Visualizing Multispecies Coalescent Trees: Drawing Gene Trees Inside Species Trees

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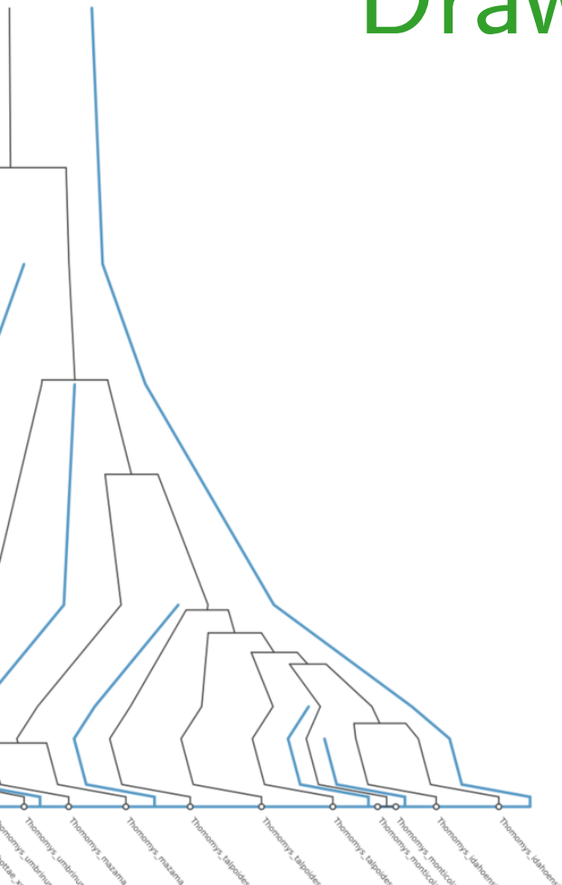
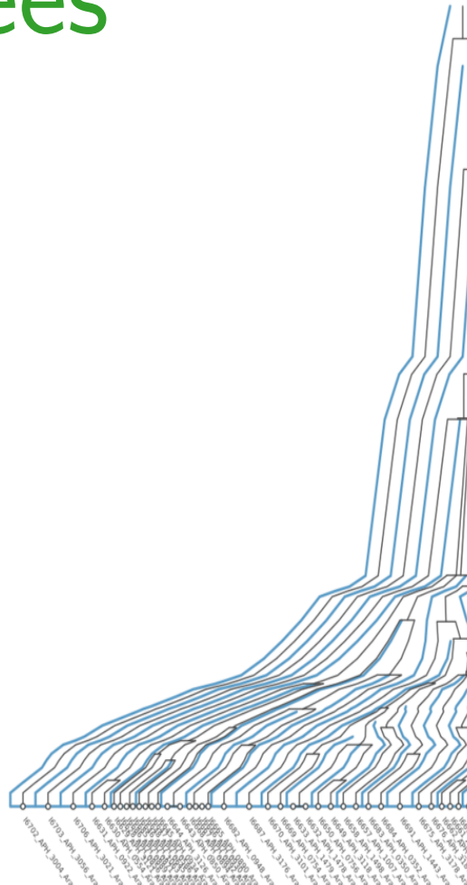
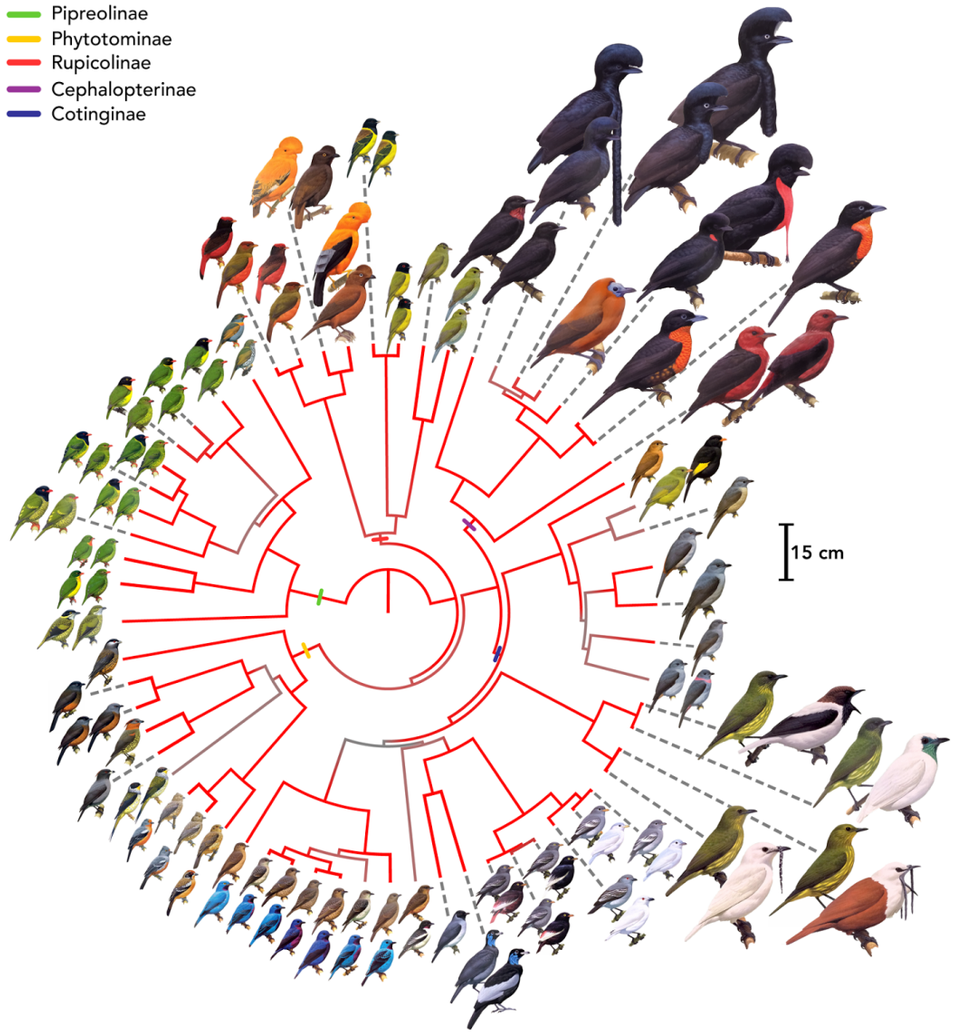
Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

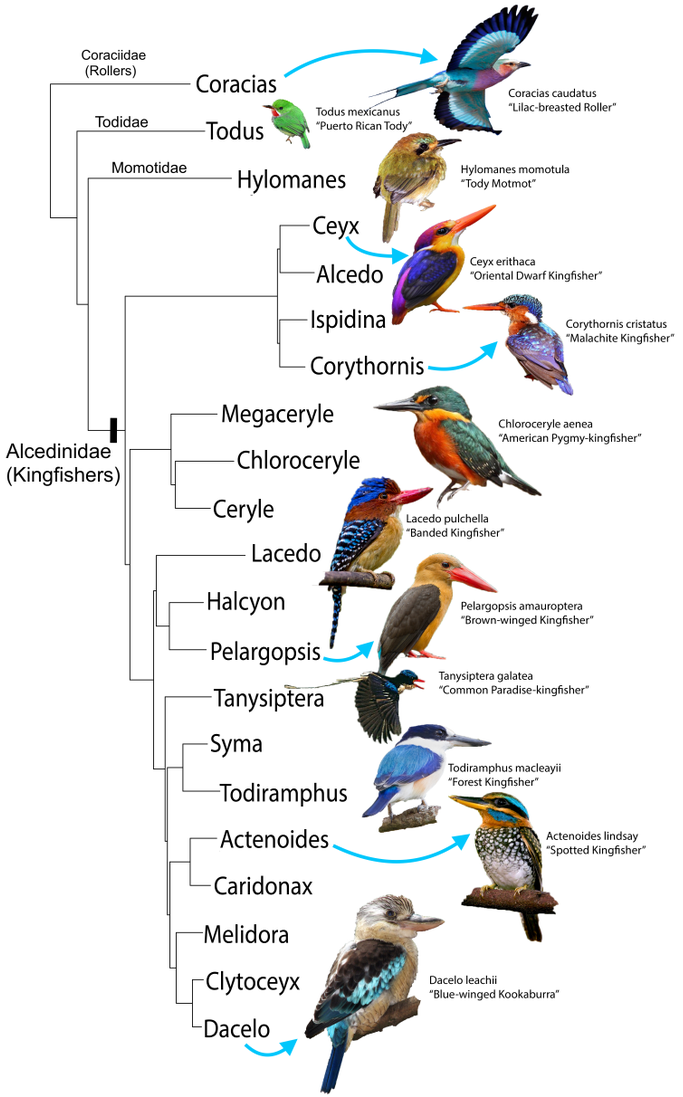




Phylogenetic trees



by Berv & Prum 2014



by Jenna McCullough 2016

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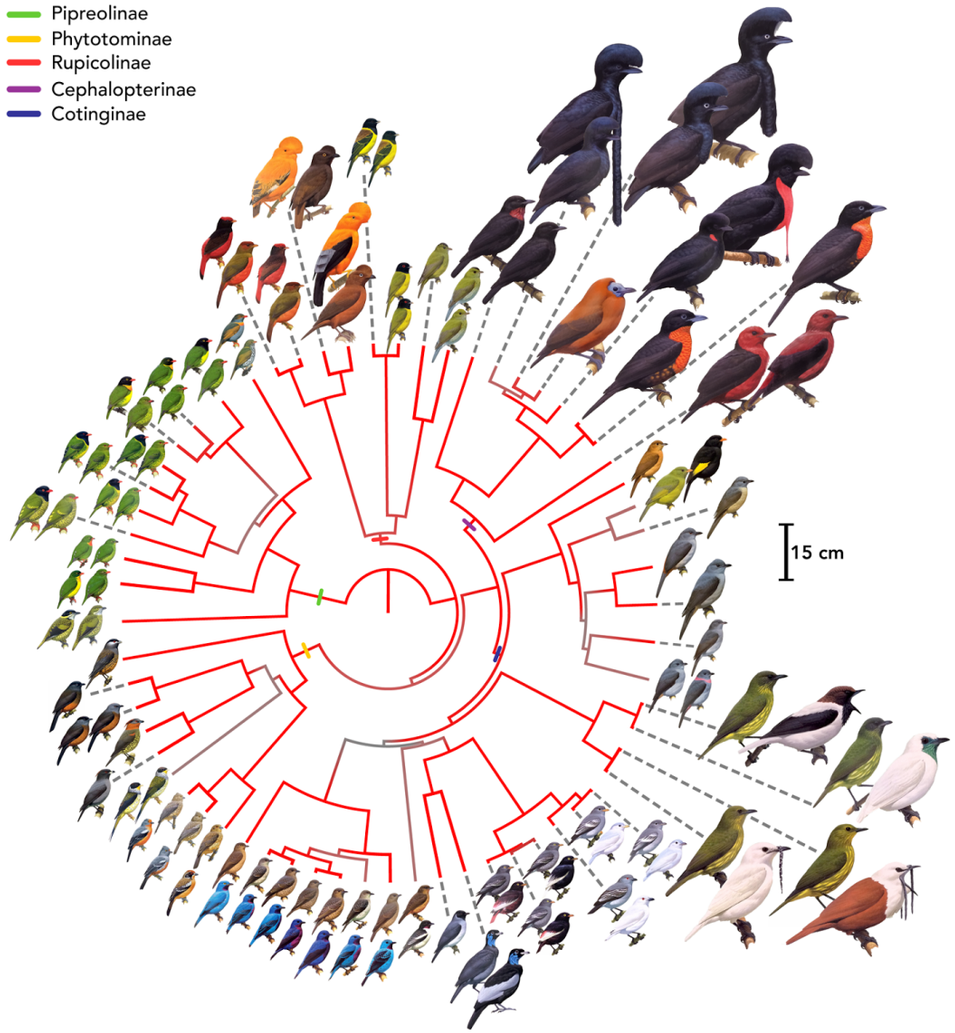

