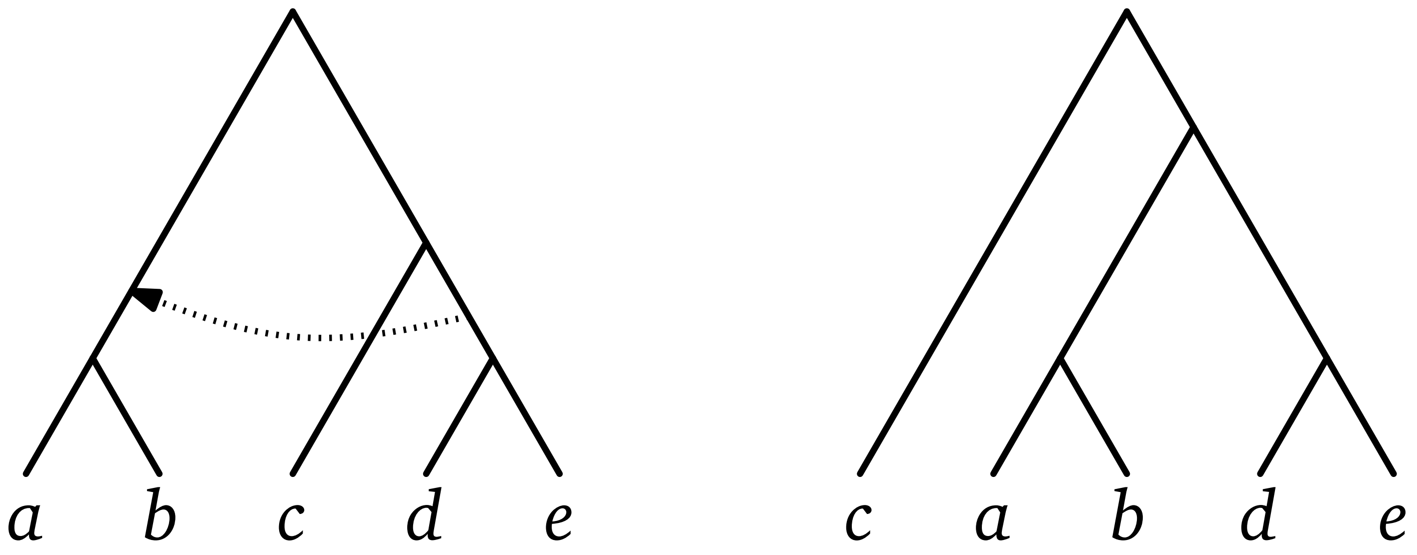

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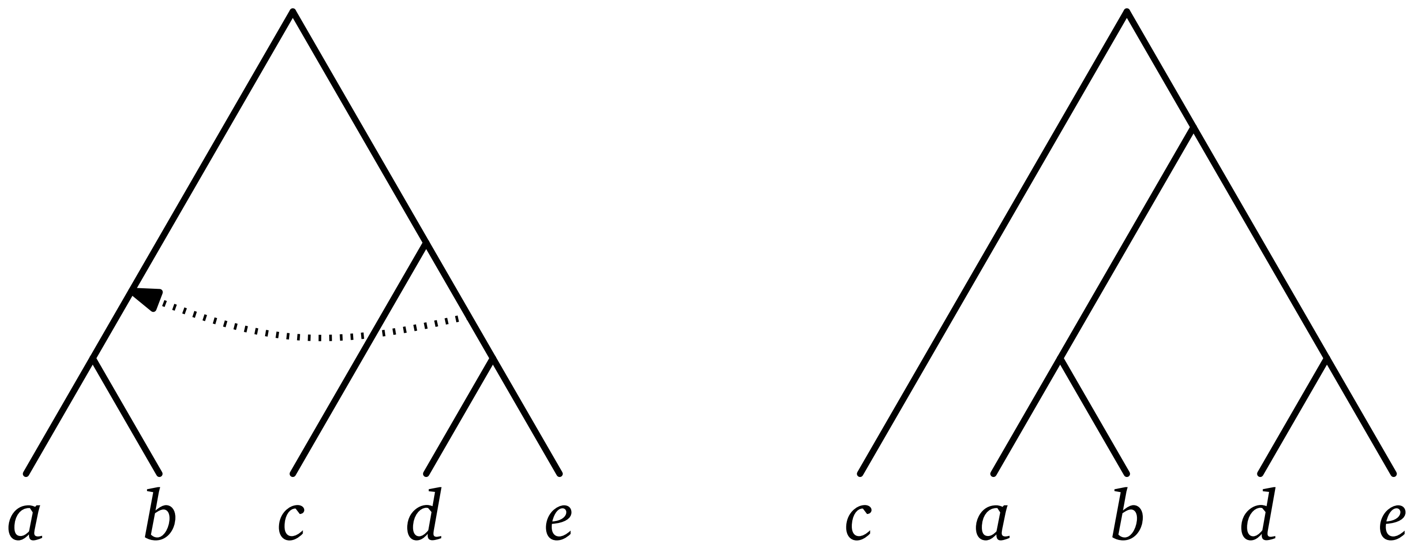

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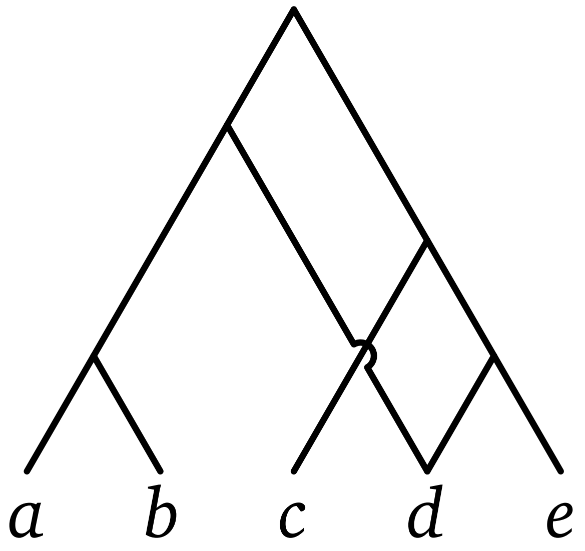

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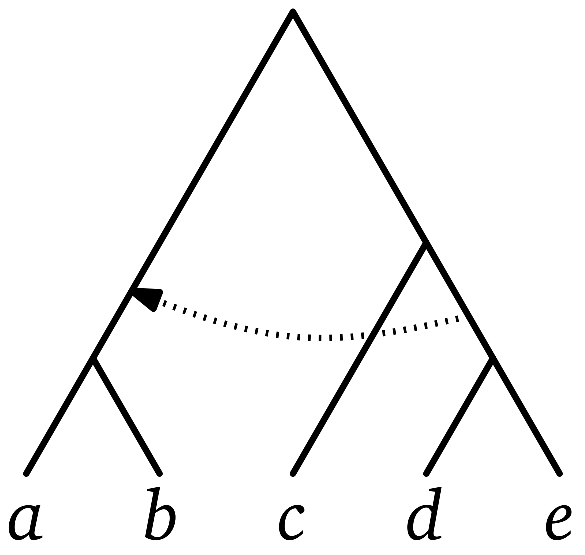

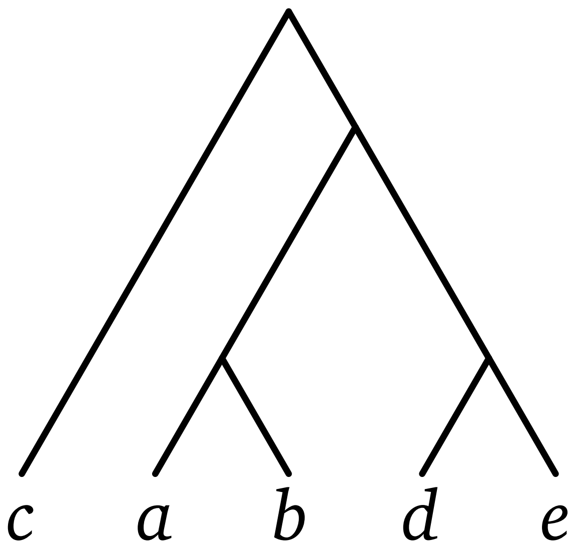

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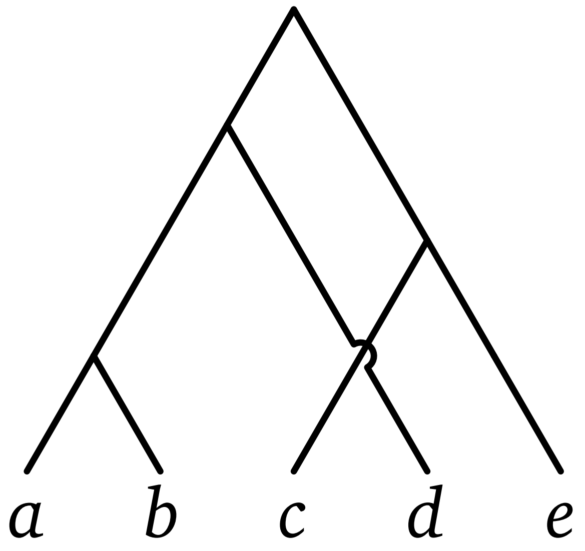

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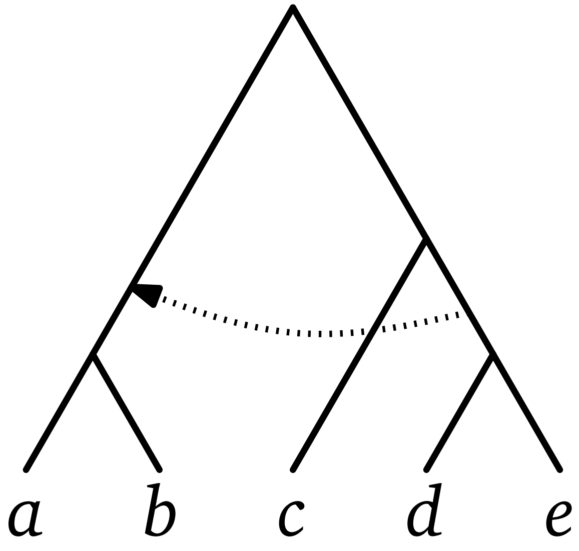

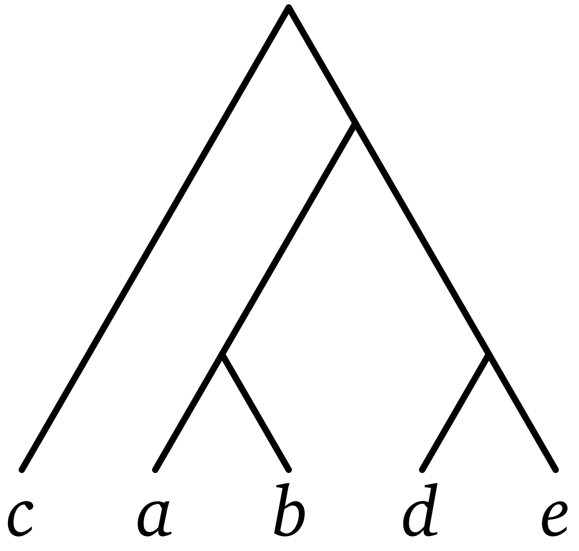

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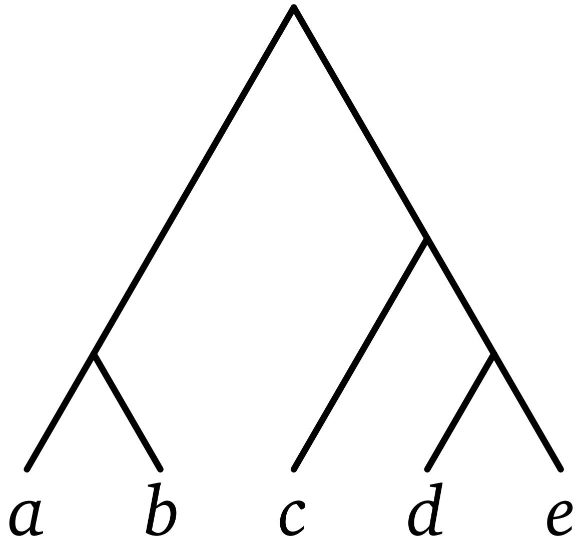

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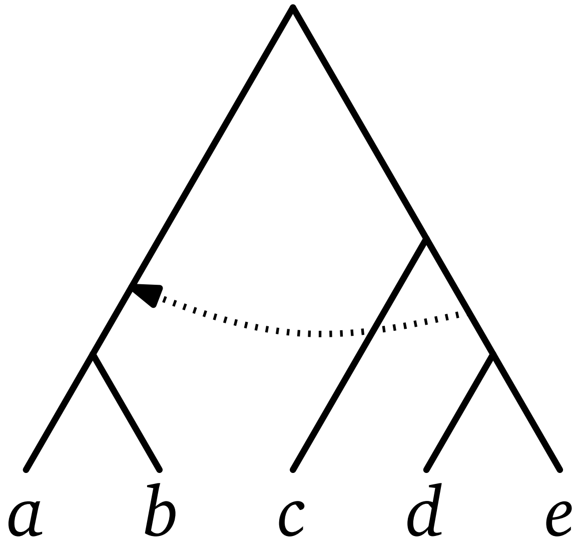

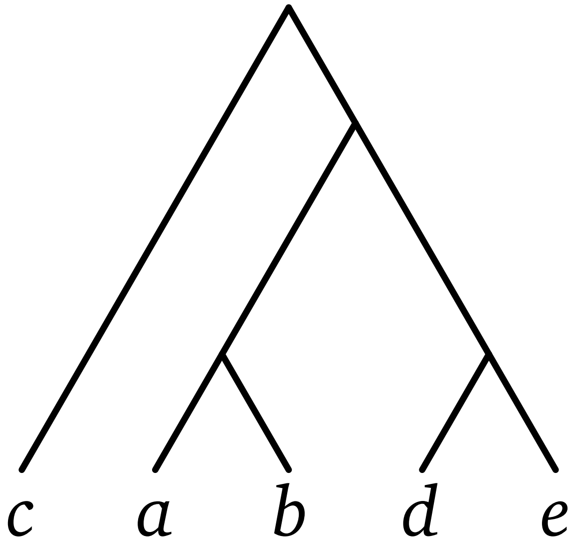

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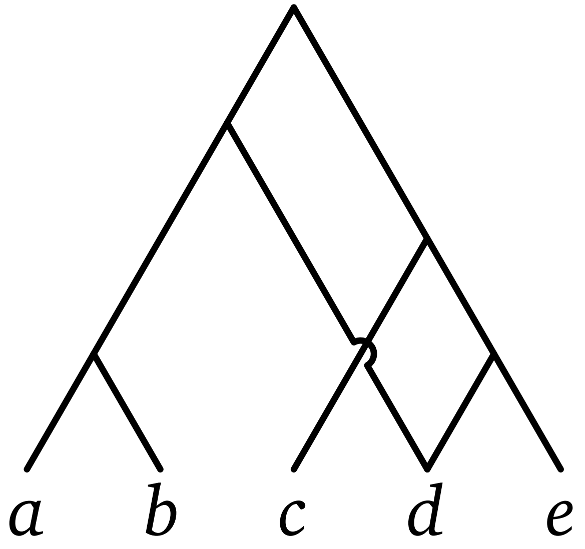


Zeina the Zonkey

Owklawn Farm Zoo, Nova Scotia

Reconciling Phylogenies

1. Tree distances

- ***SPR distance:*** number of SPR operations to transform one tree into the other

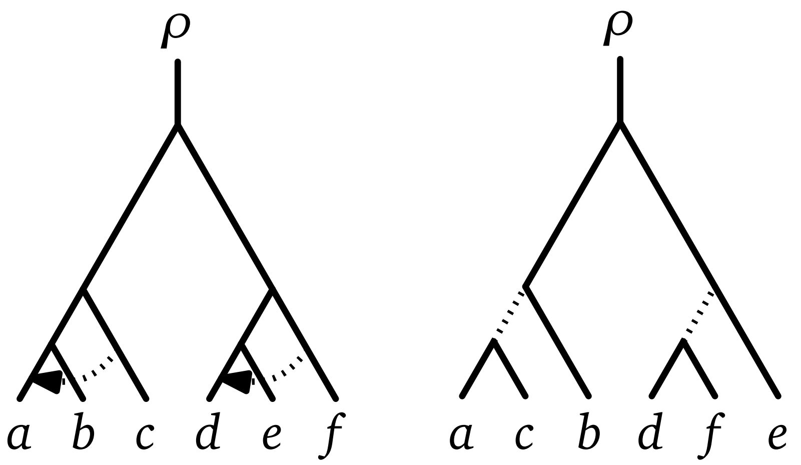
  NP-hard [Bordewich/Semple 2005]

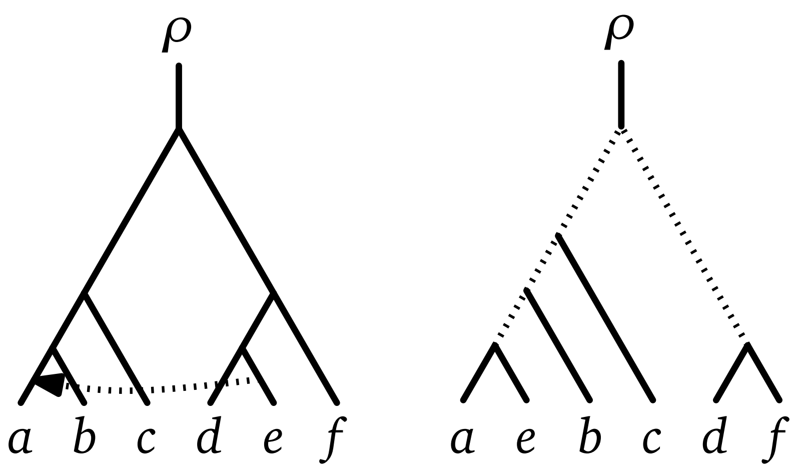
- ***Hybridization number:*** minimum number of nodes with two parents in any network that displays both trees

  NP-hard [Bordewich/Semple 2007]

- ***Robinson-Foulds distance:*** number of bipartitions that disagree

  Linear-time, but . . .





Reconciling Phylogenies

2. Supertrees

- MRP supertrees [Ragan 1992]
- RF supertrees [Bansal et al. 2010]
- SPR supertrees [Whidden/Zeh/Beiko 2012]
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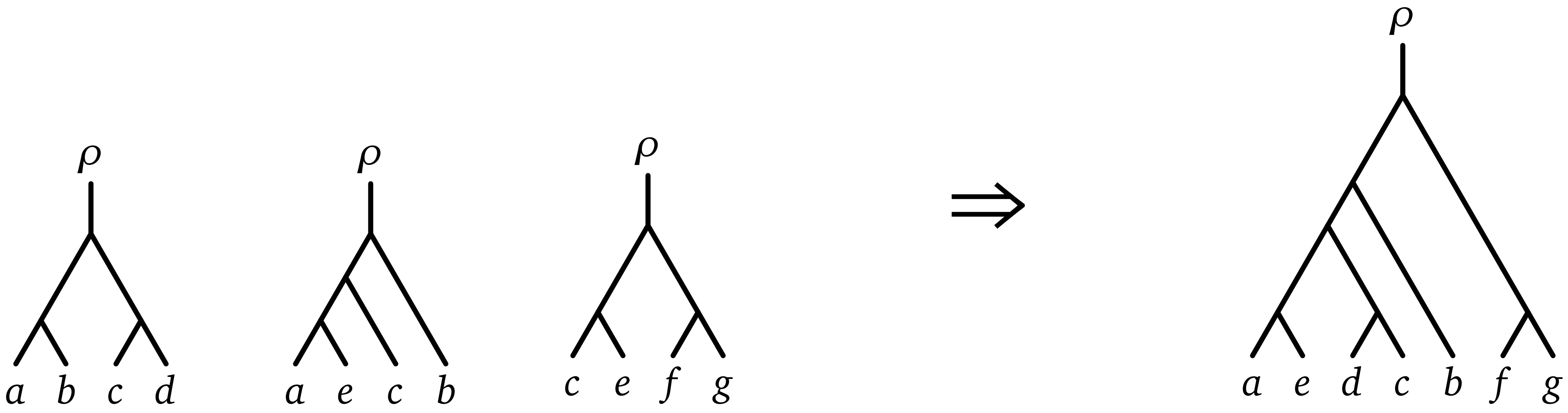

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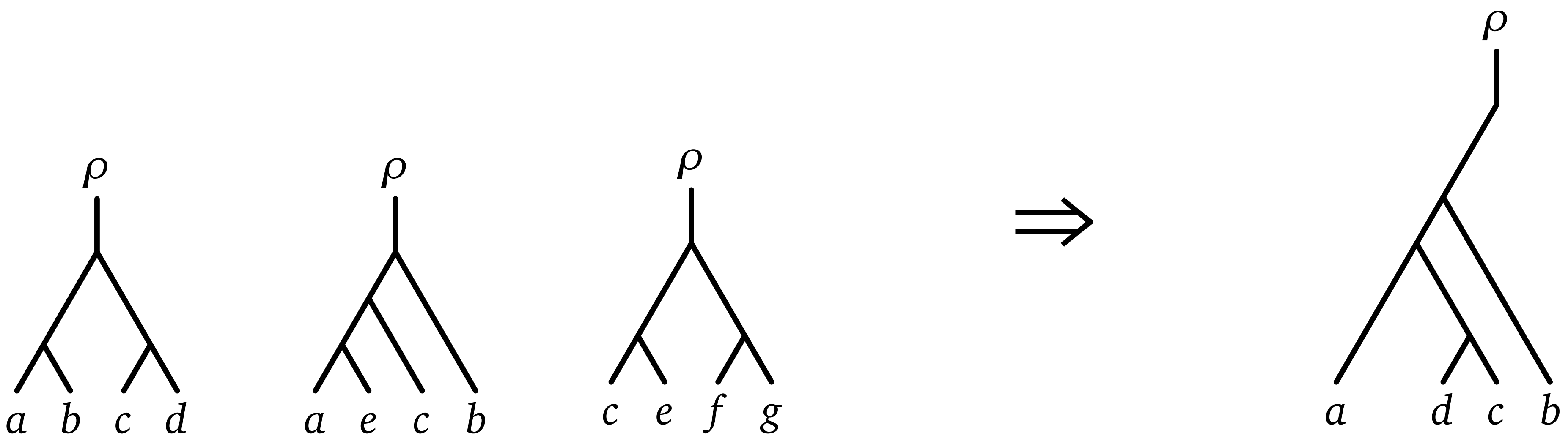

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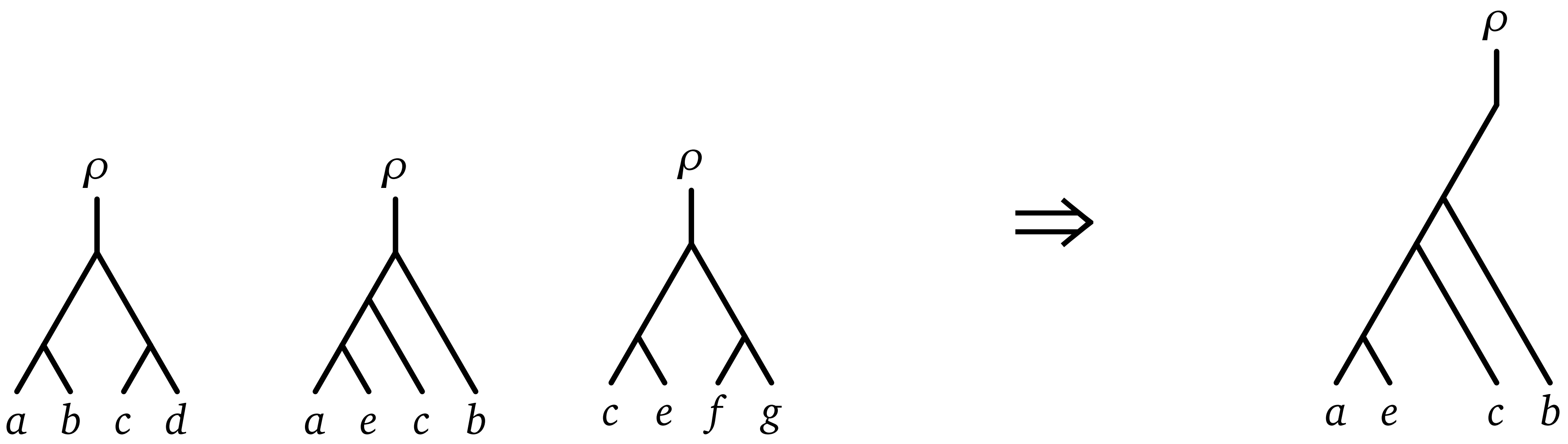

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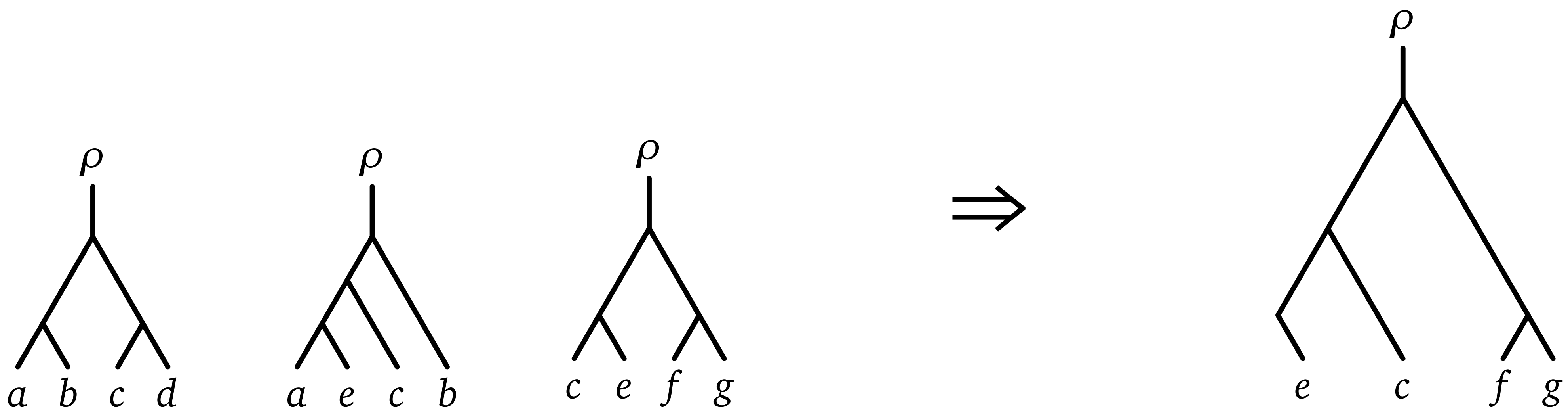

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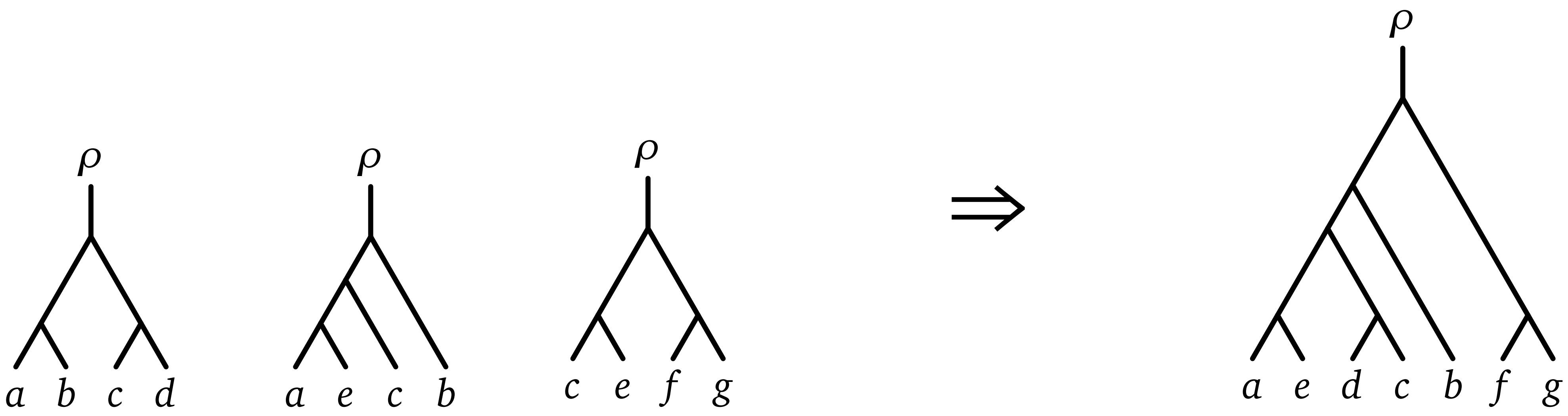


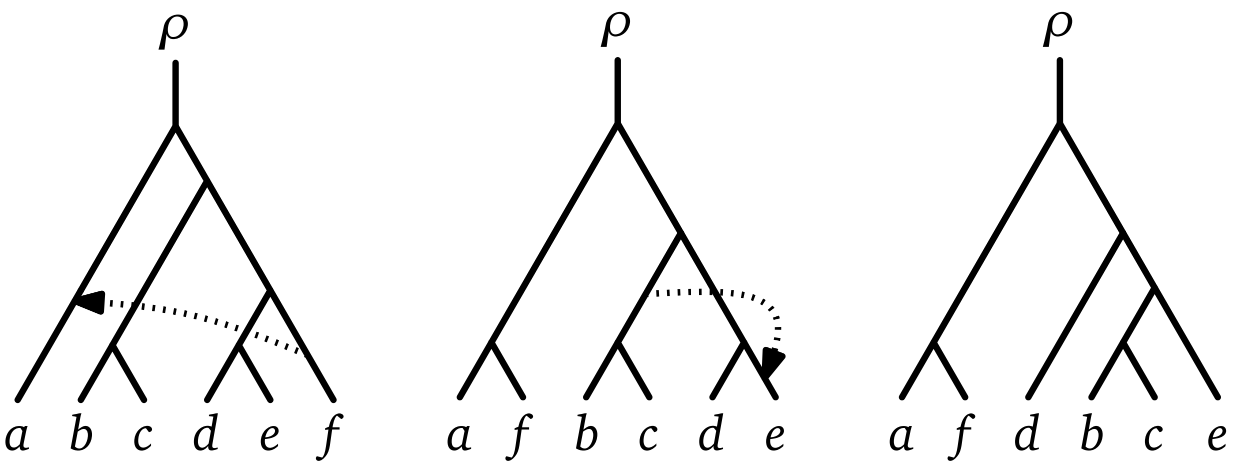
3. Phylogenetic networks

- DLT networks [Hallet/Lagergren 2011, Doyon et al. 2011]
- Recombination networks [Gusfield et al. 2003]
- Level-*k* hybridization networks [van Iersel/Kelk 2011]
- MAAF of multiple trees [Chen/Wang 2012]

Computing SPR Distance

Agreement Forests

How many SPR operations does it take to turn T_1 into T_2?



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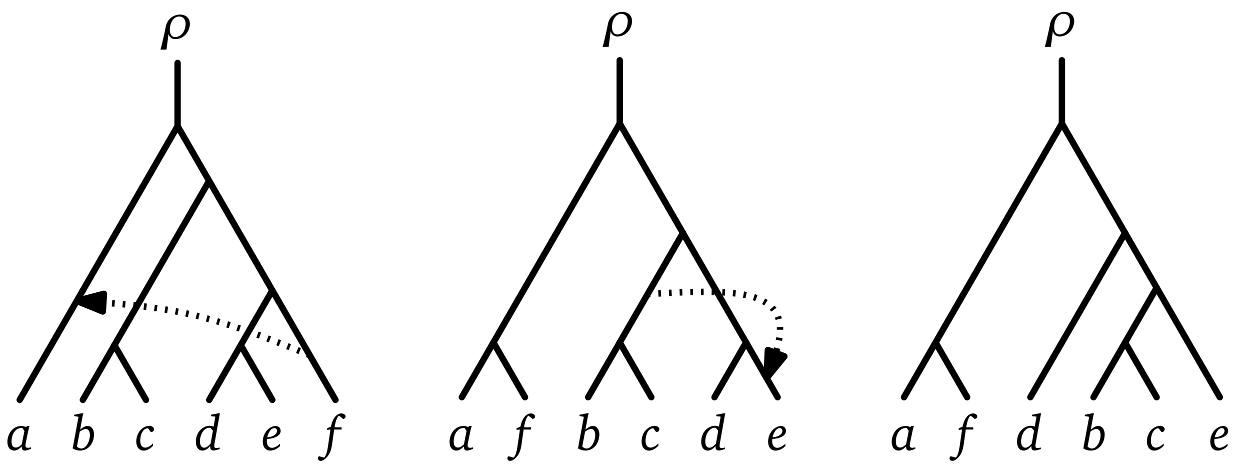

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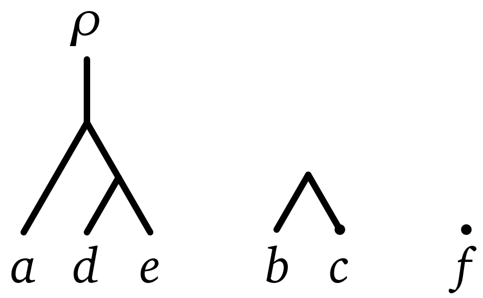

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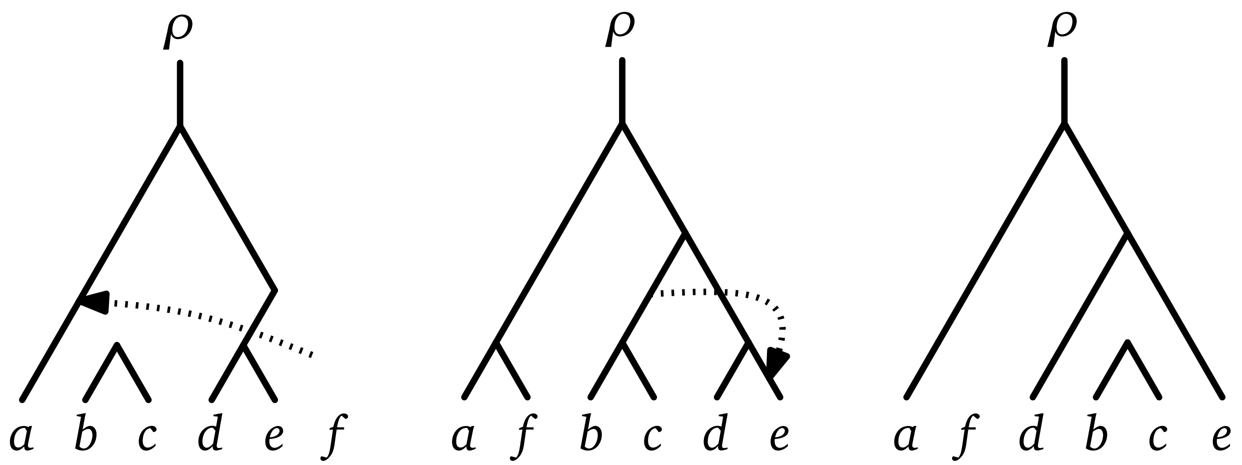