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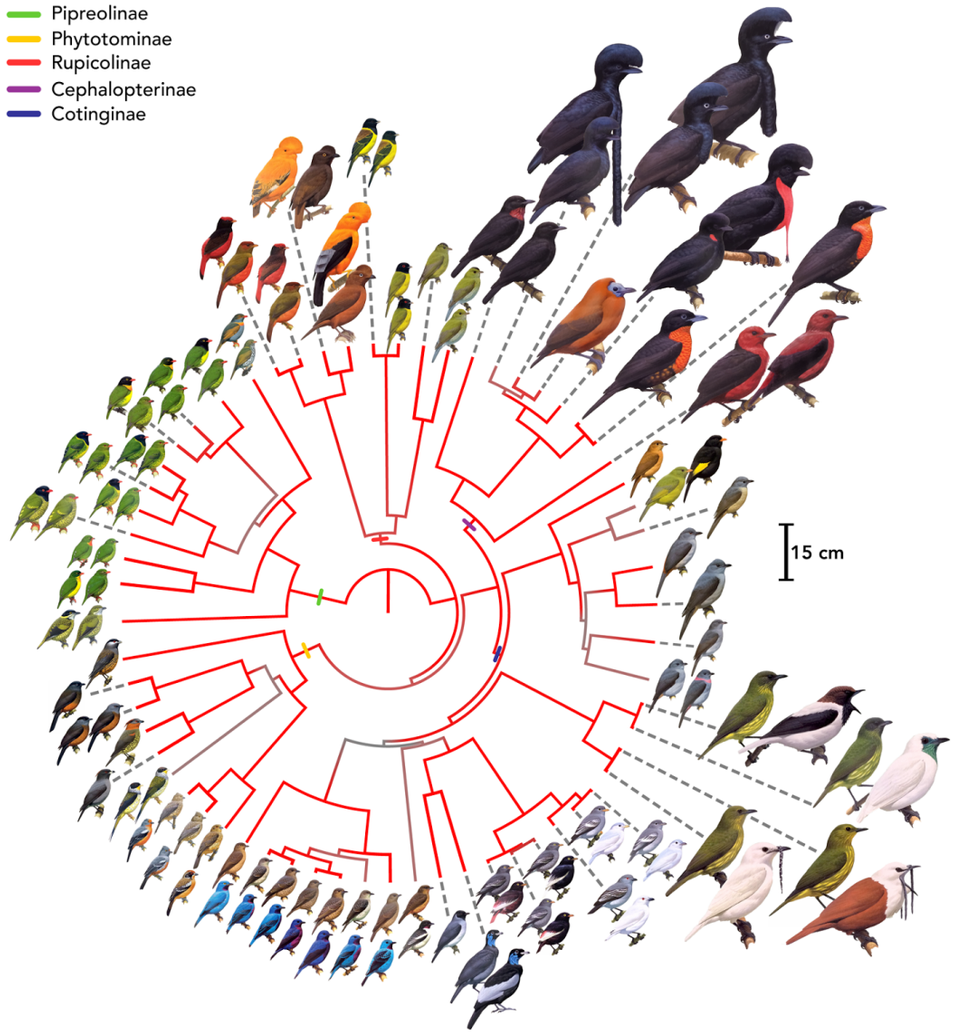
A **phylogenetic tree** T is a rooted, binary tree with labelled leaves and vertex heights.

Phylogenetic trees



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Assume all leaves have height 0.

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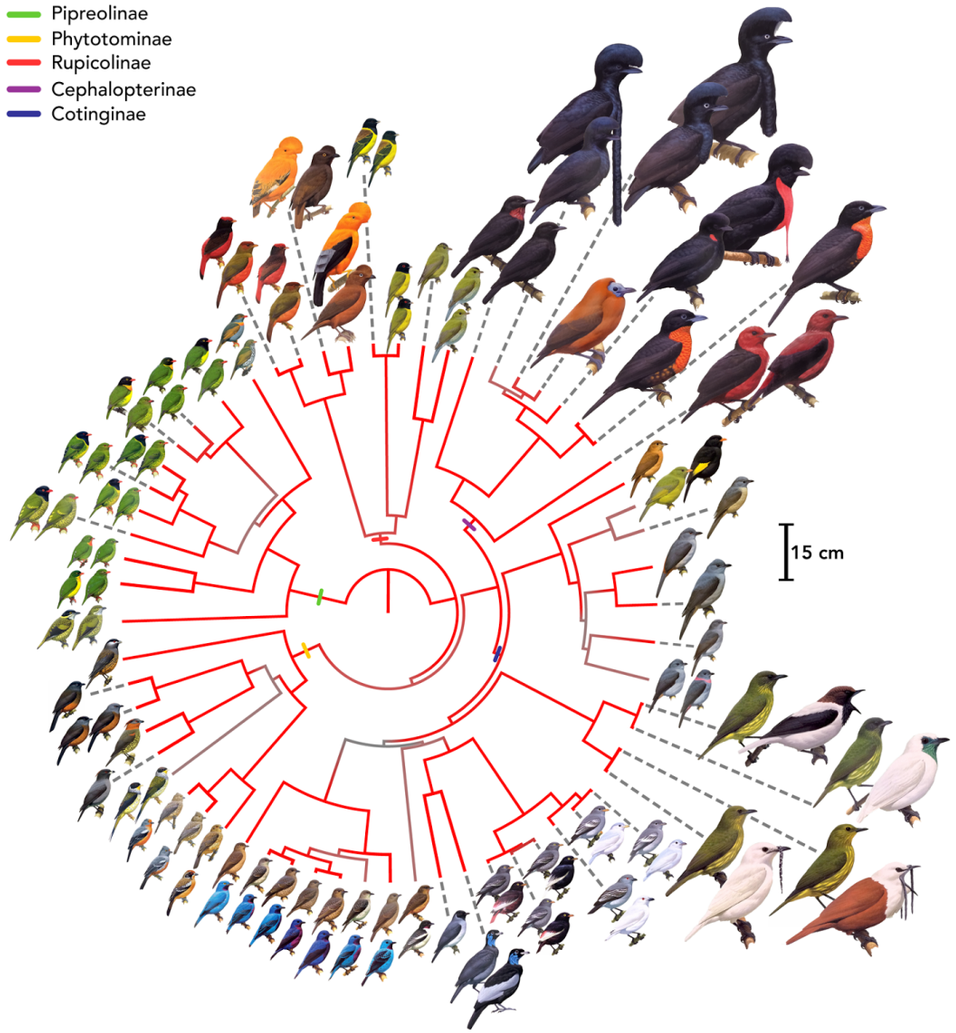

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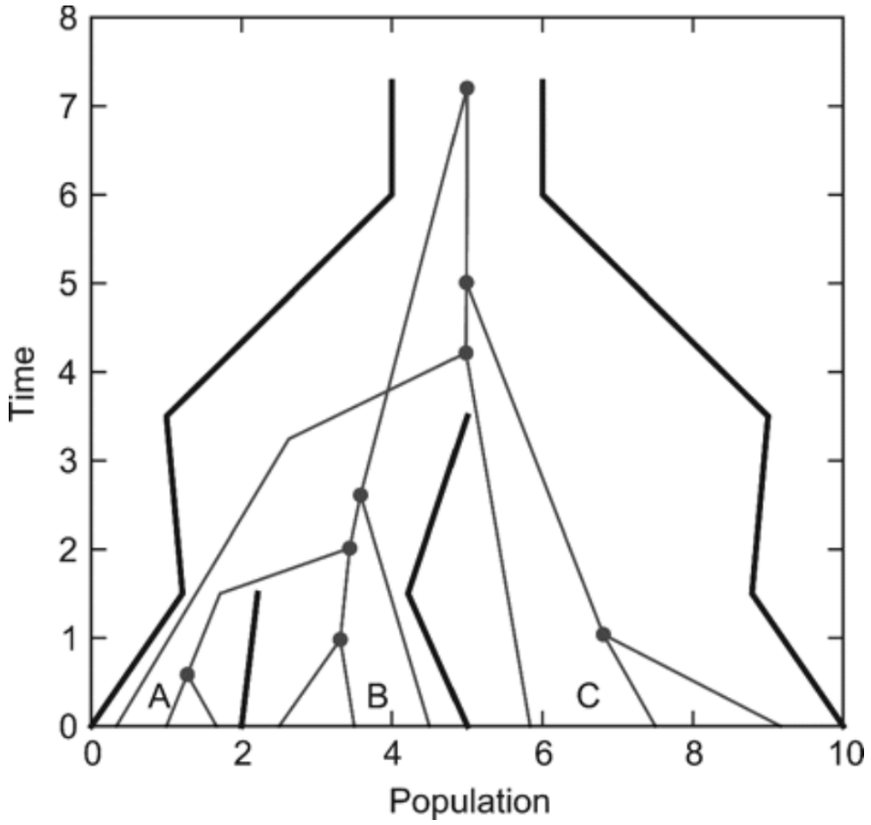
A **phylogenetic tree** T is a rooted, binary tree with labelled leaves and vertex heights.