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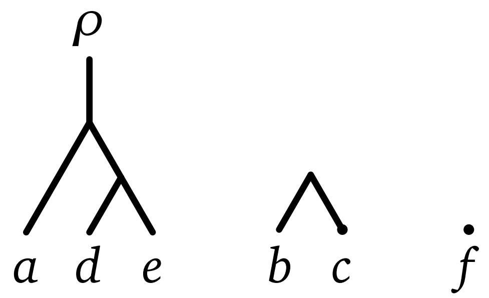

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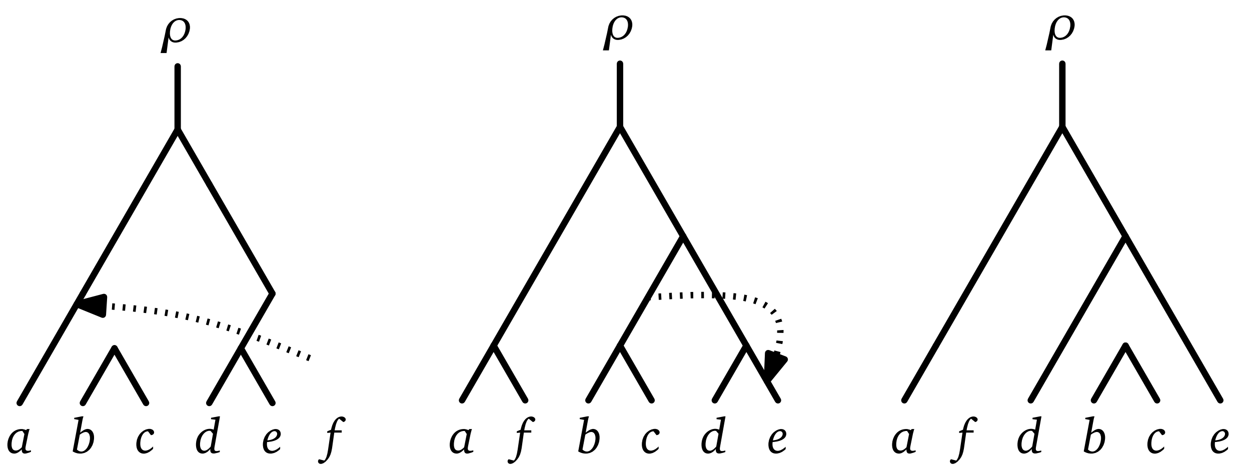

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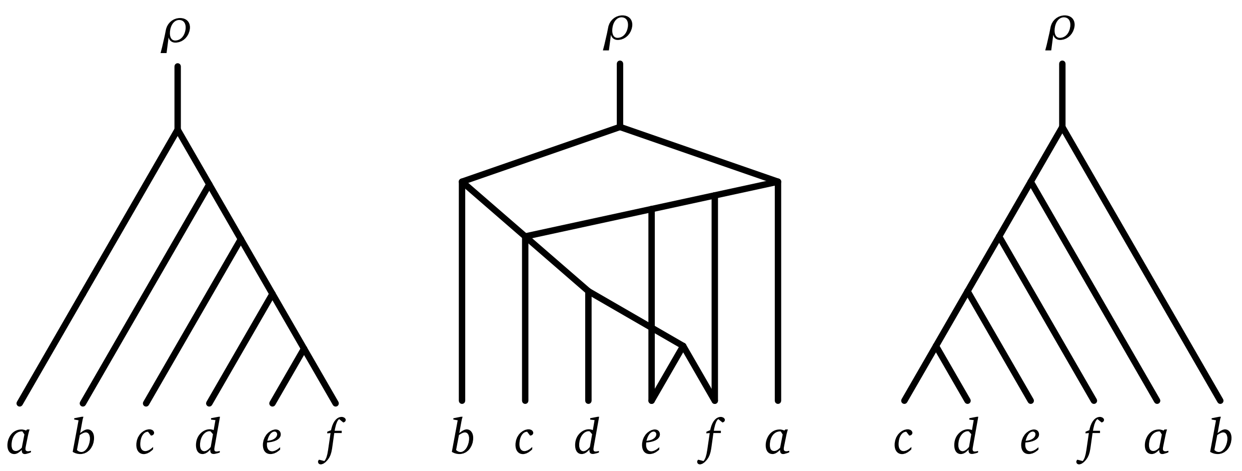

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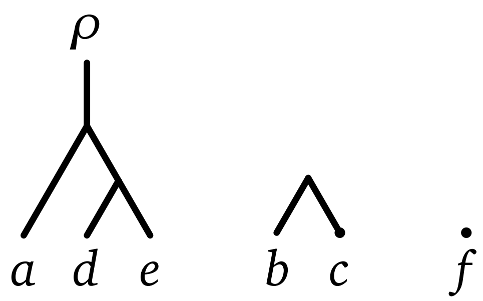

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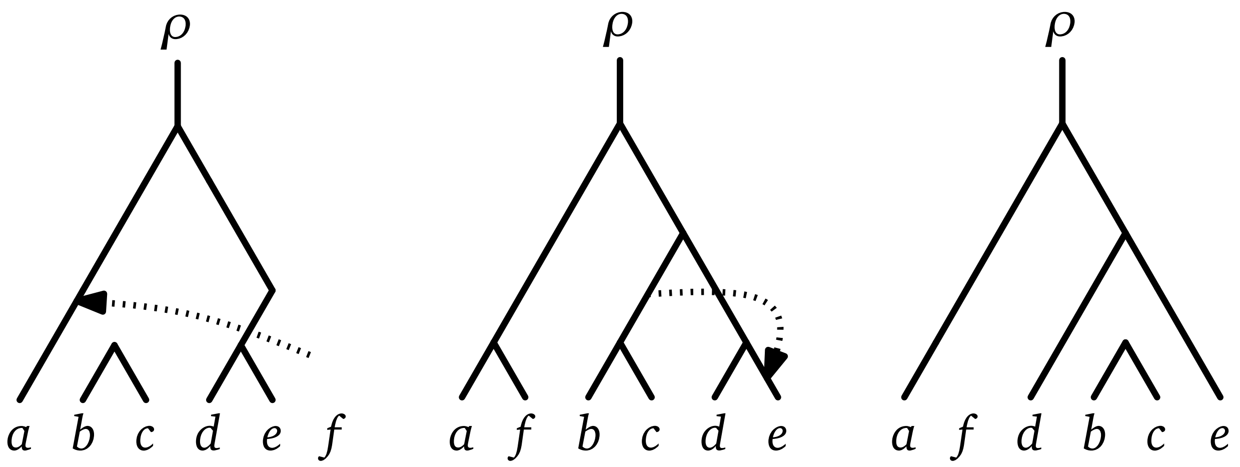

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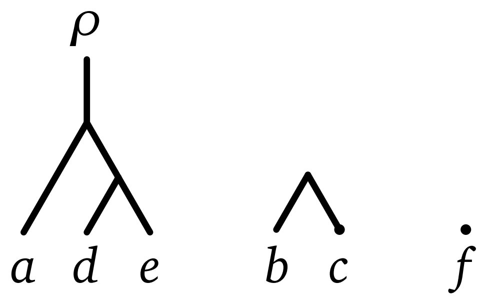

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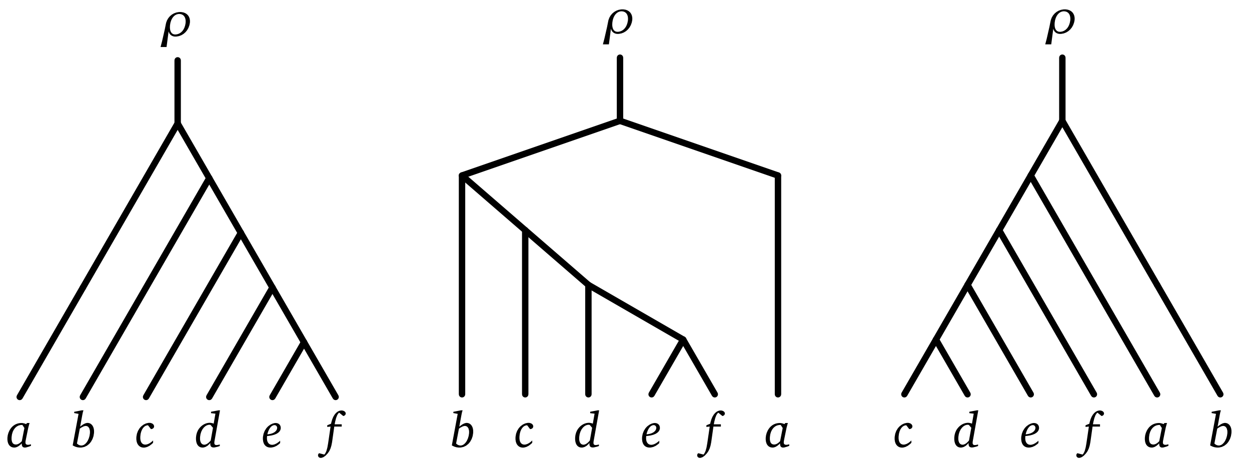

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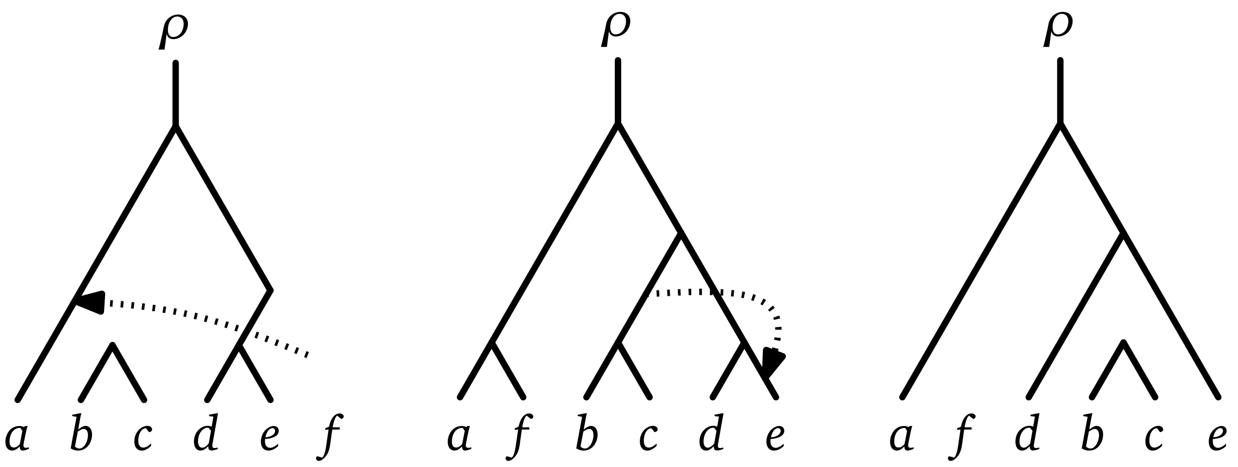

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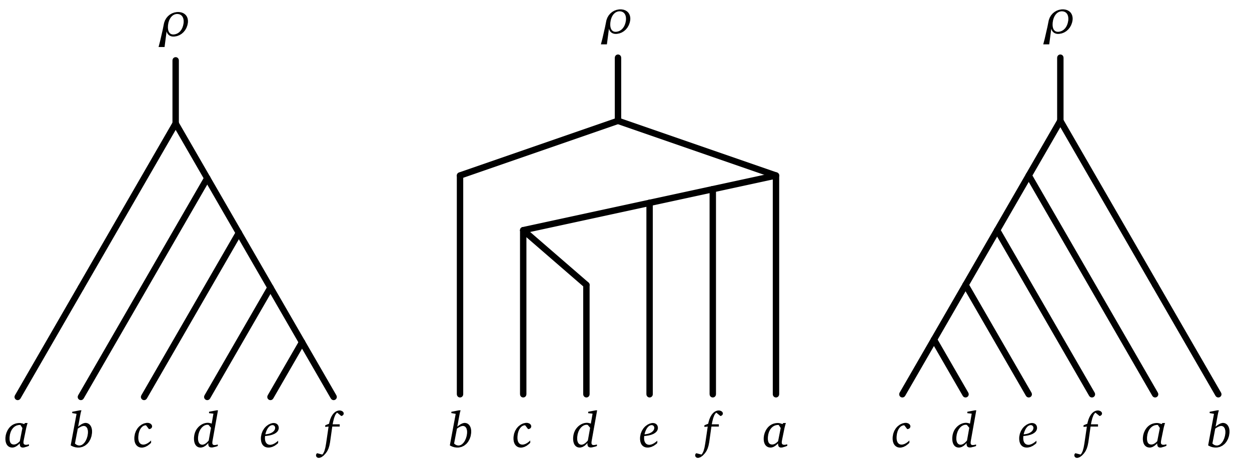

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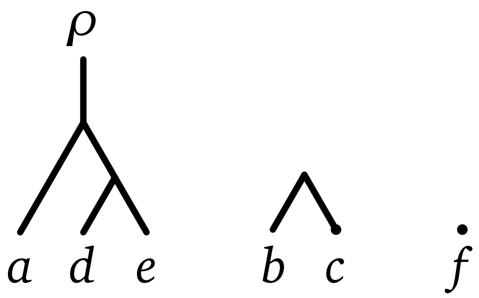

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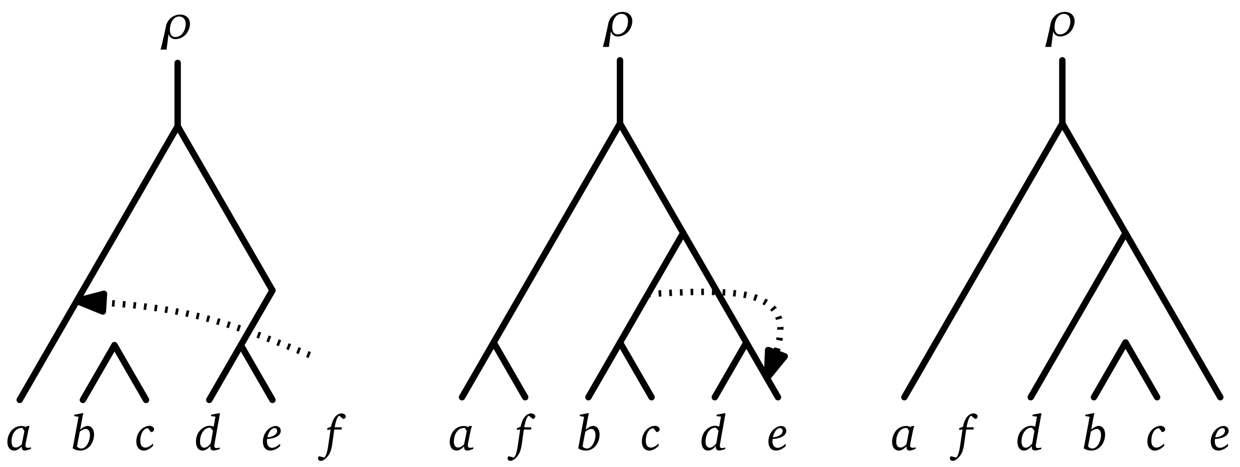

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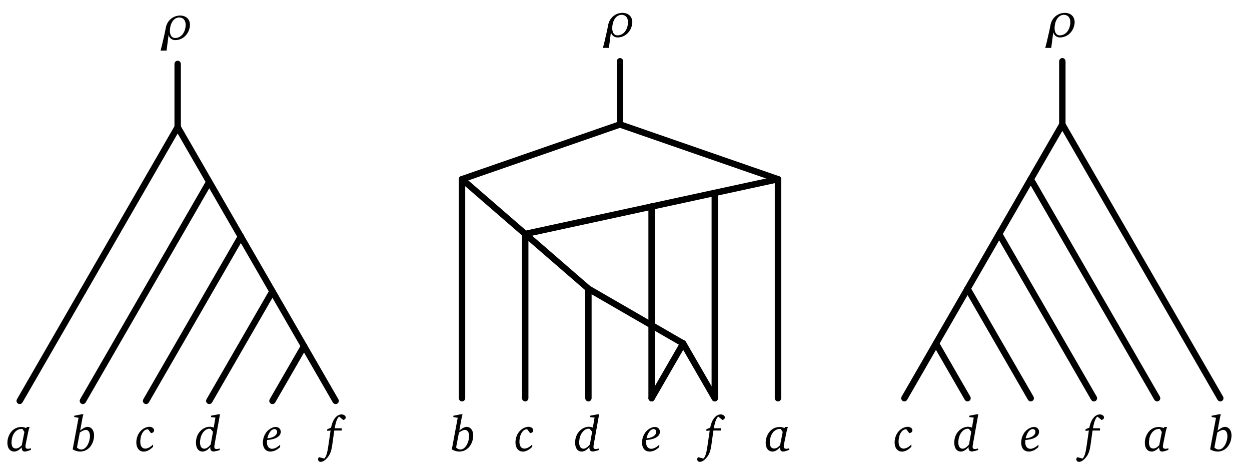

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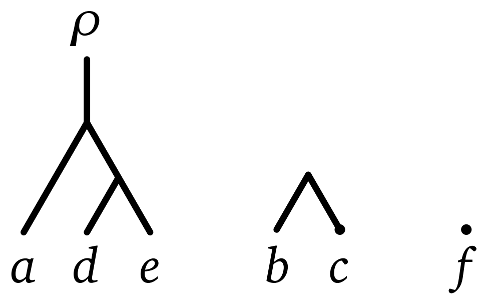

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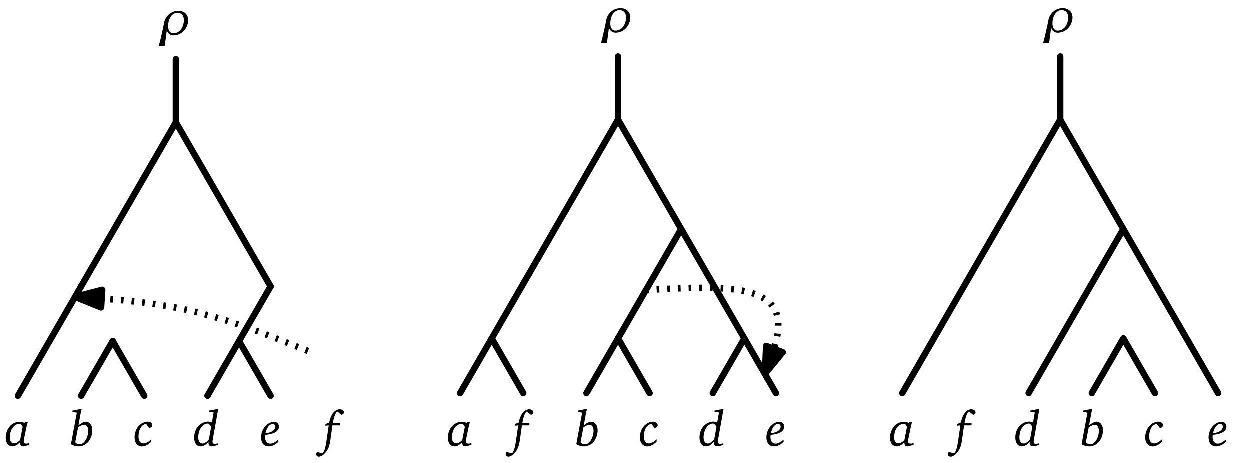

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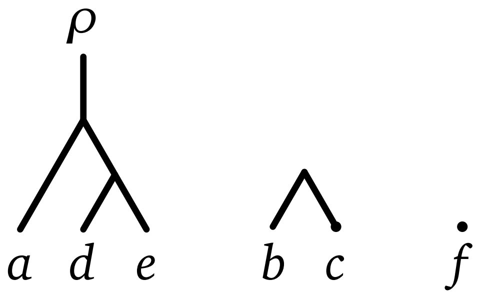

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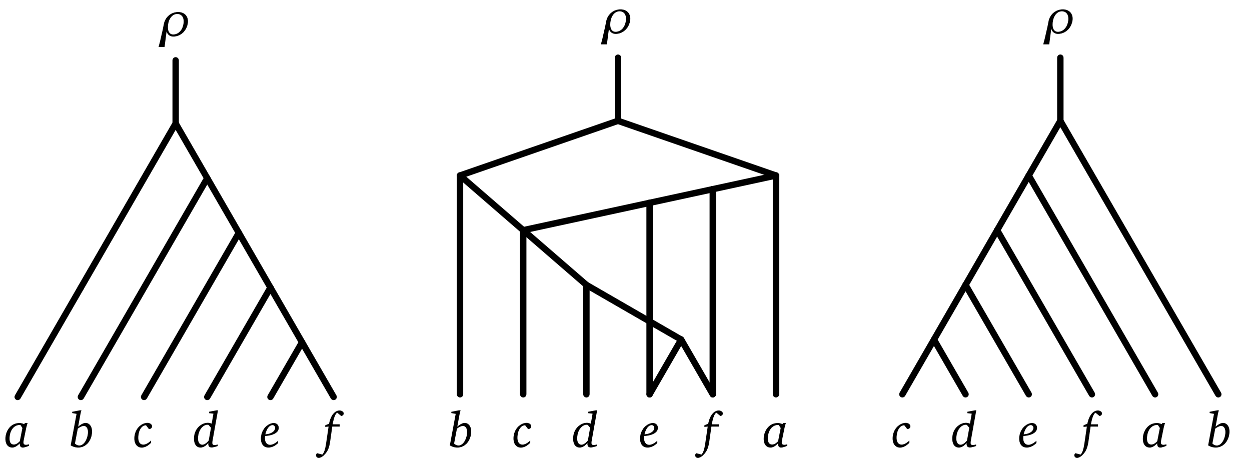

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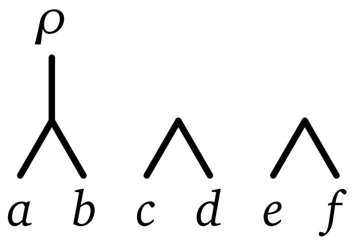

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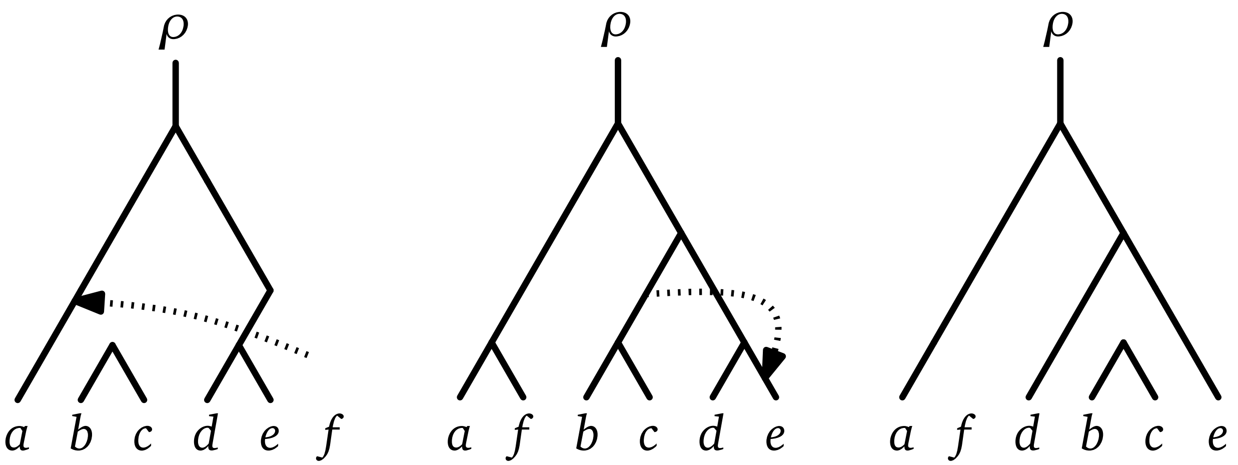

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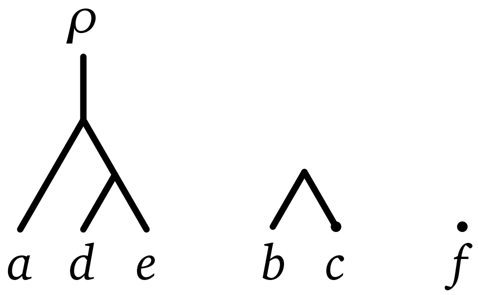

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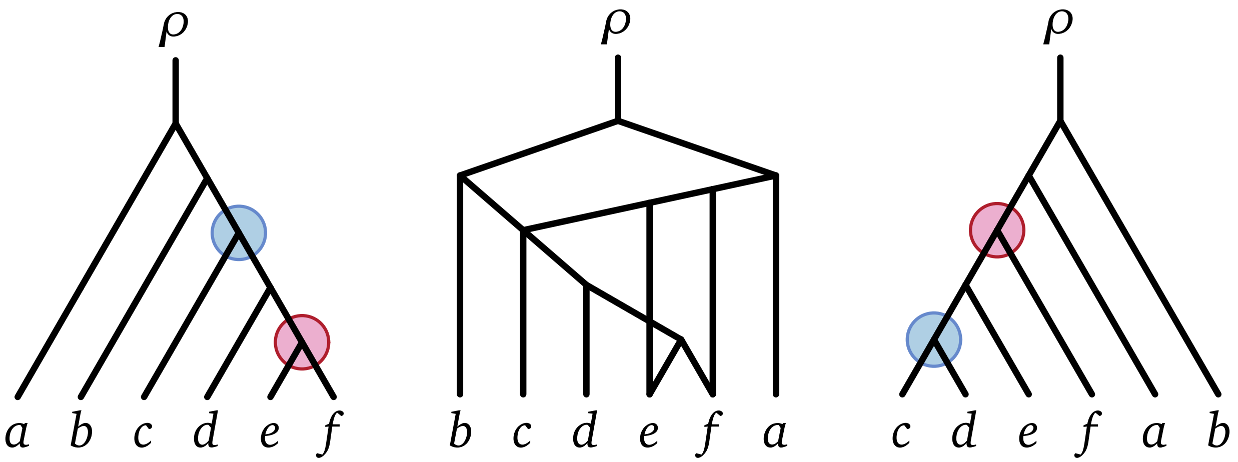

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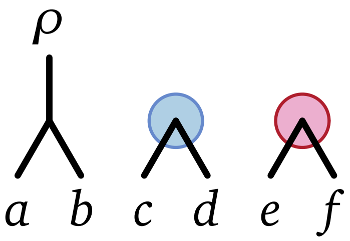

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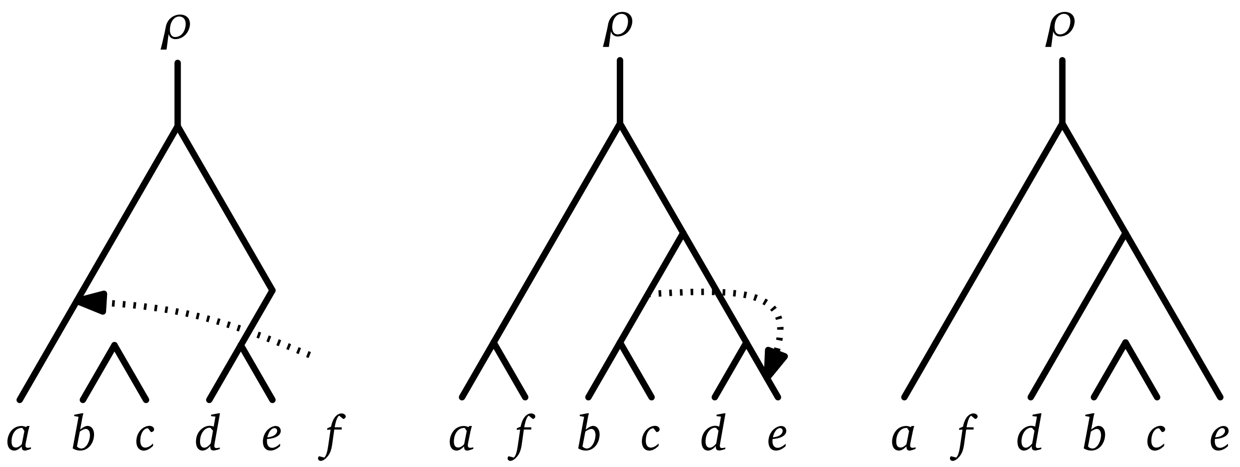

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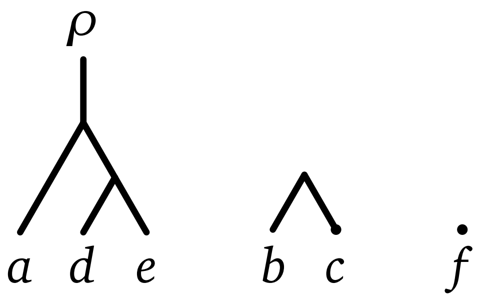

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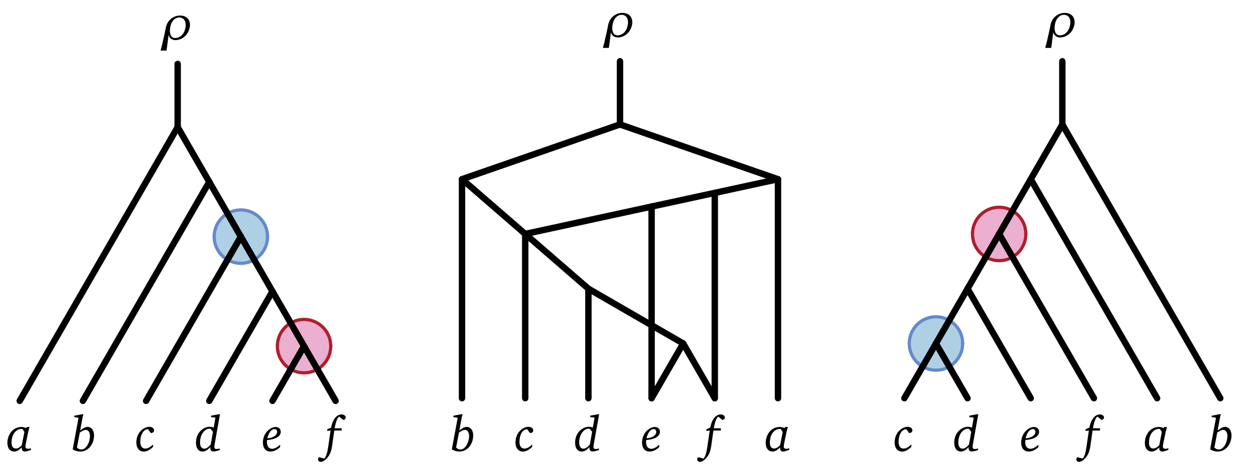

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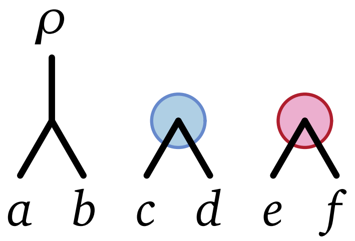

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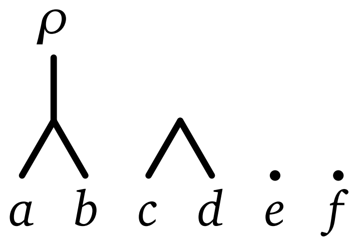

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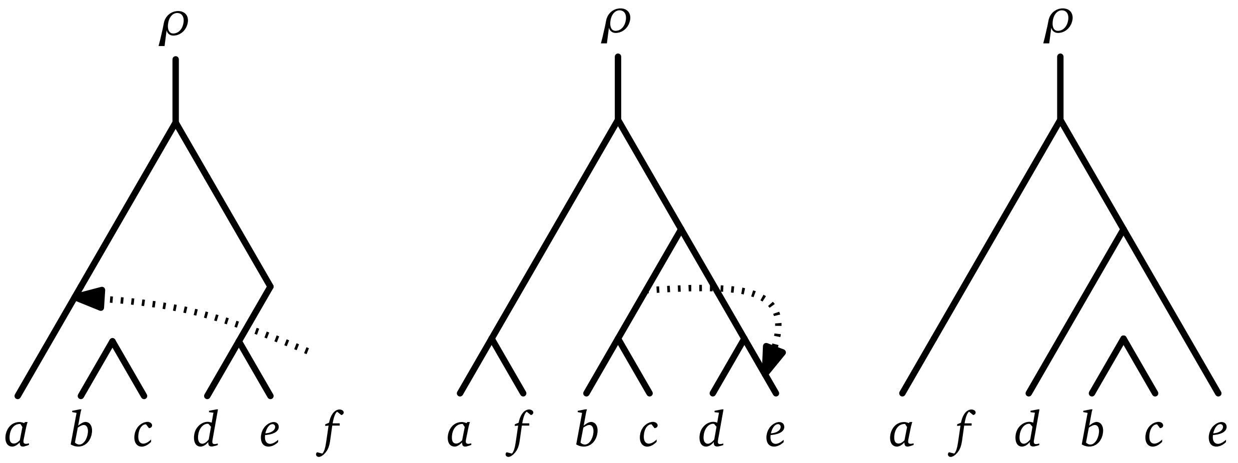

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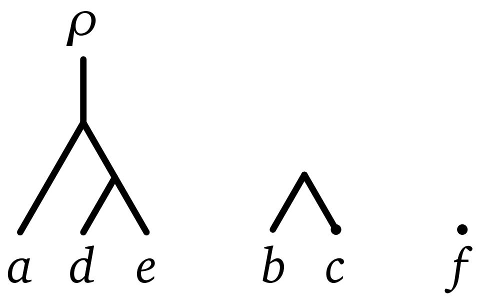