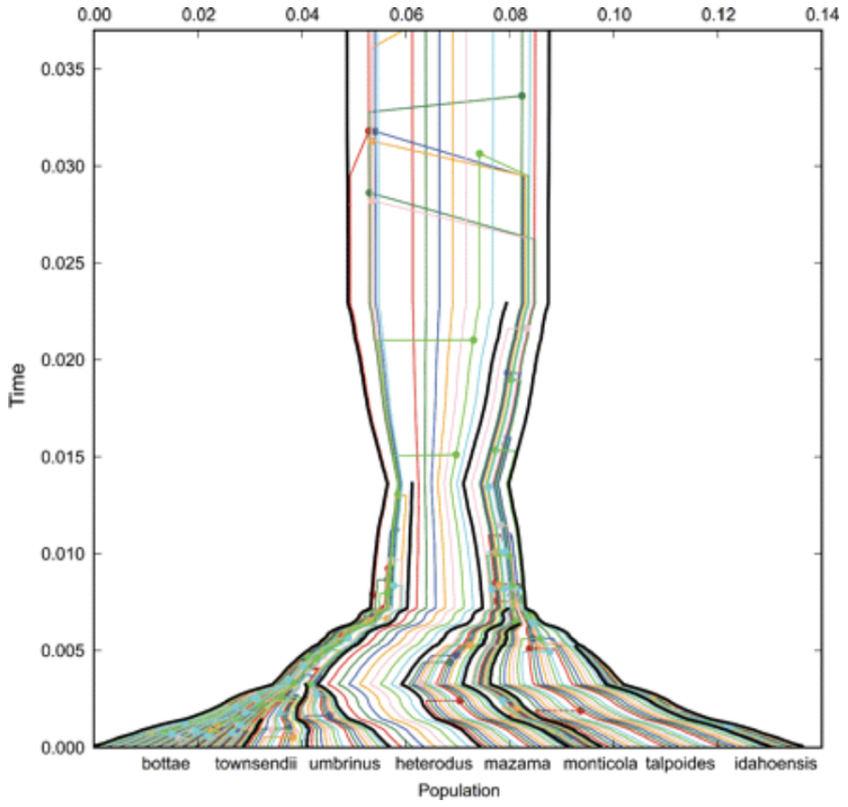
Assume all leaves have height 0.

Call T a **species/gene tree** if the leaves represent species/biological sequences.

Multispecies coalescent

- In practice, a species tree and its gene trees *differ*.





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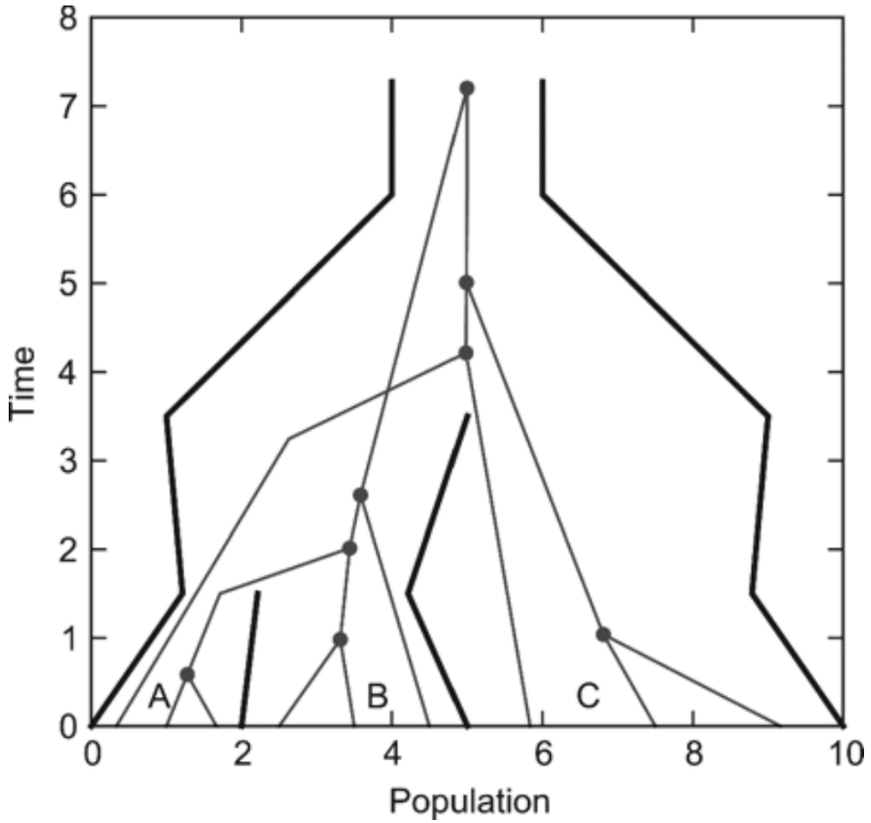

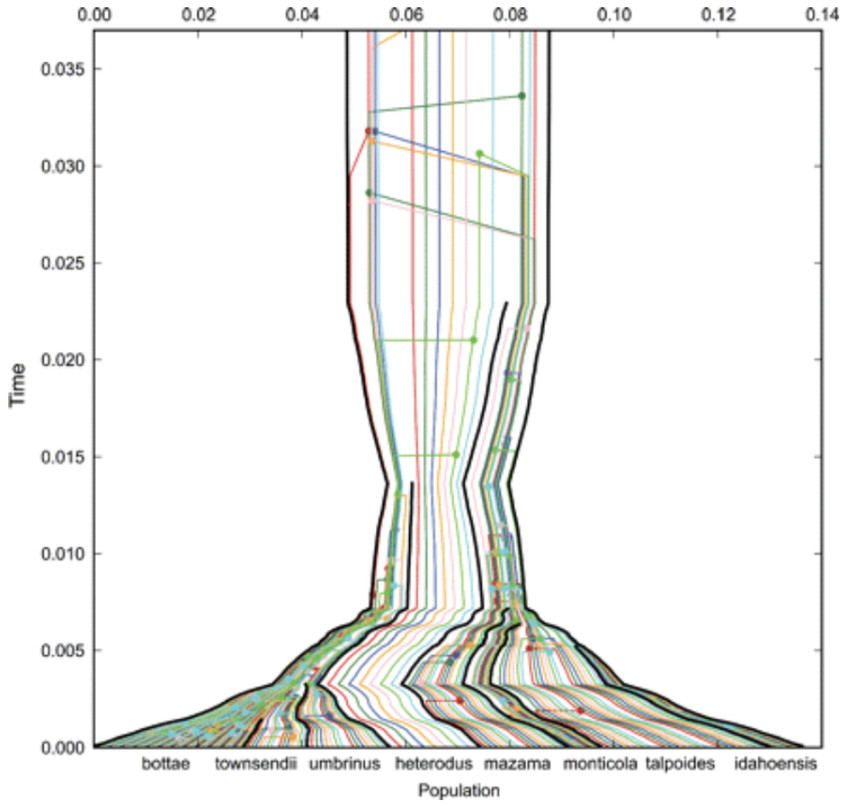

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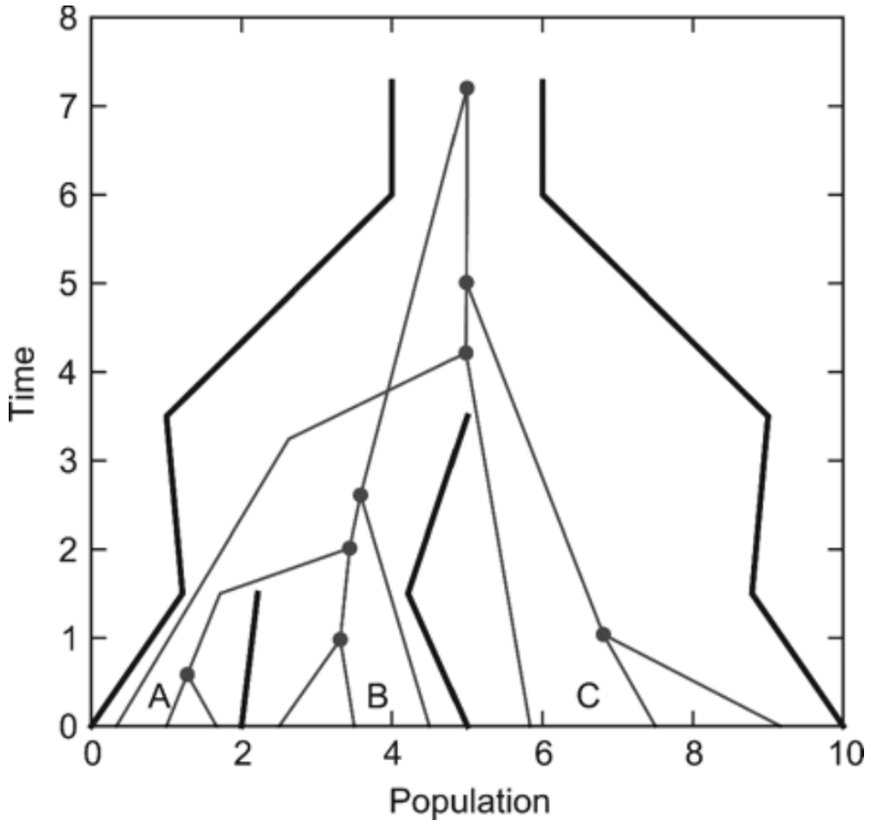

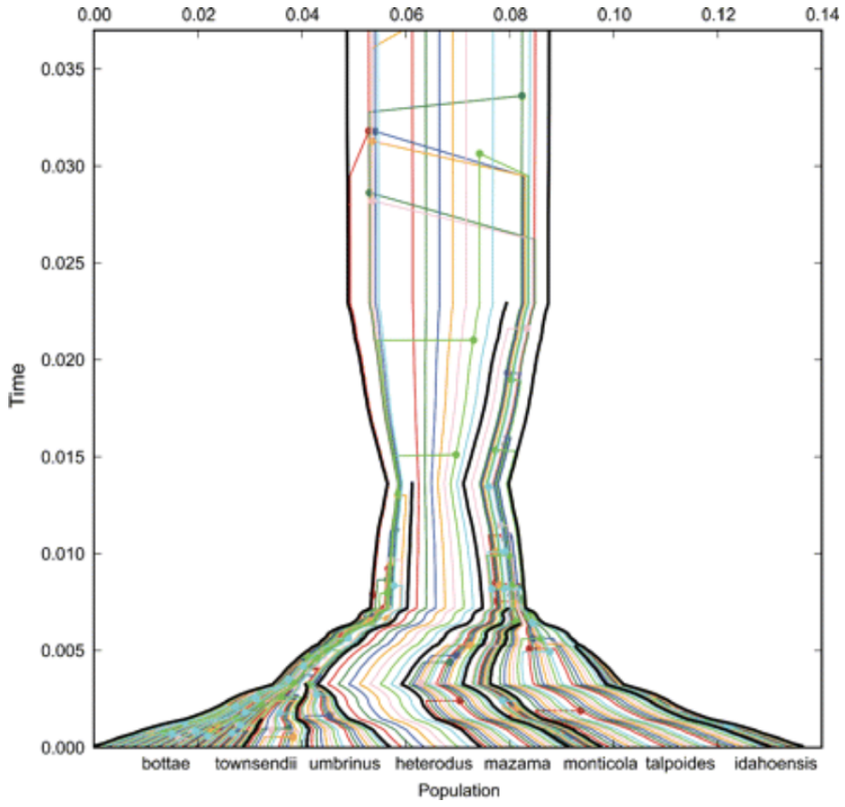

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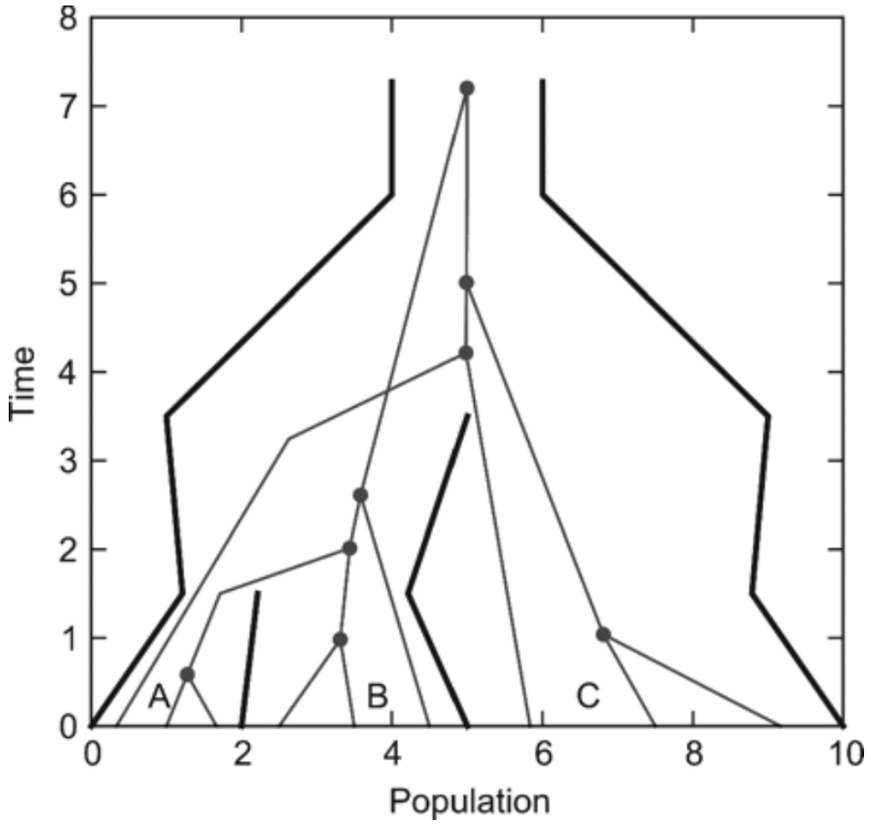
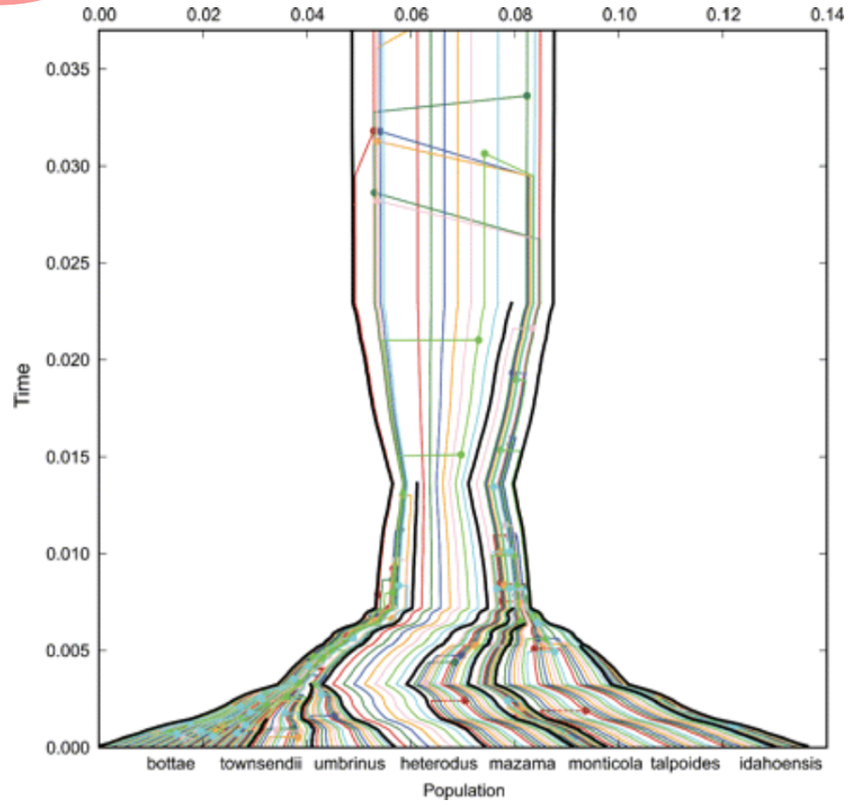


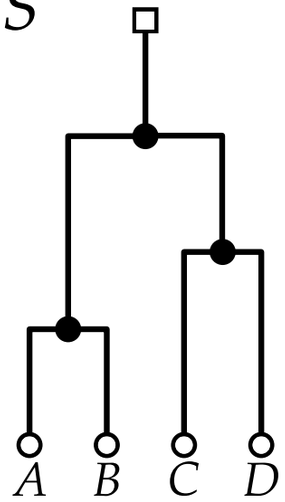


Multispecies coalescent trees

A **multispecies coalescent tree** $\langle S, T, \varphi \rangle$ consists of

Multispecies coalescent trees

Species tree S



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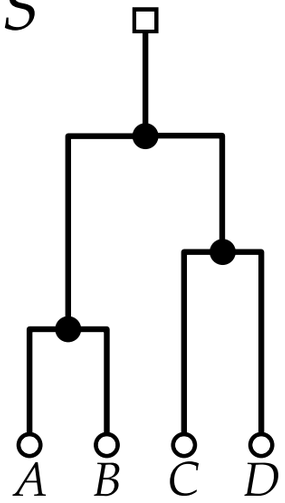

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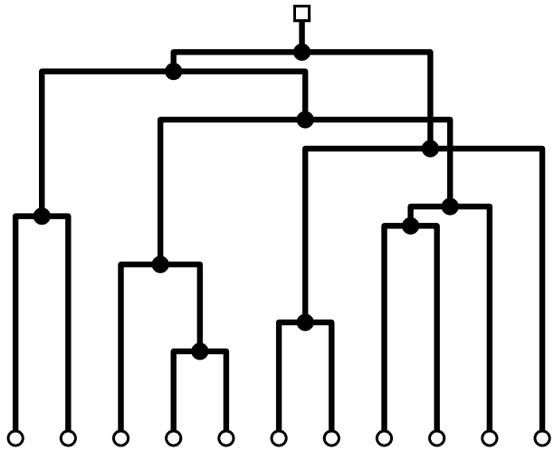

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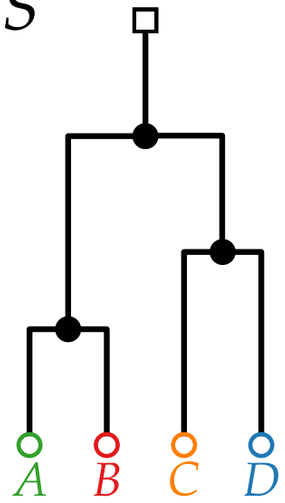

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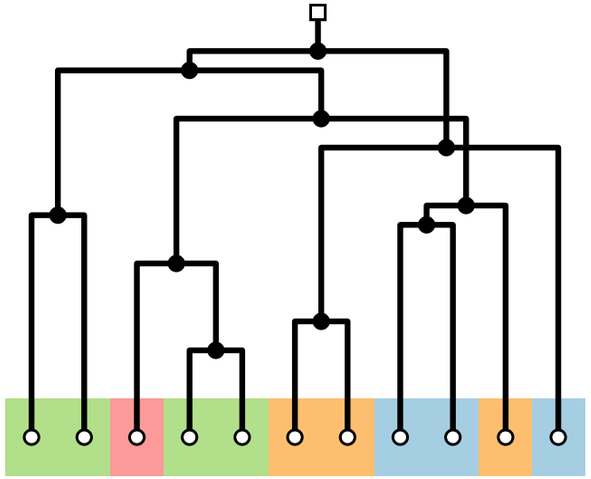

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- a mapping φ of the leaves of T (**genes**) to the leaves of S (**species**).

Multispecies coalescent trees

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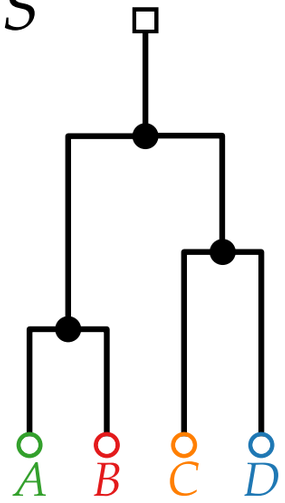

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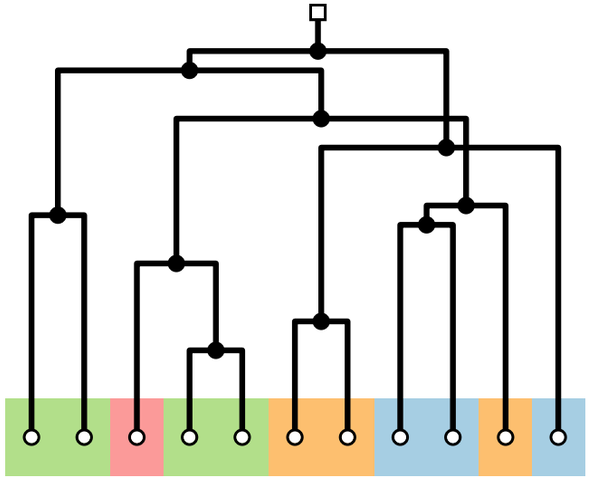

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Additionally:

- Effective population size – branch widths

Multispecies coalescent trees

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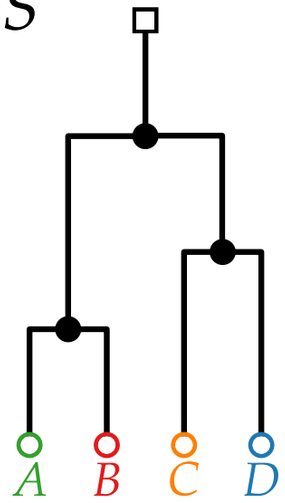