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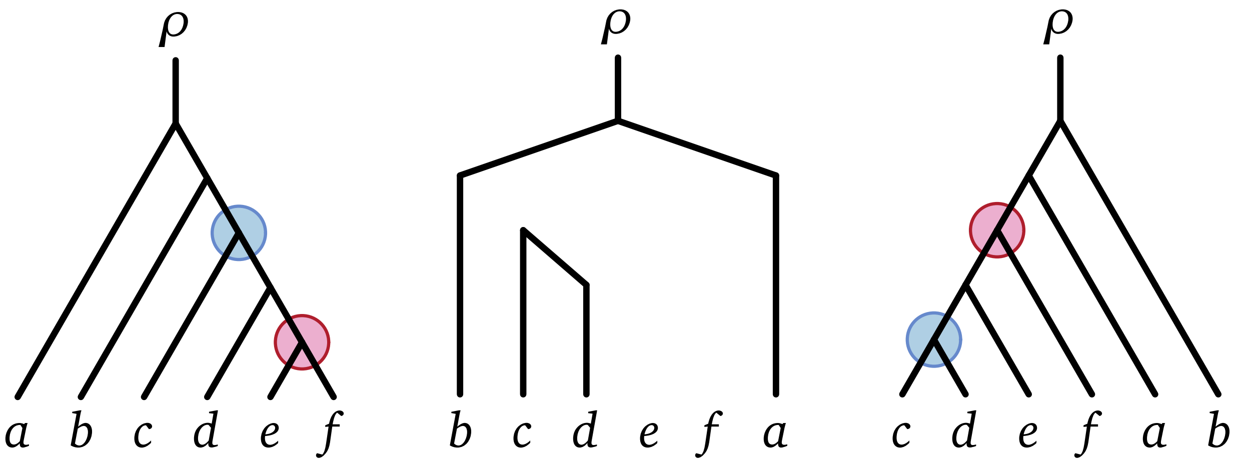

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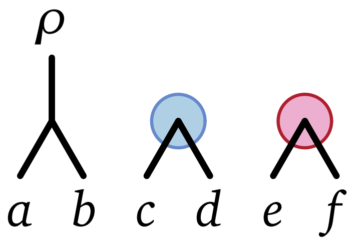

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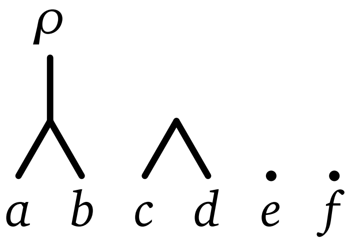
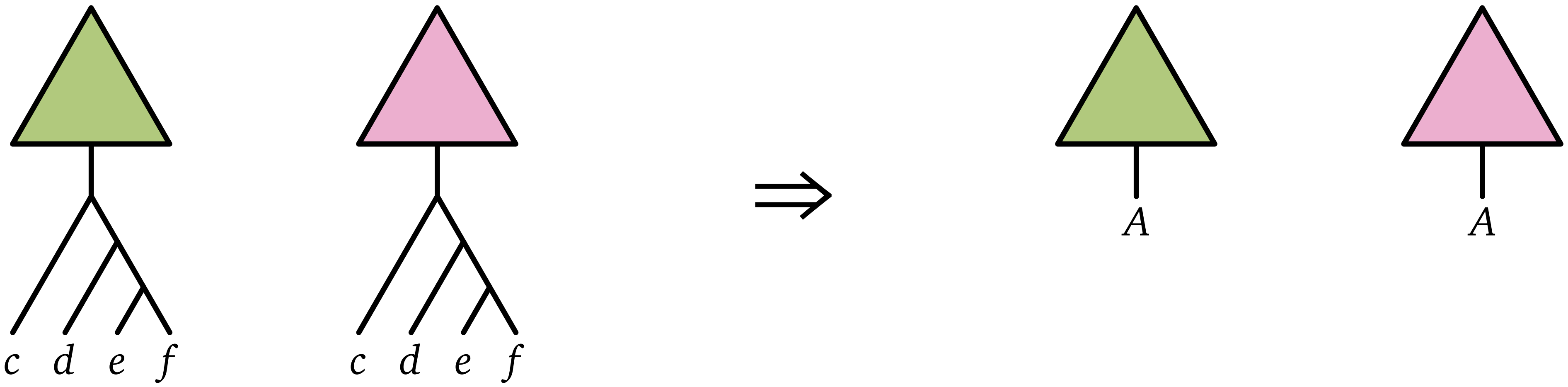


acyclic
agreement forest

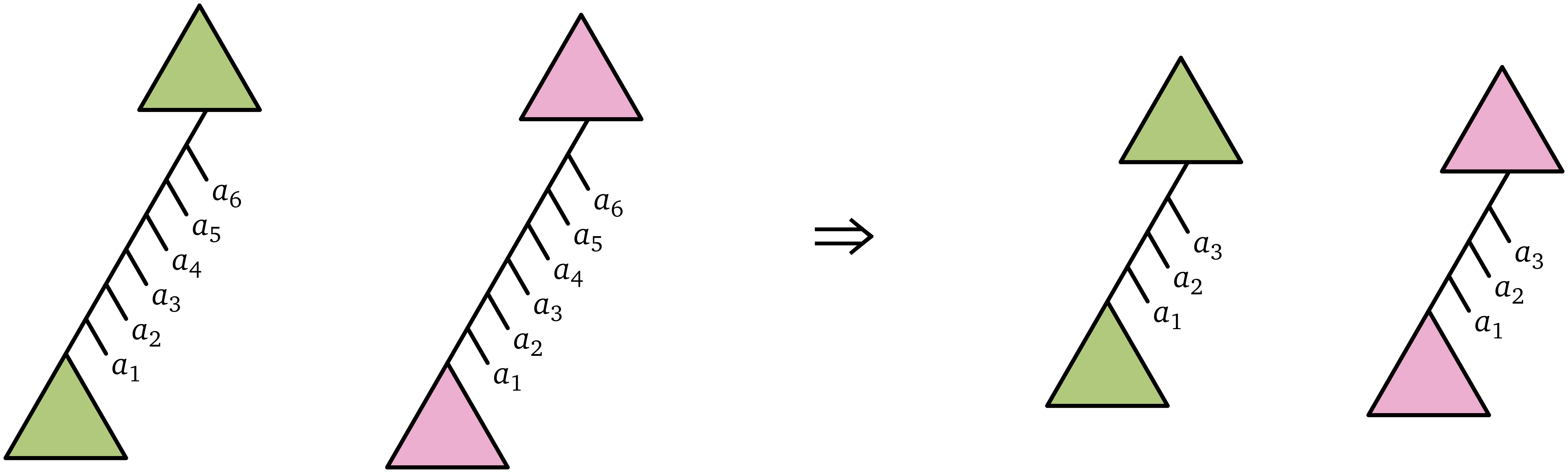
[Bordewich/Semple 2007]

Kernelization for Maximum Agreement Forest (SPR Distance)

Rule 1: Prune agreeing subtrees



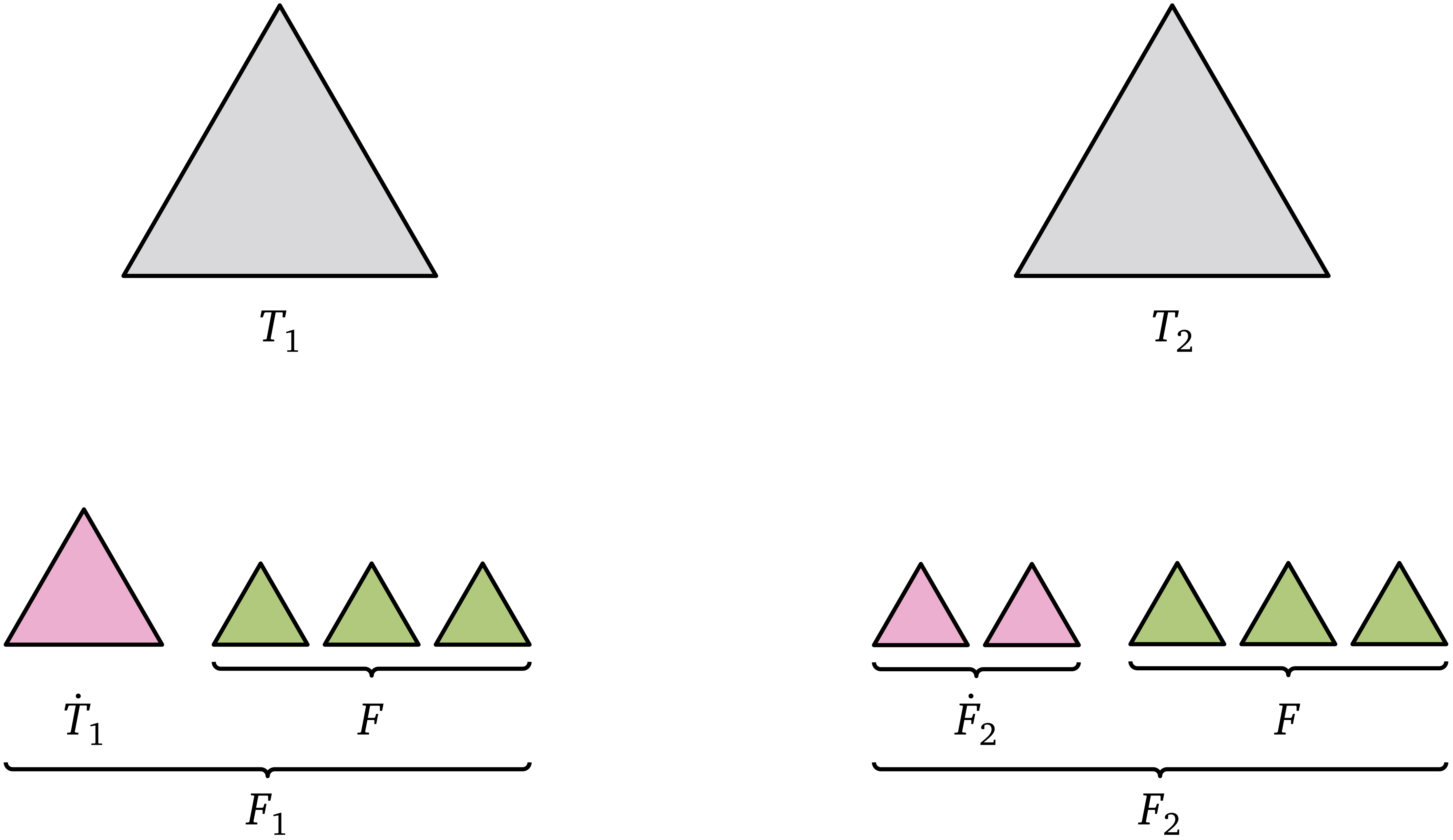
Rule 2: Compress agreeing chains



Running time: $O((56k)^k + \text{poly}(n))$

[Bordewich/Semple 2005]

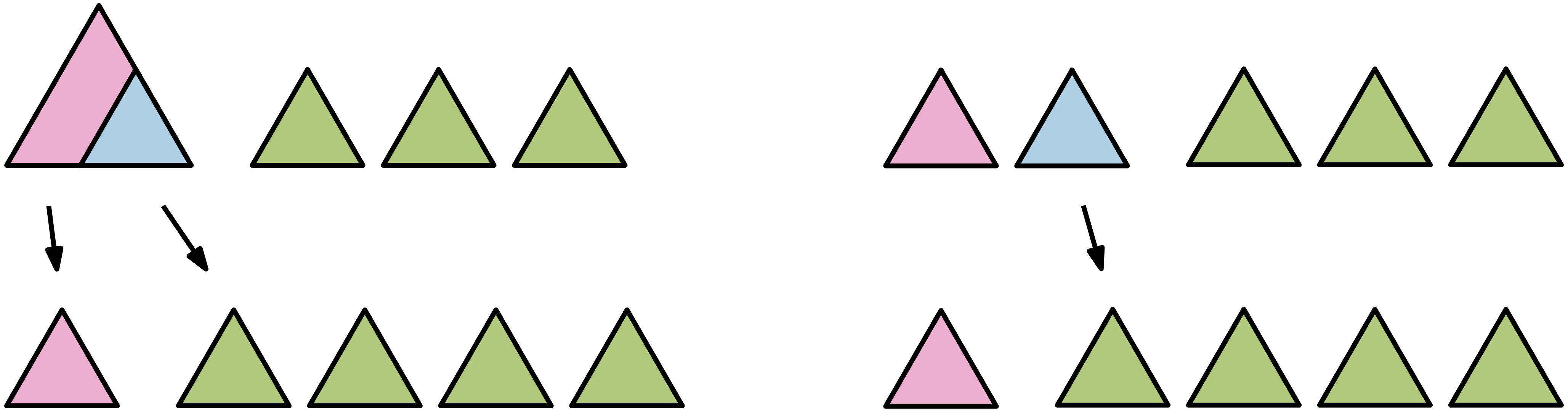
Depth-Bounded Search for MAF [Whidden/Zeh 2009]



An MAF of T_1 and T_2 can be obtained by cutting edges in F_2.

Depth-Bounded Search for MAF [Whidden/Zeh 2009]

Case 1: A whole tree in $\dot{F}_2$ agrees with a subtree of $\dot{T}_1$



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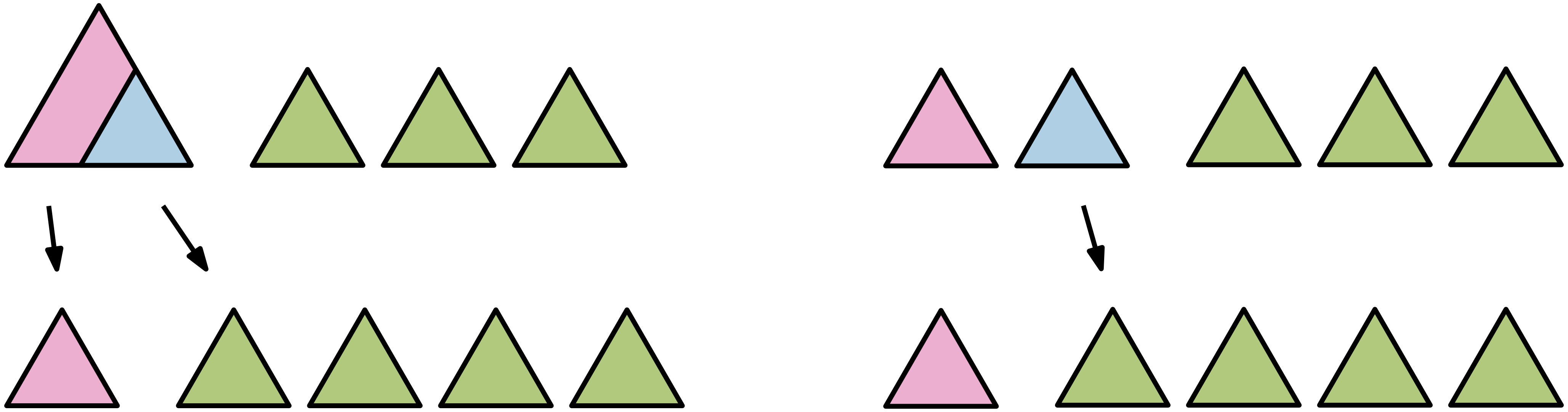
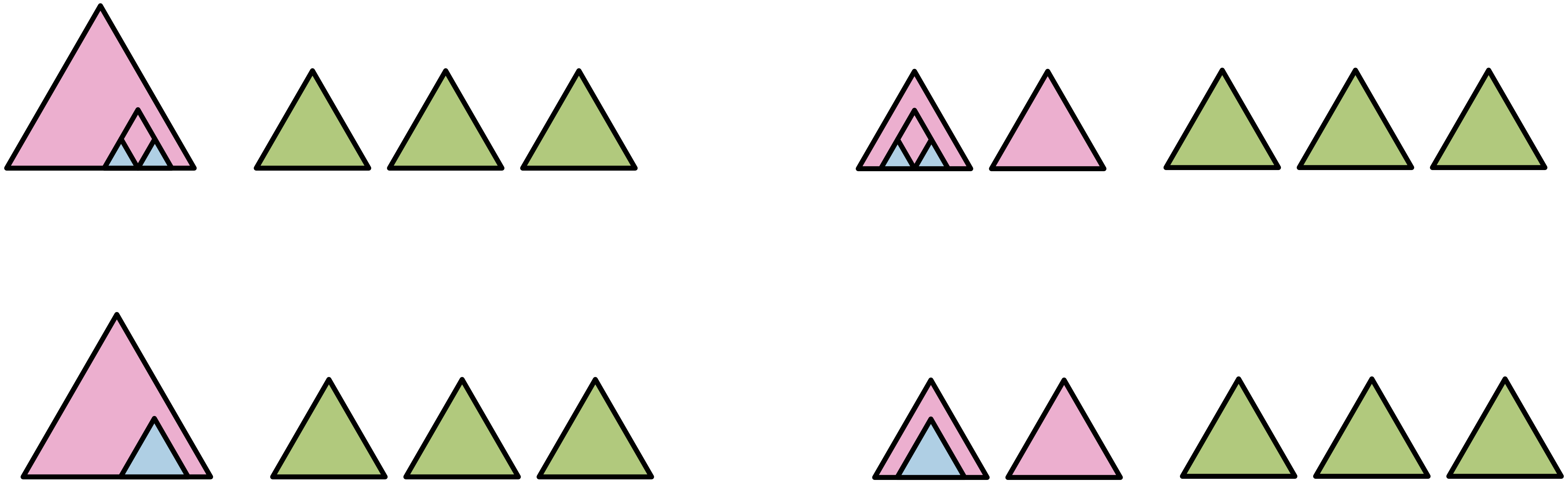