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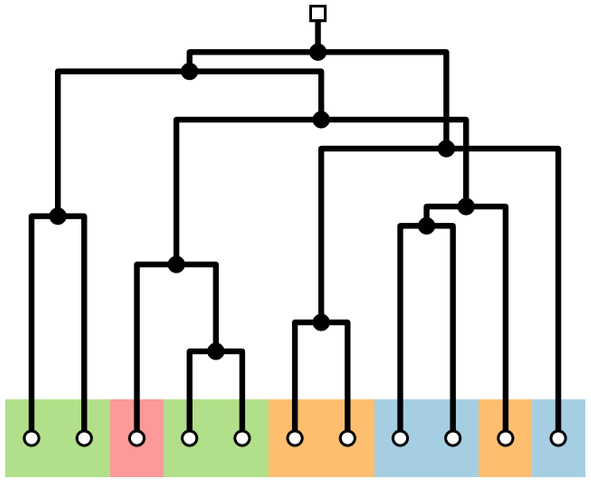

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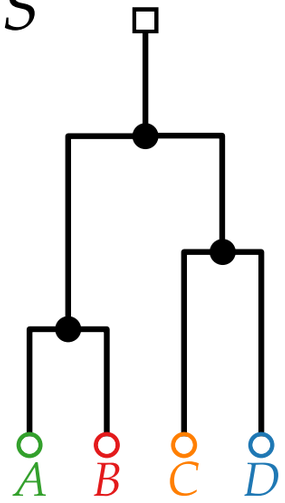
Drawing style

Species tree S



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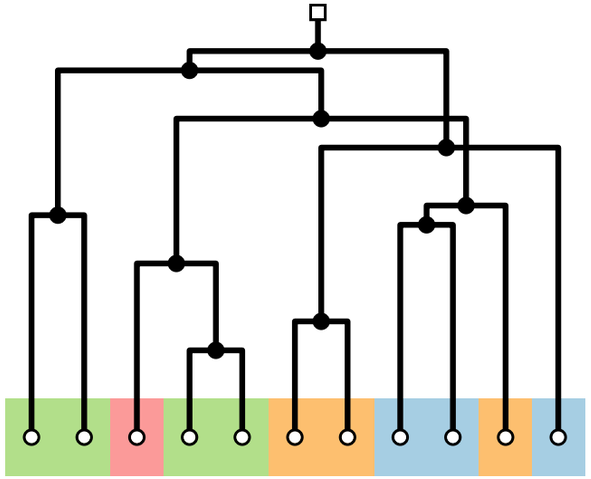

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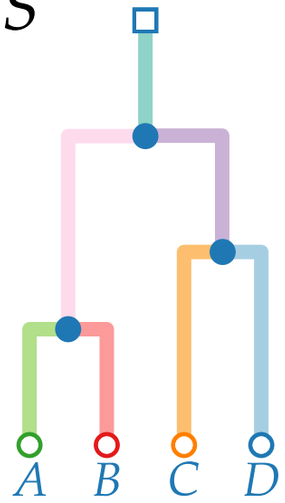

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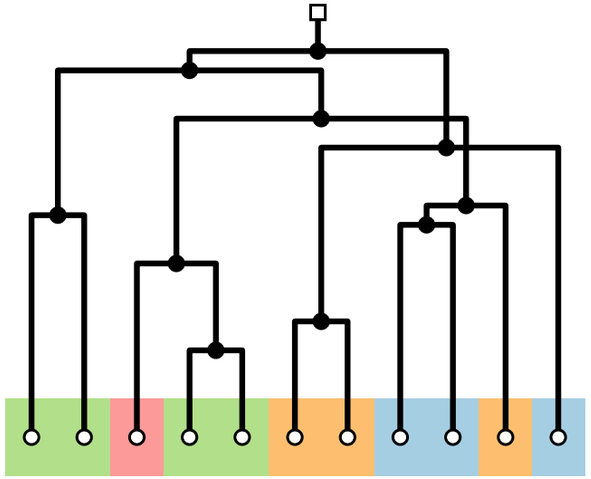

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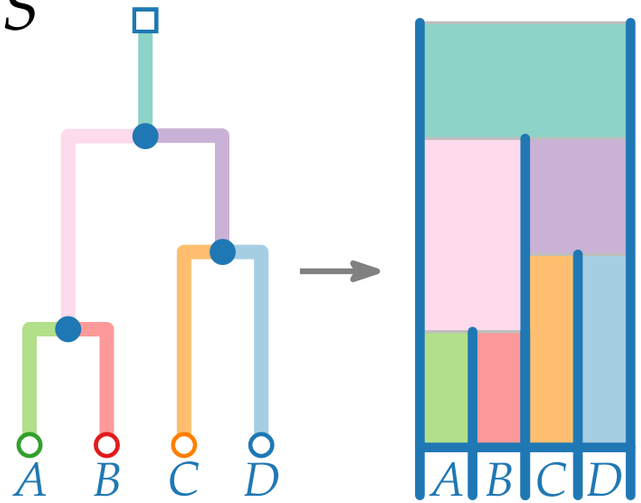

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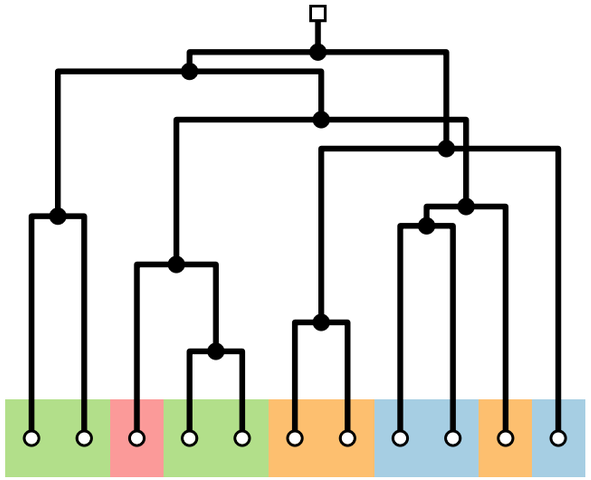

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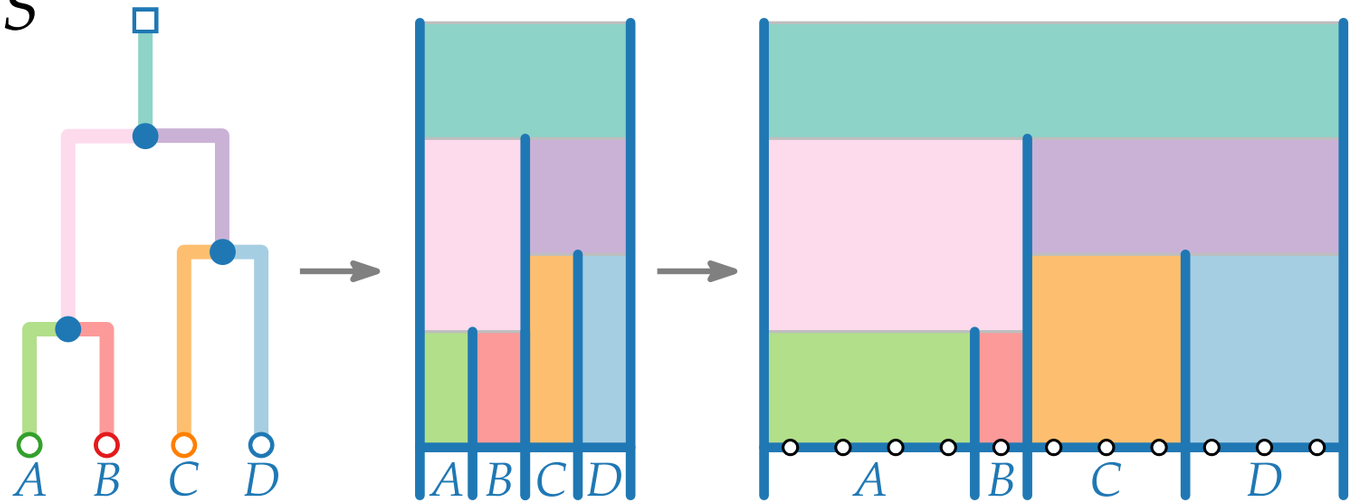

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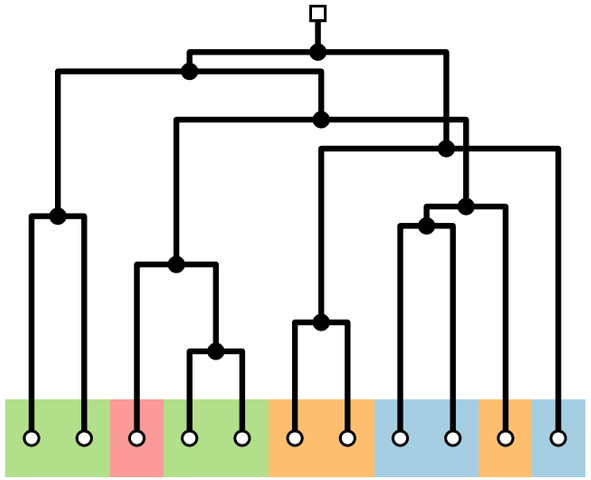

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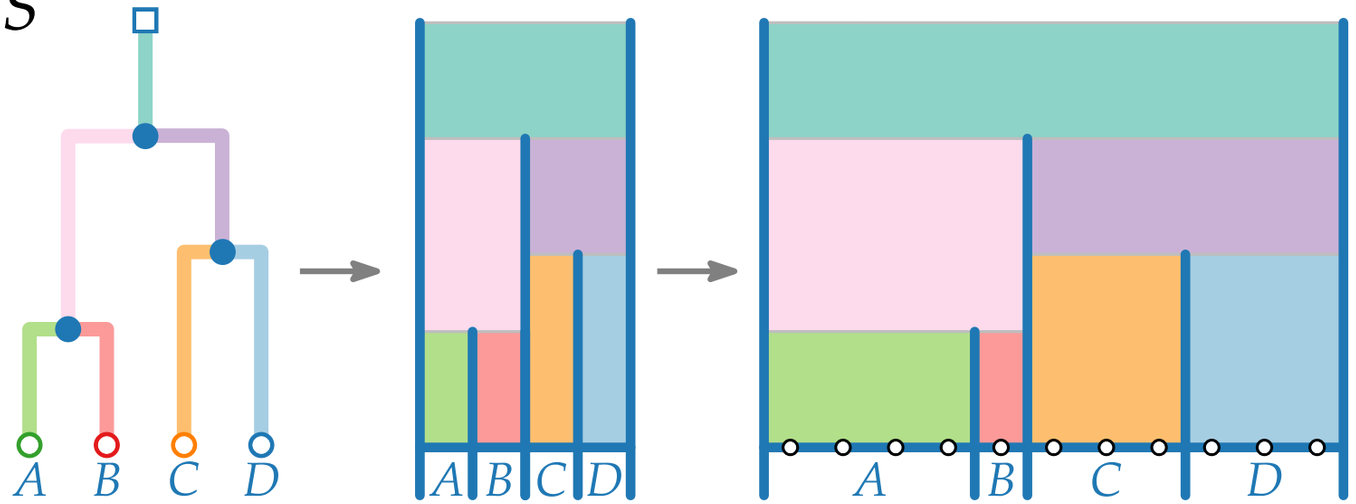

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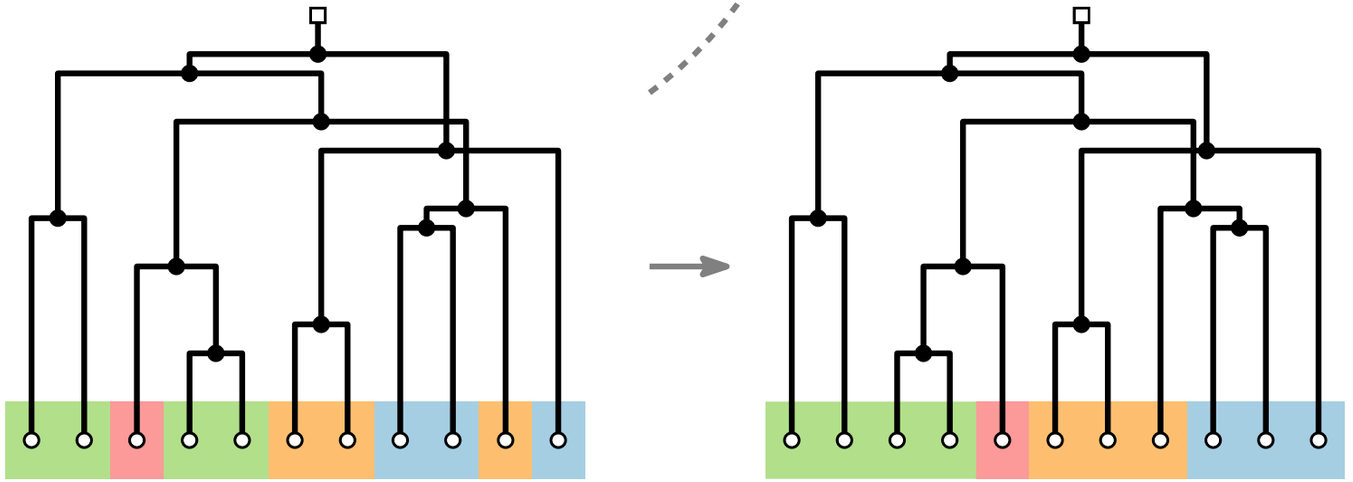

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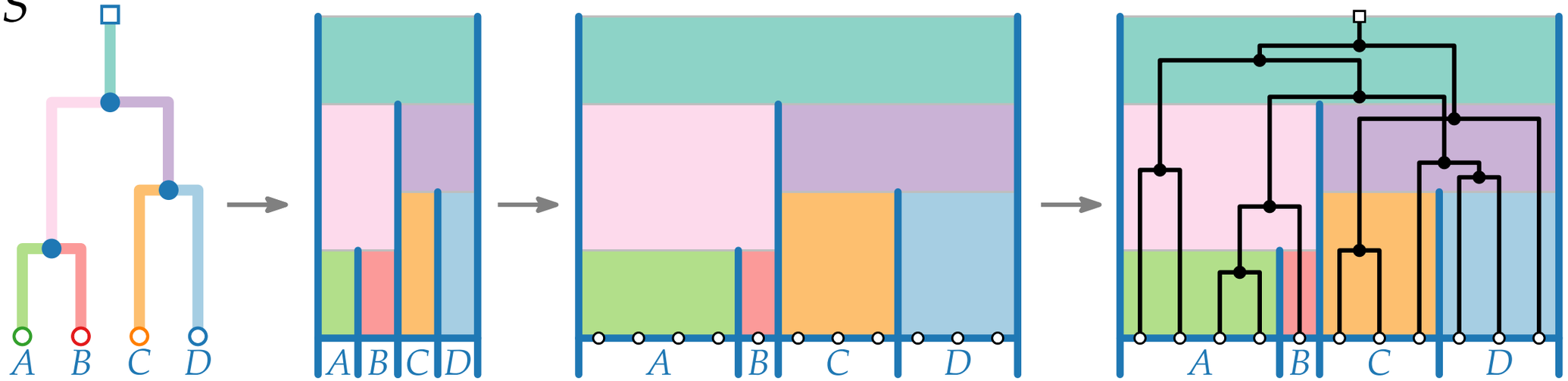

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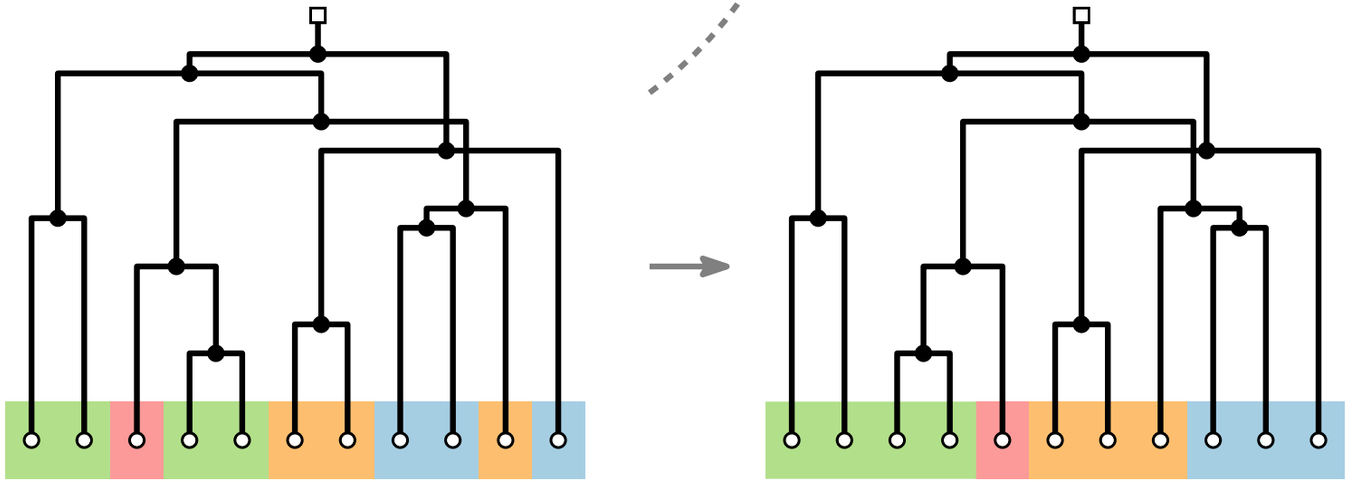

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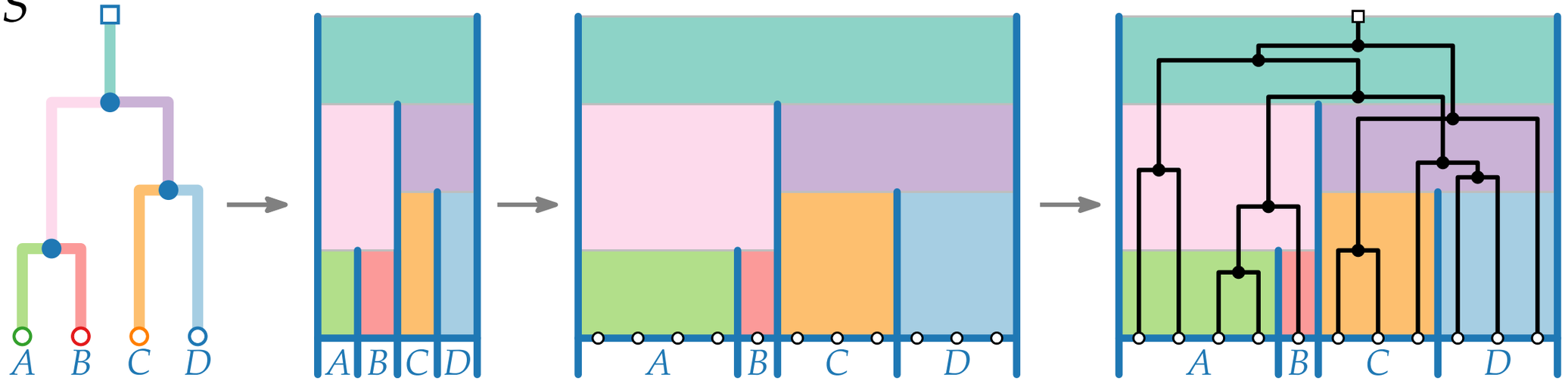