Case 2: Two agreeing subtrees are adjacent in $\dot{T}_1$ and $\dot{F}_2$



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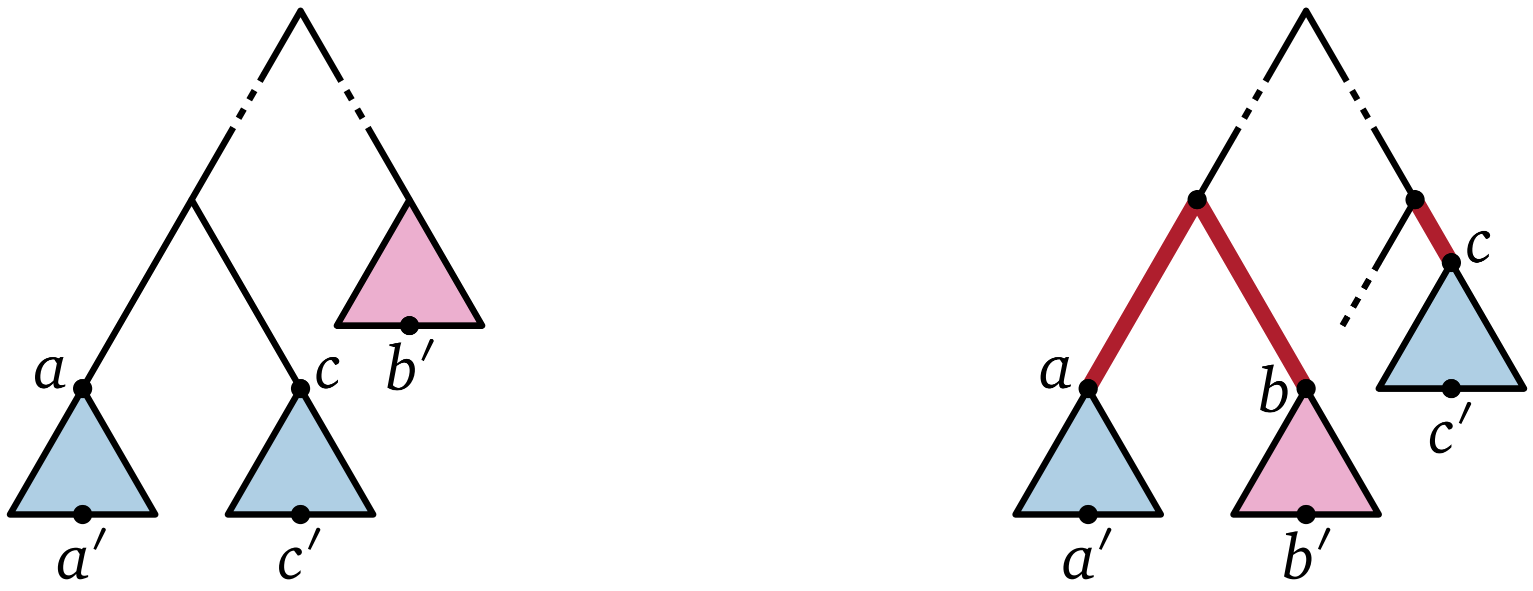

One branch per edge

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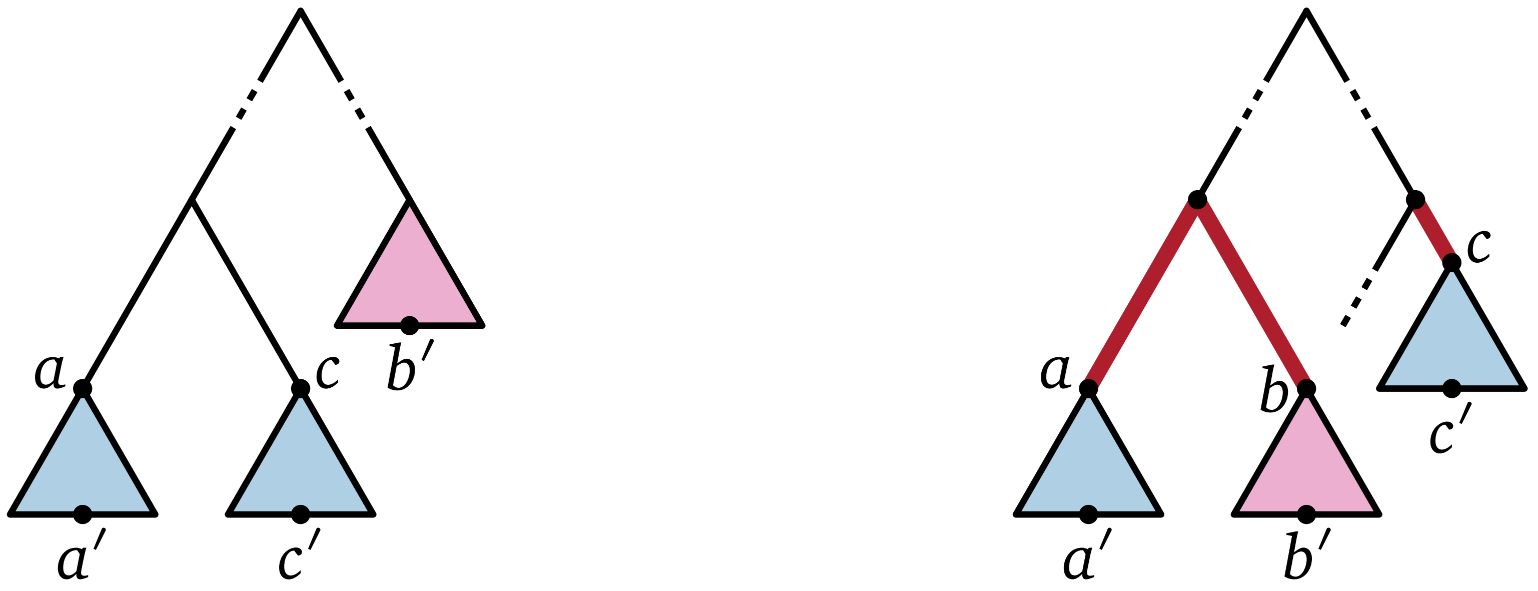


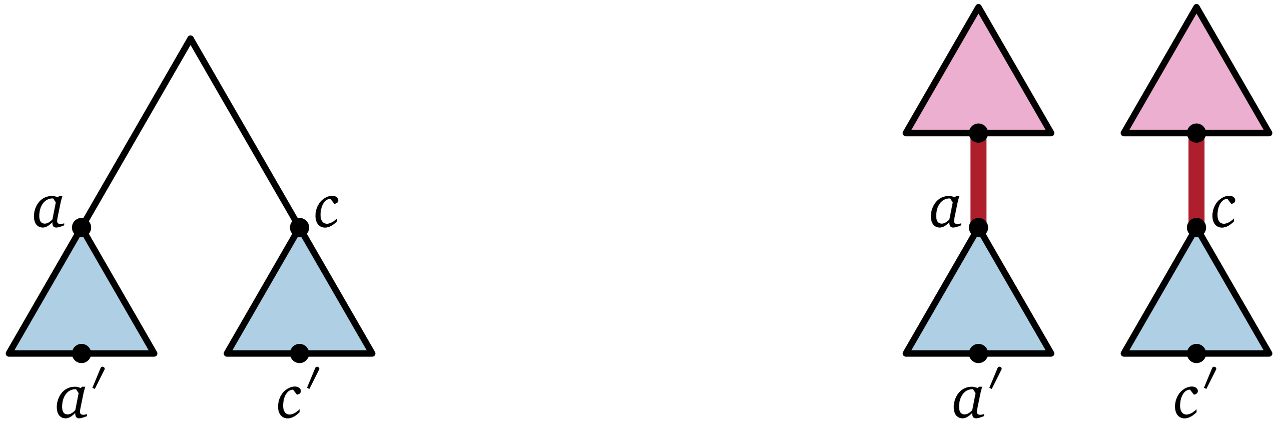
One branch per edge

- Number of recursive calls $= 3^k$
- Each costs $O(n)$ time

Running time: $O(3^k n)$

Improved Branching Rules [Whidden/Beiko/Zeh 2010]

Case 3.1: a and b belong to different subtrees of $\dot{F}_2$



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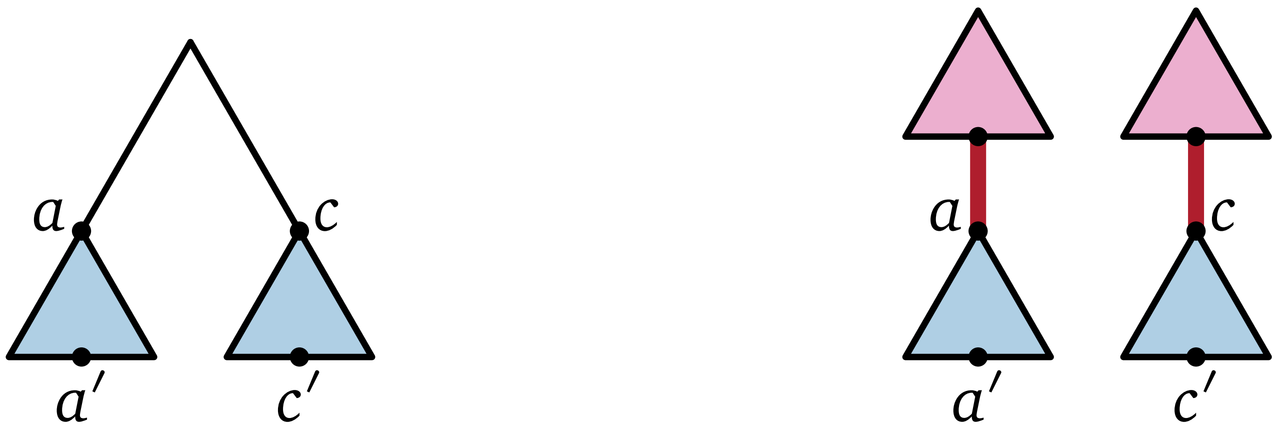

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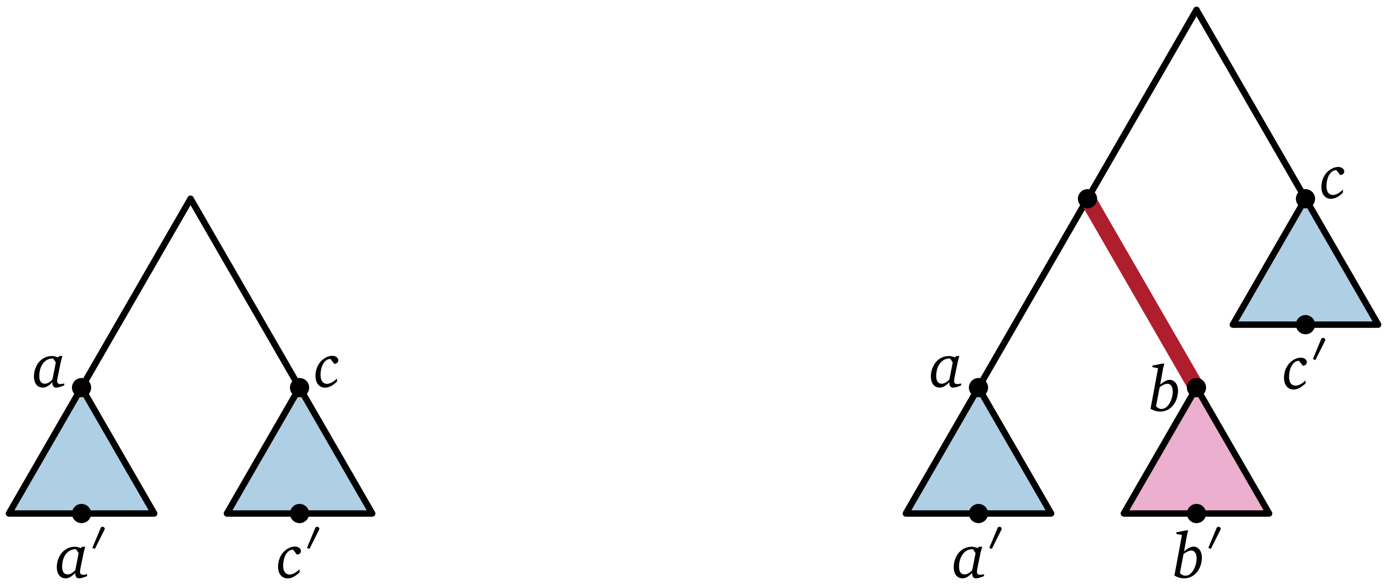

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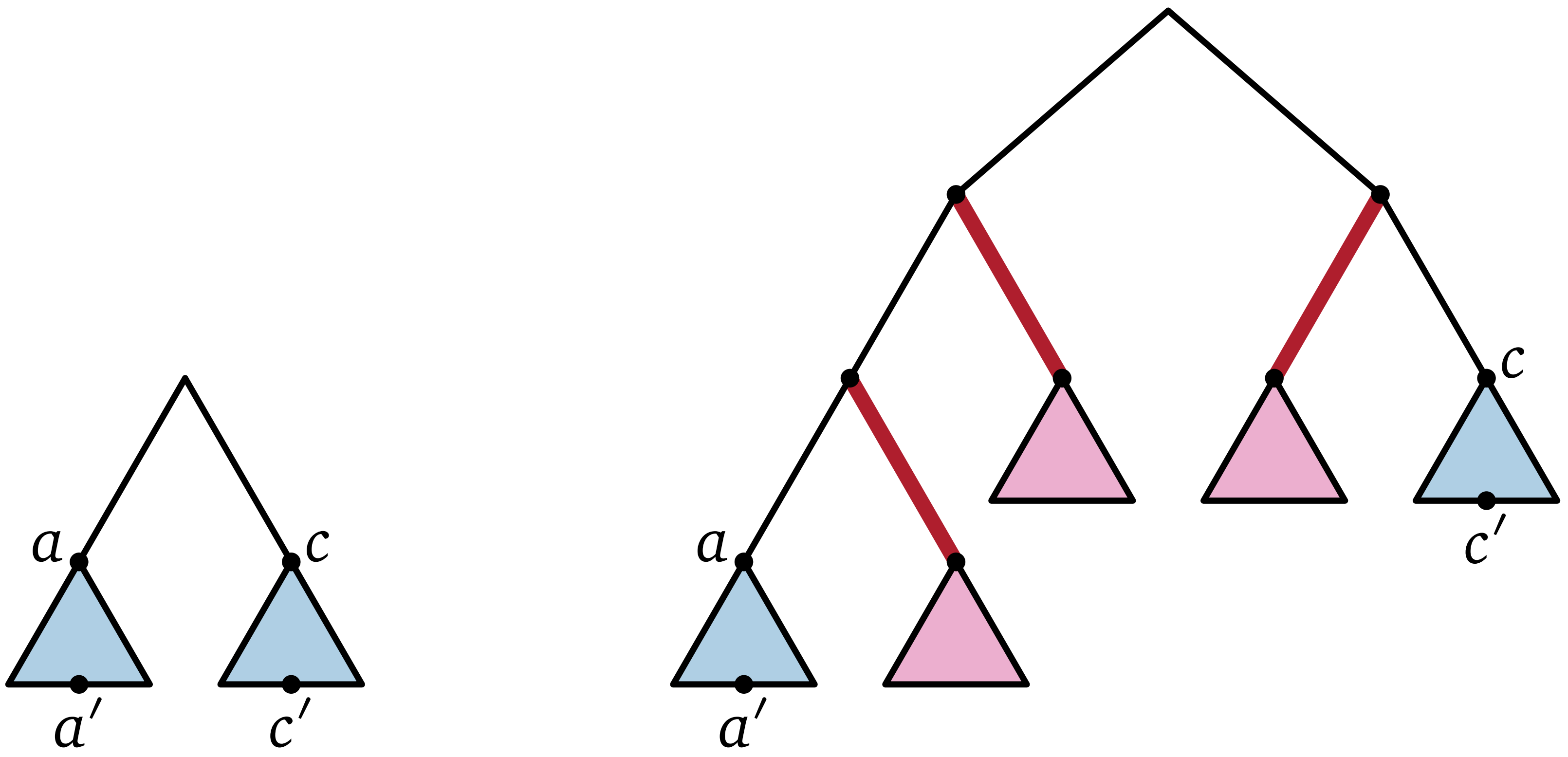