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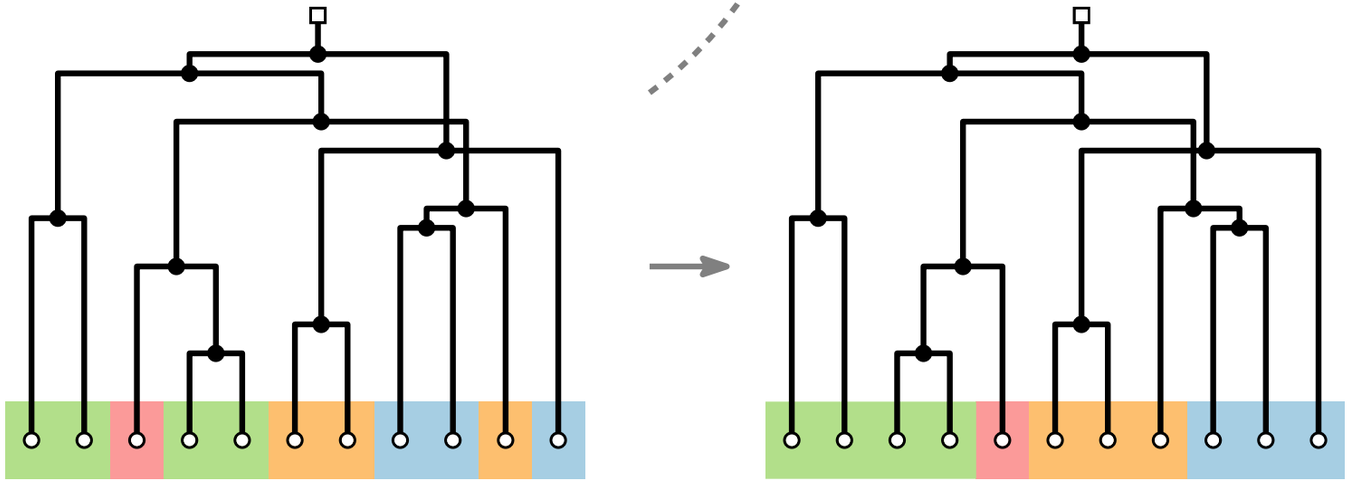
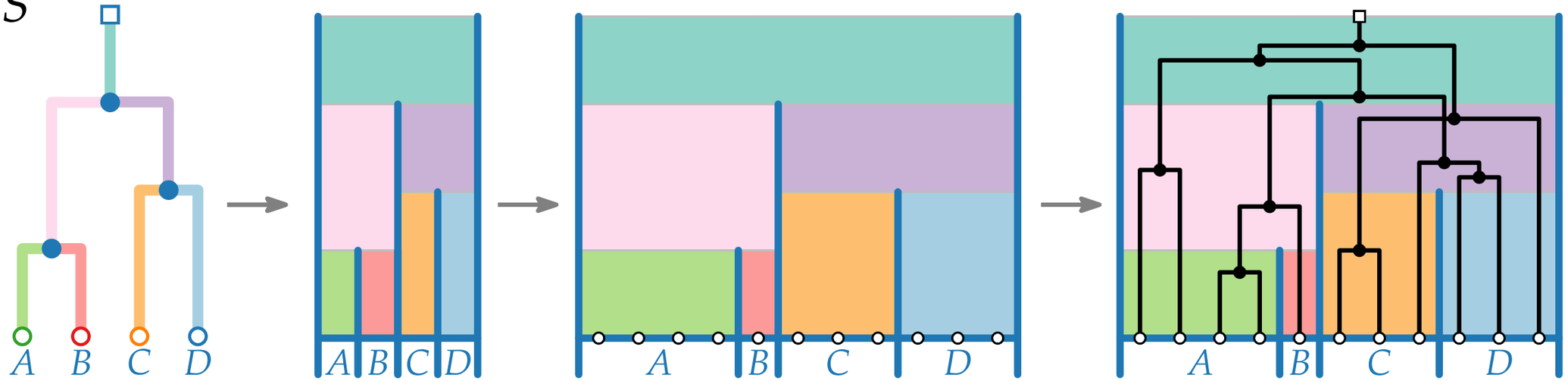


Drawing rules:

Drawing style

Species tree S



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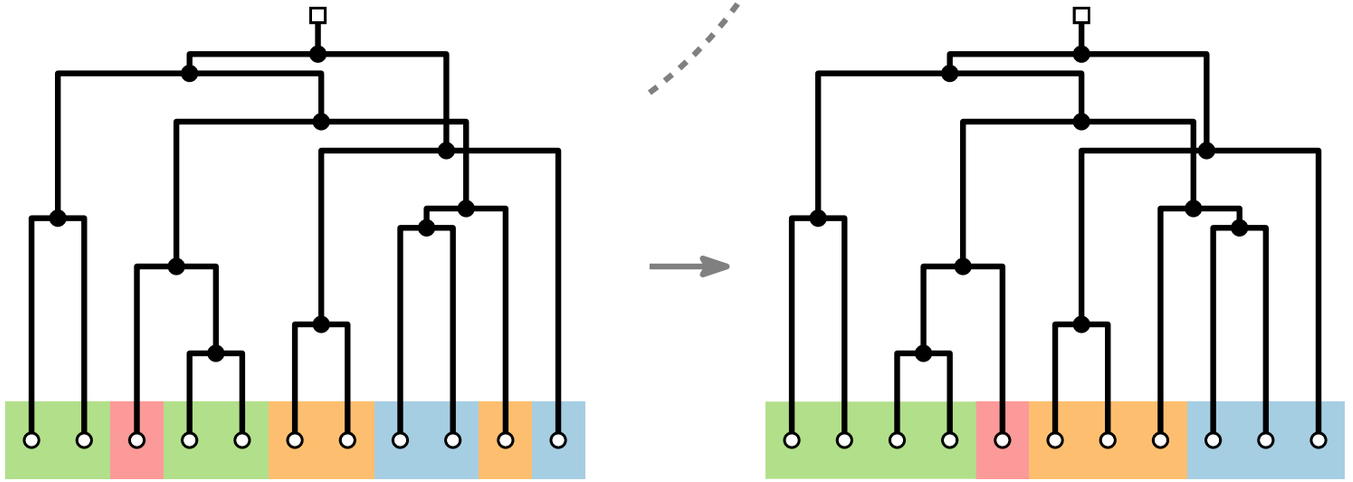

Drawing rules:

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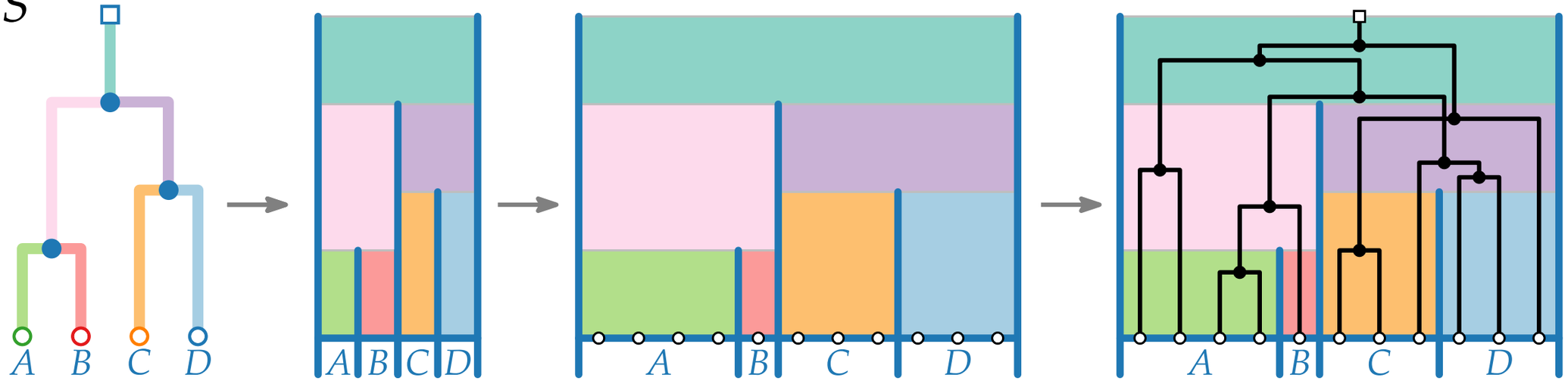

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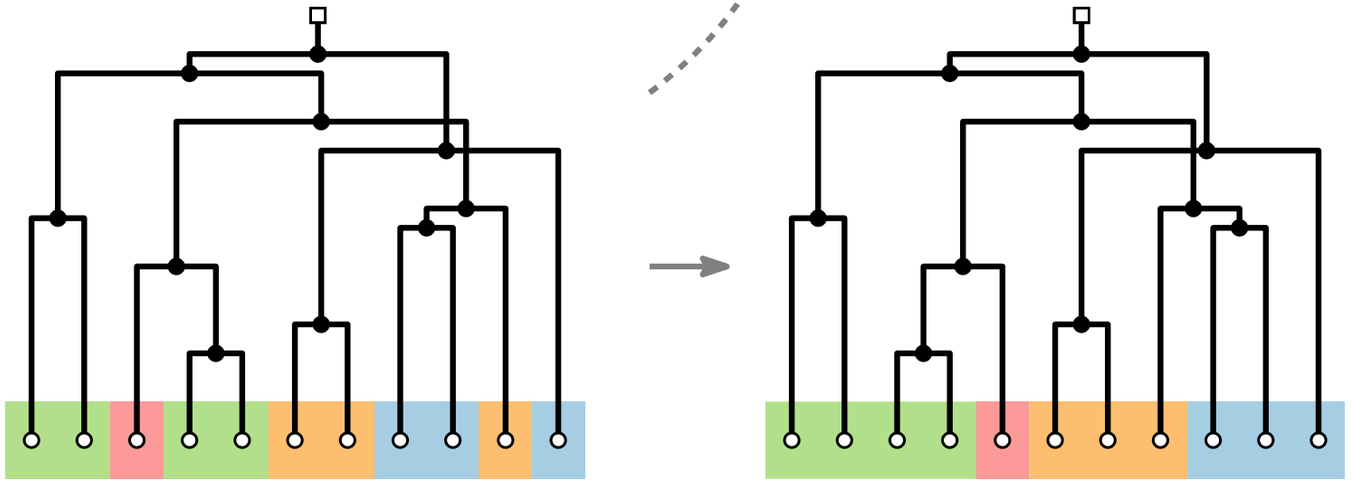

Drawing rules:

- orthogonal style
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Drawing style

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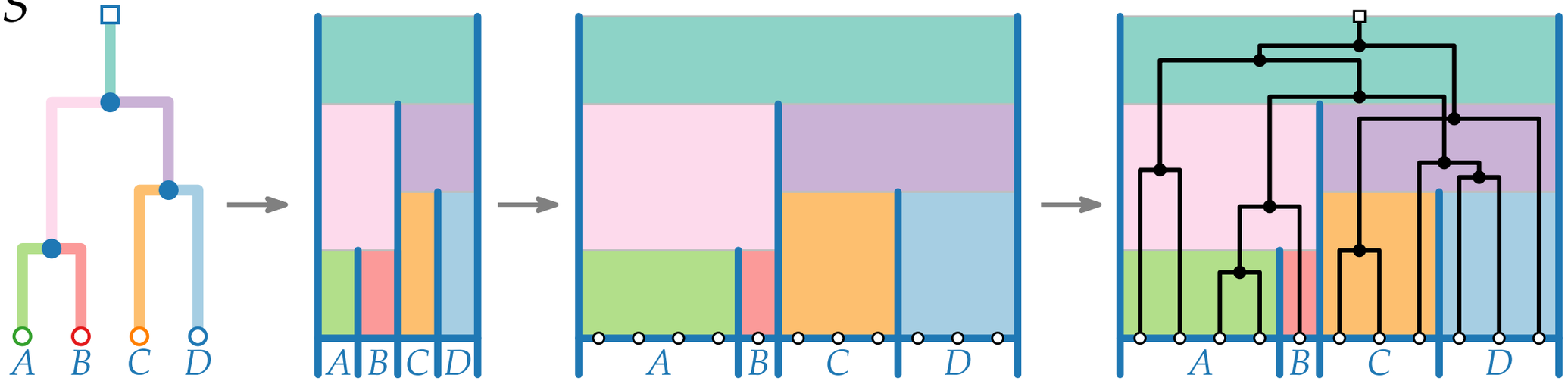