3 recursive calls with parameters

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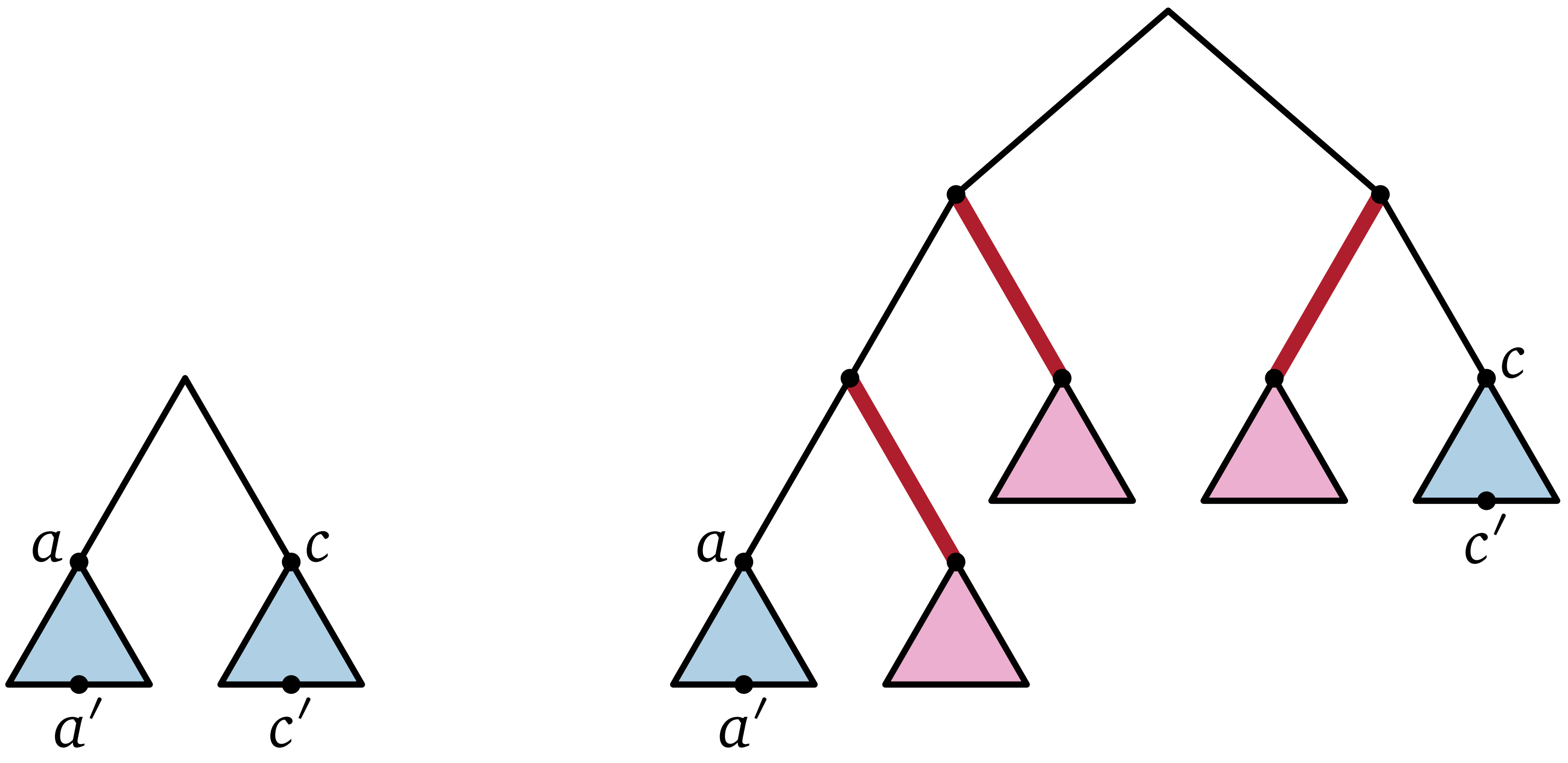

3 recursive calls with parameters

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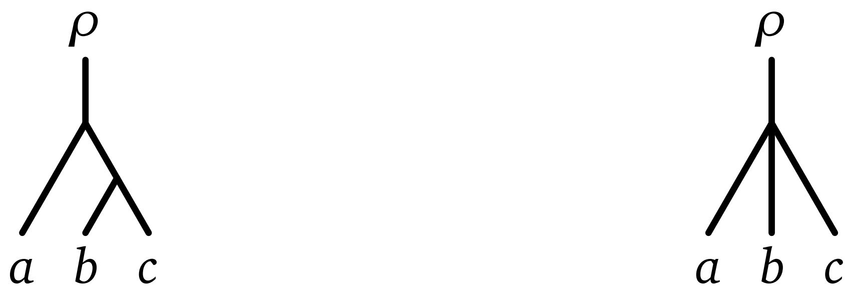
Number of recursive invocations

$$I(k) \leq 2I(k-1) + I(k-2) \leq (1+\sqrt{2})^k \approx 2.41^k$$

Multifurcating Trees [Whidden/Beiko/Zeh 2012]

Problem 1: What is a meaningful definition of an agreement forest?



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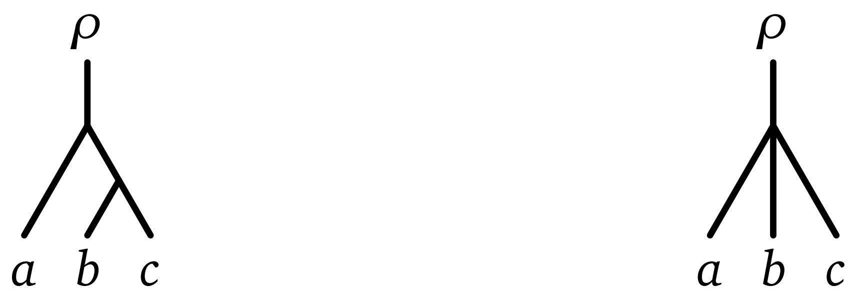

An MAF of two multifurcating phylogenies T_1 and T_2 is the largest forest that is an AF of two binary resolutions of T_1 and T_2.

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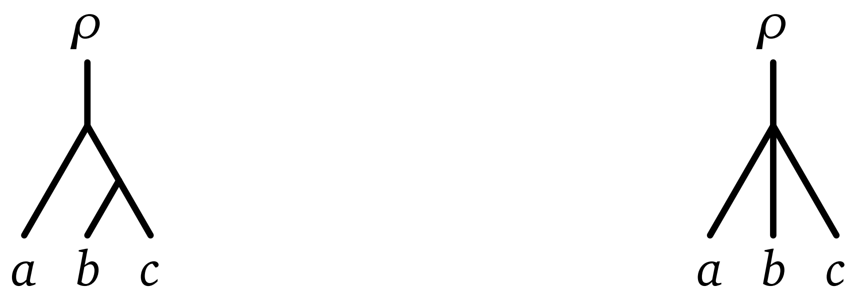

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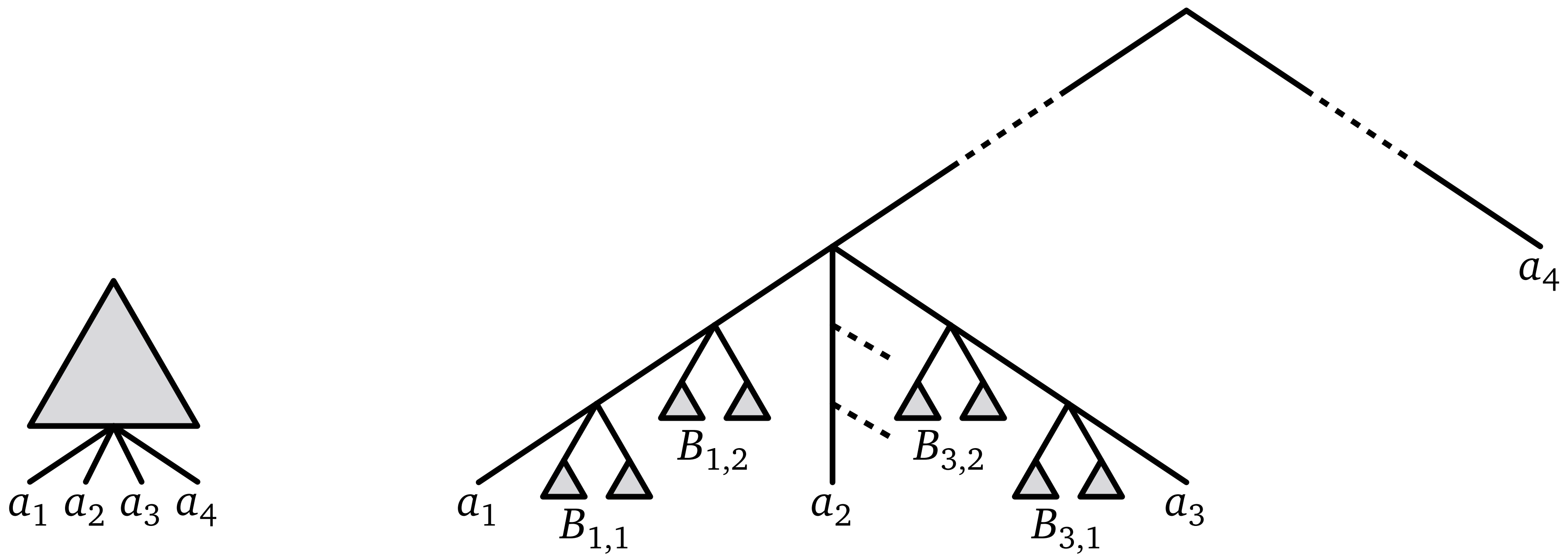
Problem 2: Sibling pairs become sibling groups.



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It’s FPT, alright . . .

- 5 cases depending on the structure of F_2
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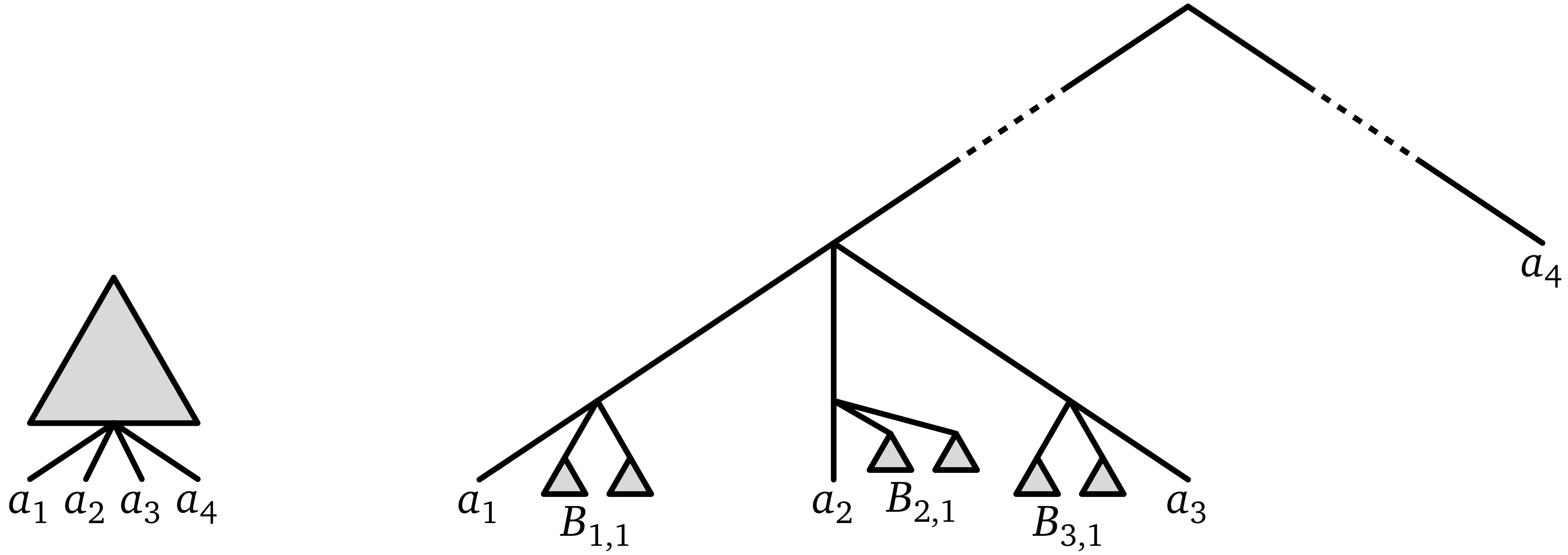

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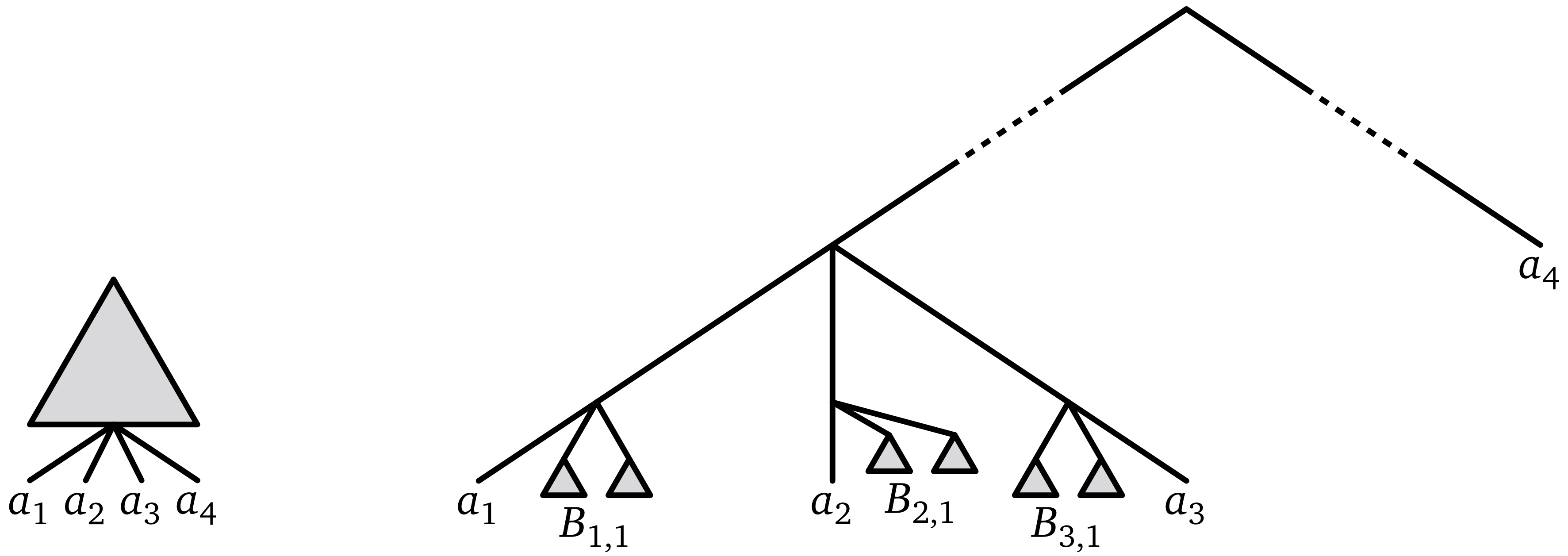


- Until the protected edges are eliminated, every recursive call becomes a 2-way branch.
- Each such sequence of 2-way branches ends in a “1-way branch”.

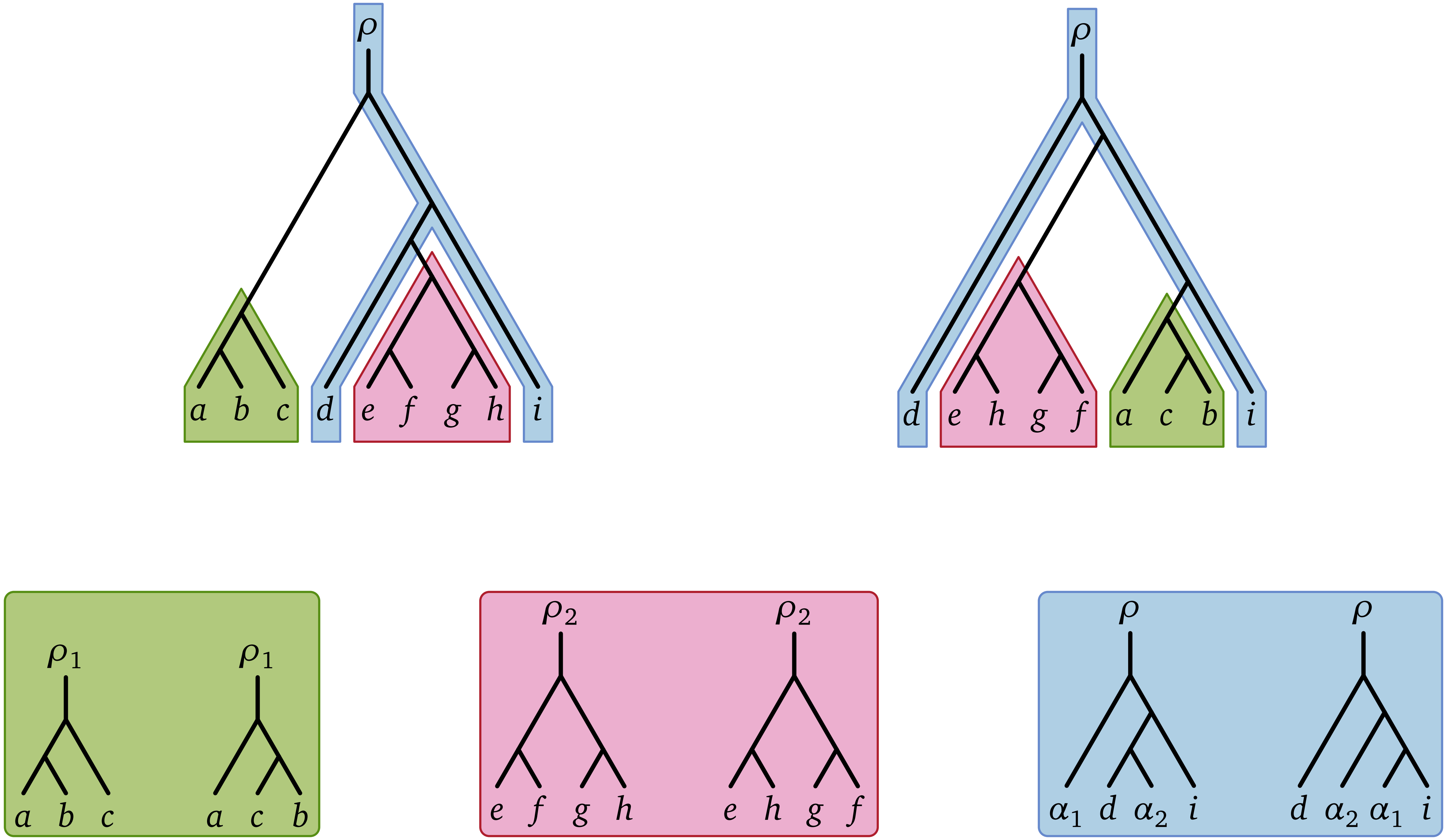
Running time: $O(2.42^k n)$

Binary Trees Even Faster [Whidden/Beiko/Zeh 2012]

- Edge protection idea from the multifurcating algorithm
- A couple of new cases
- A hairy analysis

Running time: $O(2^k n)$

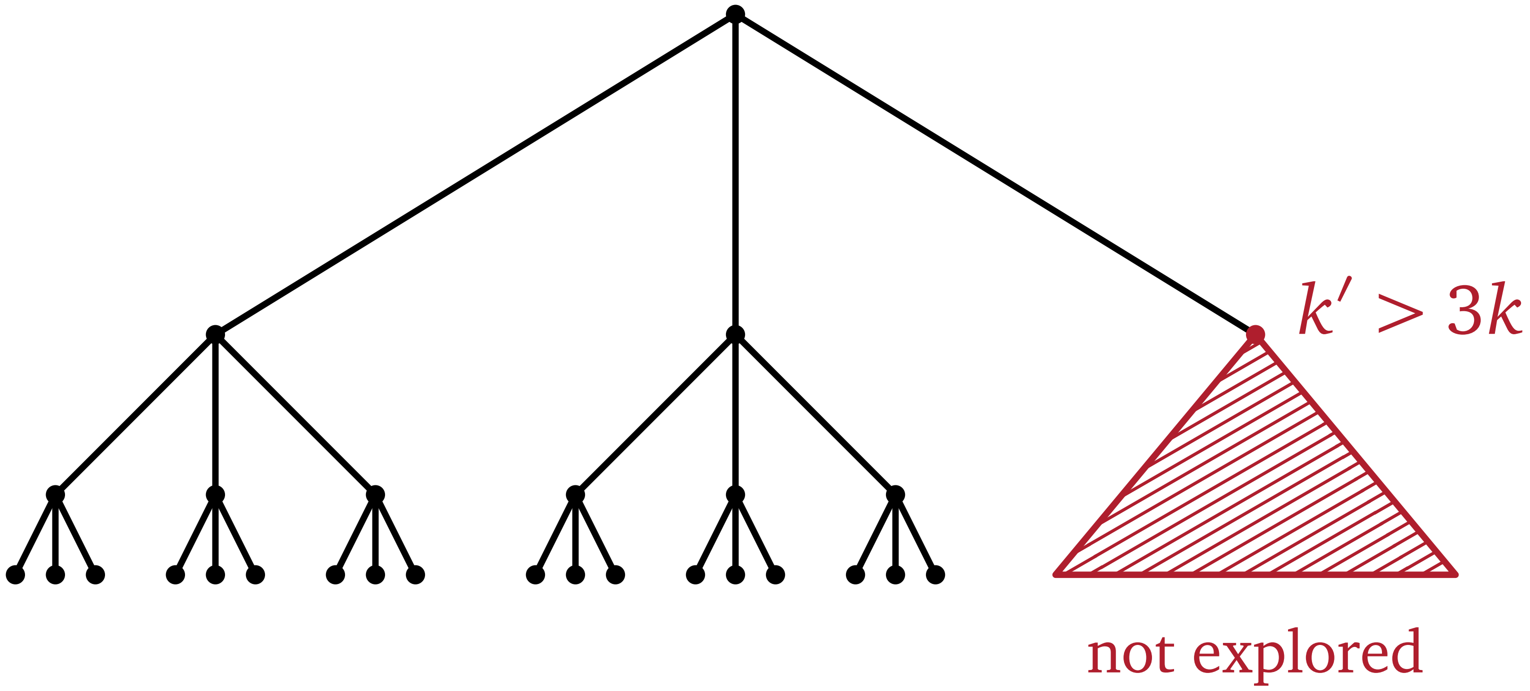
Clustering [Linz/Semple 2009]



An MAF of the two input trees can be computed by computing MAFs of the clusters . . . with a twist.

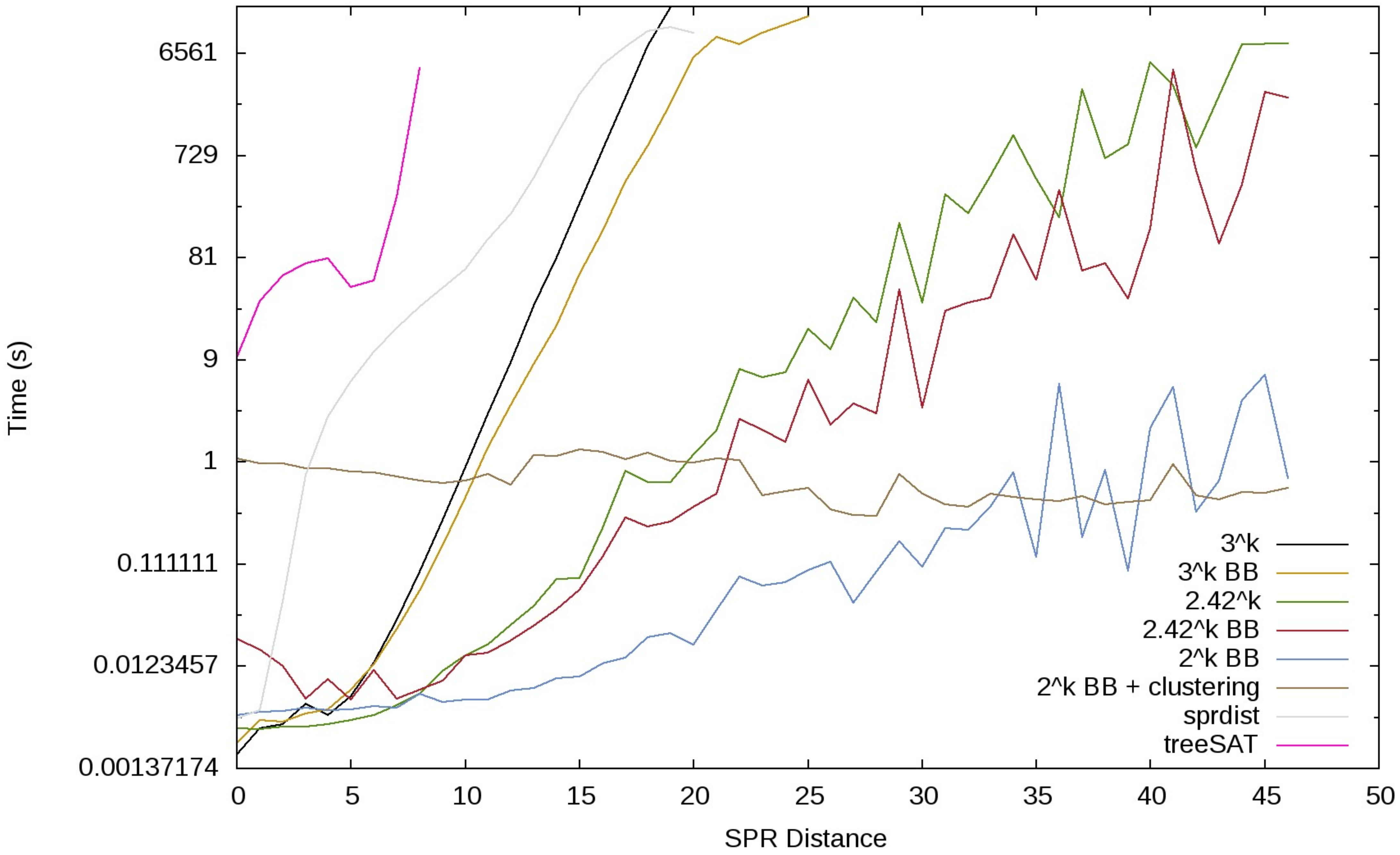
Branch and Bound

- For each invocation, compute 3-approximation k' of number of edges left to be cut.
- If $k' > 3k$, abort.



Added cost per invocation: $O(n)$ [Whidden/Zeh 2009]

Experimental Results



Hybridization [Whidden/Beiko/Zeh 2012]

Observation: While F_2 is not an AF of T_1 and T_2, at least one of the branches in each case of the MAF algorithm makes progress towards an MAAF.

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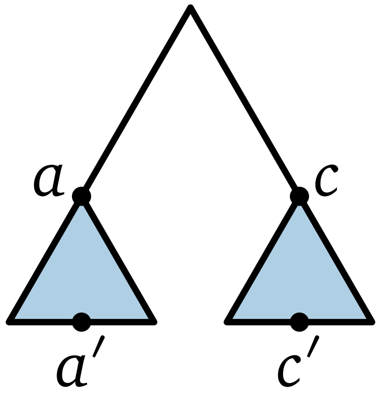

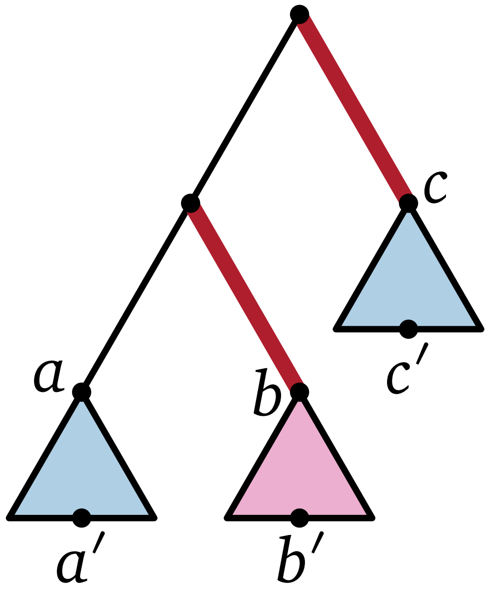

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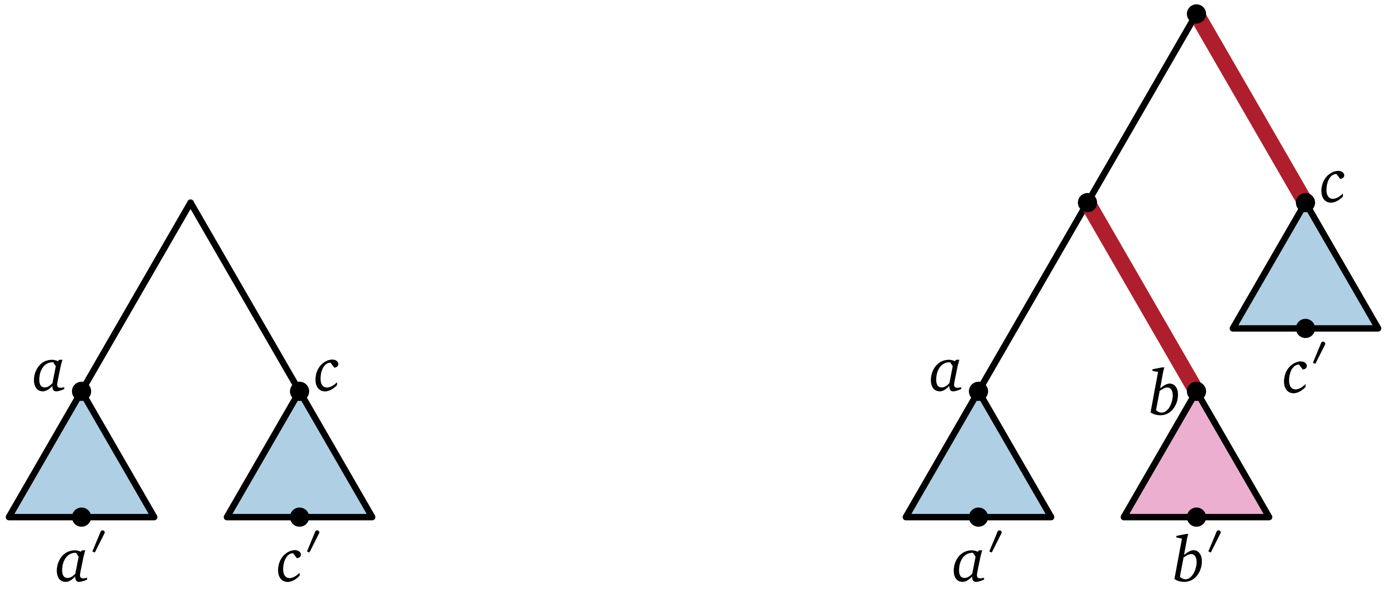

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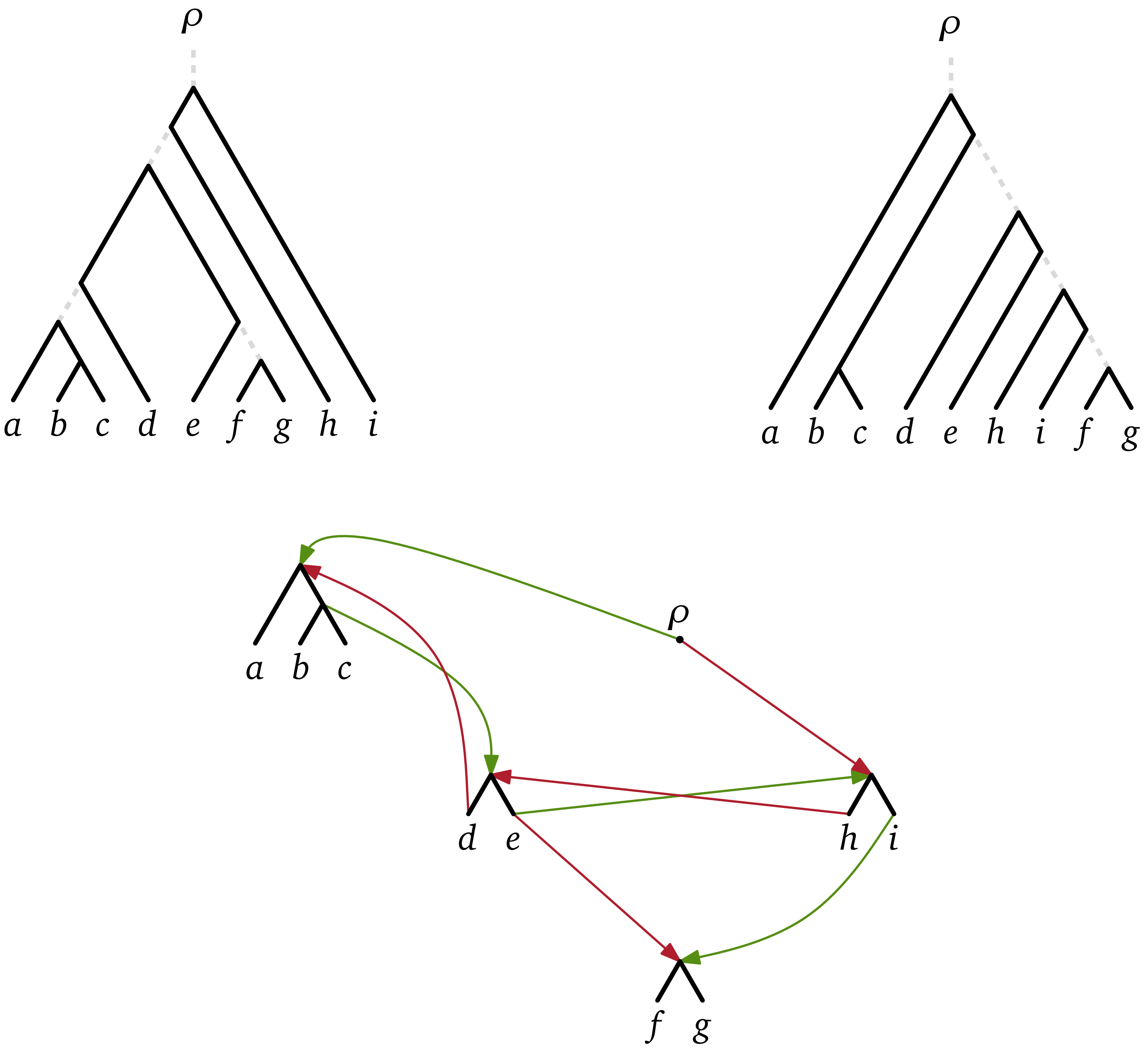
Once an AF is obtained, cut edges to eliminate cycles.

Hybridization [Whidden/Beiko/Zeh 2012]

Cycle graph



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- $2k$ edges between components
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Reducing the number of candidate edges

- Can get away with considering only k of the $2k$ edges

$\Rightarrow O(2^k \cdot 2.42^k n) = O(4.84^k n)$ time

Hybridization [Whidden/Beiko/Zeh 2012]

A better analysis

- If the AF has $k' \approx k$ edges, the refinement step considers $\binom{k}{k-k'} \ll 2^k$ choices
- If the AF has $k' \approx 0$ edges, the refinement step considers at most $2^{k'} \ll 2^k$ choices
- If the AF has $k' \approx k/2$ edges, the refinement step considers $\binom{k}{k-k'} \approx 2^k$ choices, but this situation can arise only $2.42^{k'} \ll 2.42^k$ times

$\Rightarrow O(3.18^k n)$ time

Application: SPR Supertrees

SPR Supertrees [Whidden/Zeh/Beiko 2012]

Open problem: Computational complexity of computing an optimal SPR supertree.

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Iterative improvement

- Try all $O(n^2)$ SPR operations on current supertree and choose the one that minimizes the SPR distance from gene trees

SPR Supertrees [Whidden/Zeh/Beiko 2012]

Limit number of SPR moves to consider

- Consider only SPR operations across $r = O(1)$ edges $\Rightarrow O(n)$ moves

$\Rightarrow O(tn)$ exact SPR computations

- Rank moves based on approximate SPR distance of resulting tree to gene trees
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MAF-driven improvements

- In each iteration, every gene tree initiates one SPR move on supertree that reduces its distance by one
- Choose this move using the MAF of gene tree and supertree

$\Rightarrow t$ exact SPR computations

Conclusions

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Compute *all* M(A)AFs [Abrecht et al. 2012]

- Provide more biological insight