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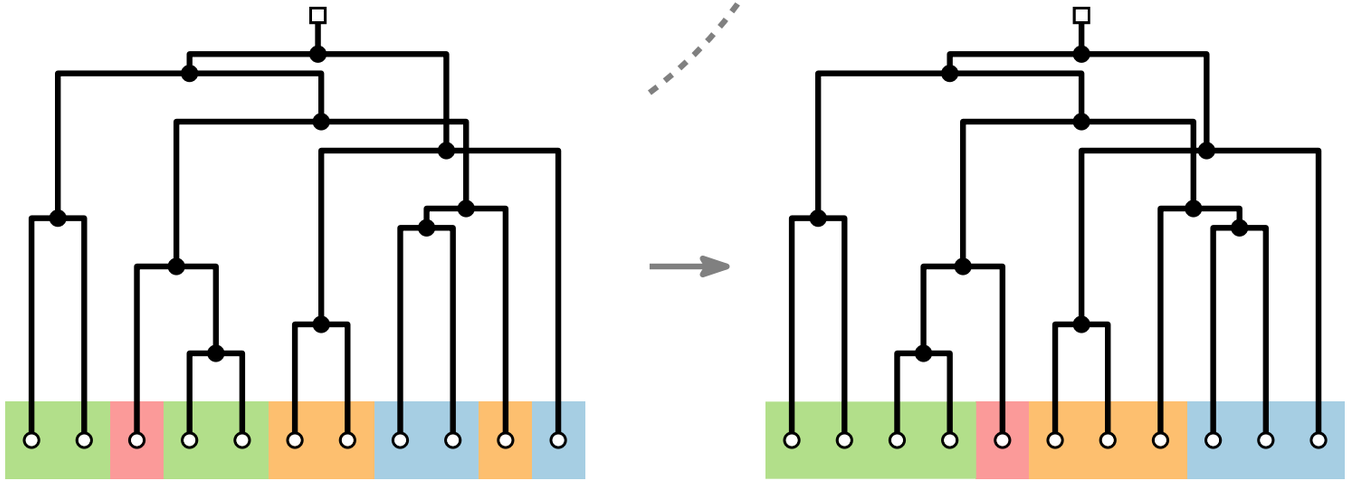

Drawing rules:

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- species tree:
  show only “frame”

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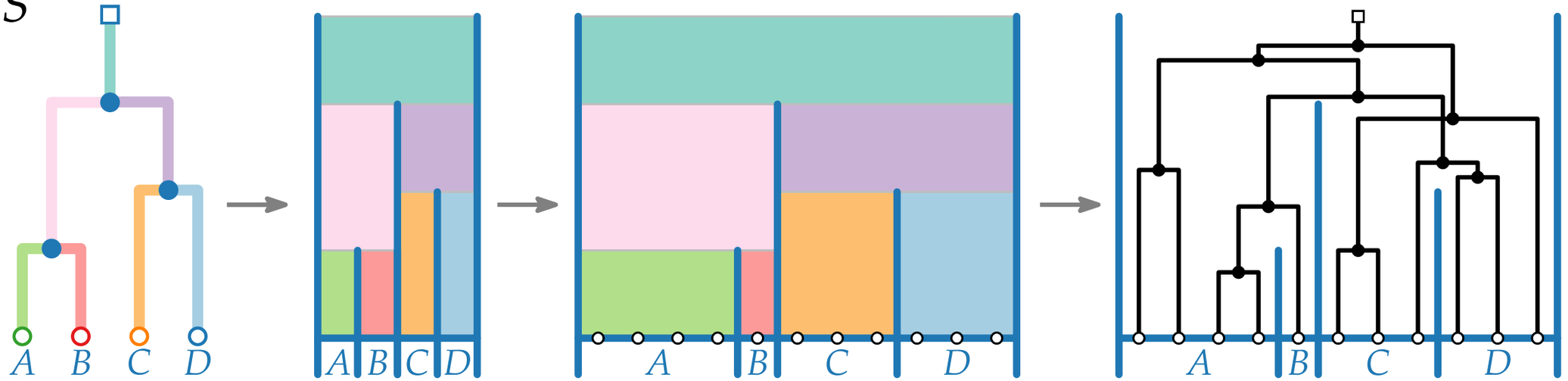

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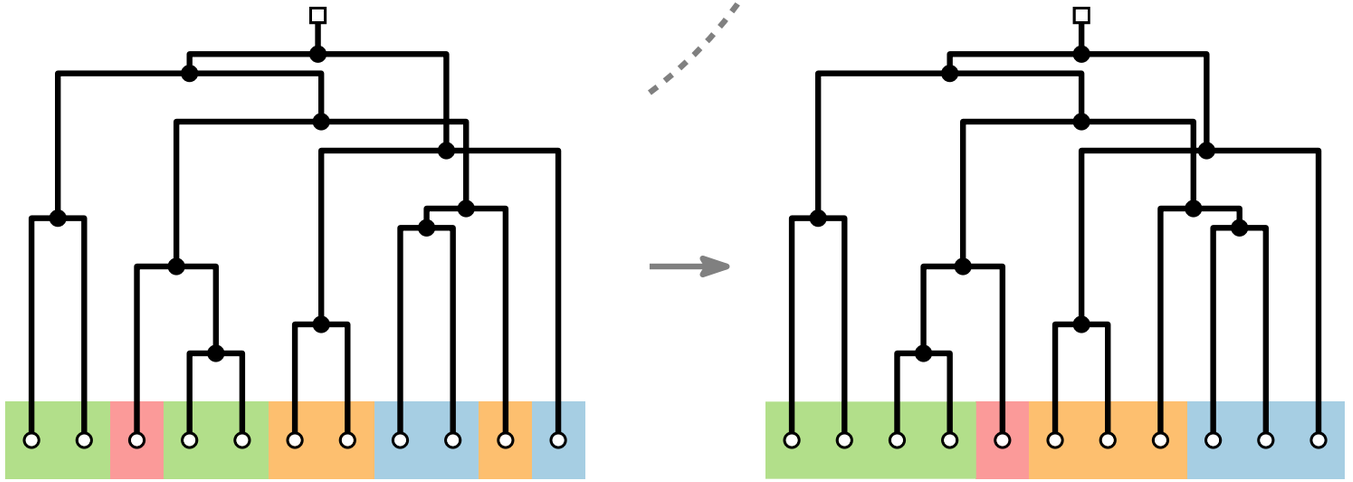

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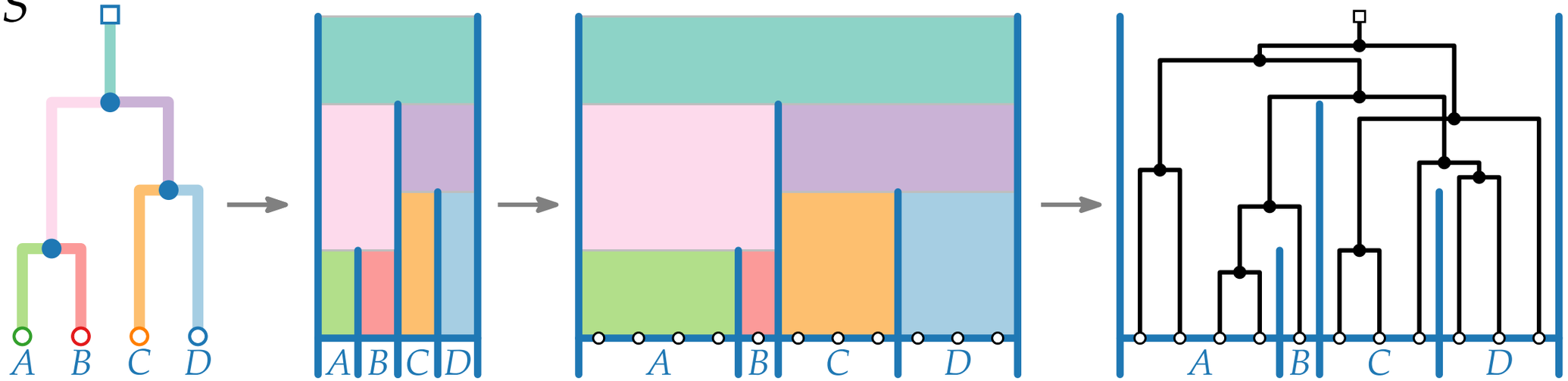

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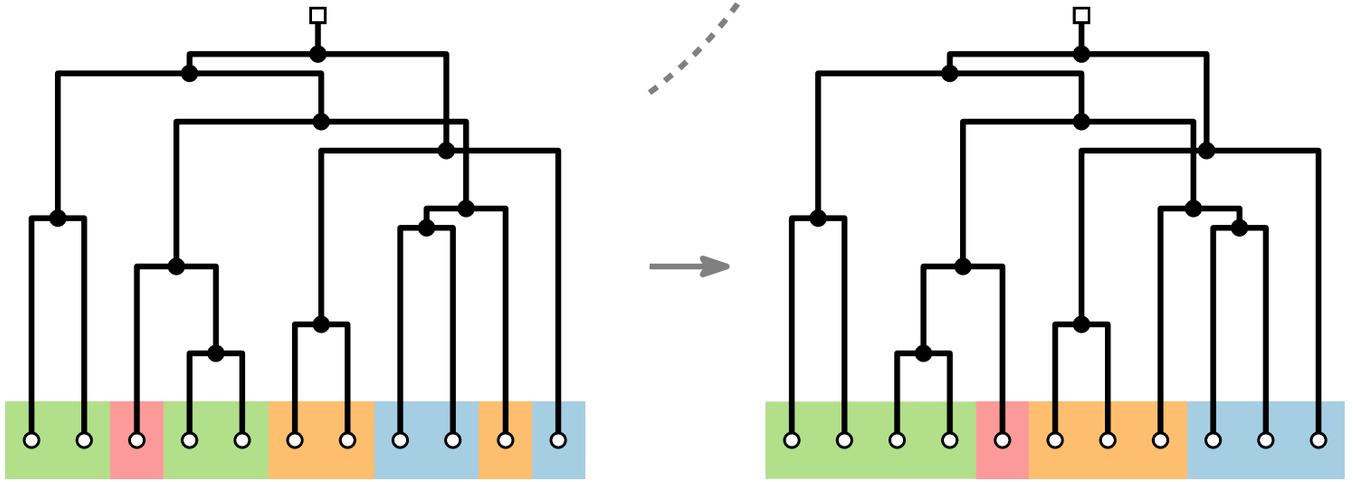

Drawing rules:

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- species tree: show only “frame”
- gene tree: center vertices horizontally

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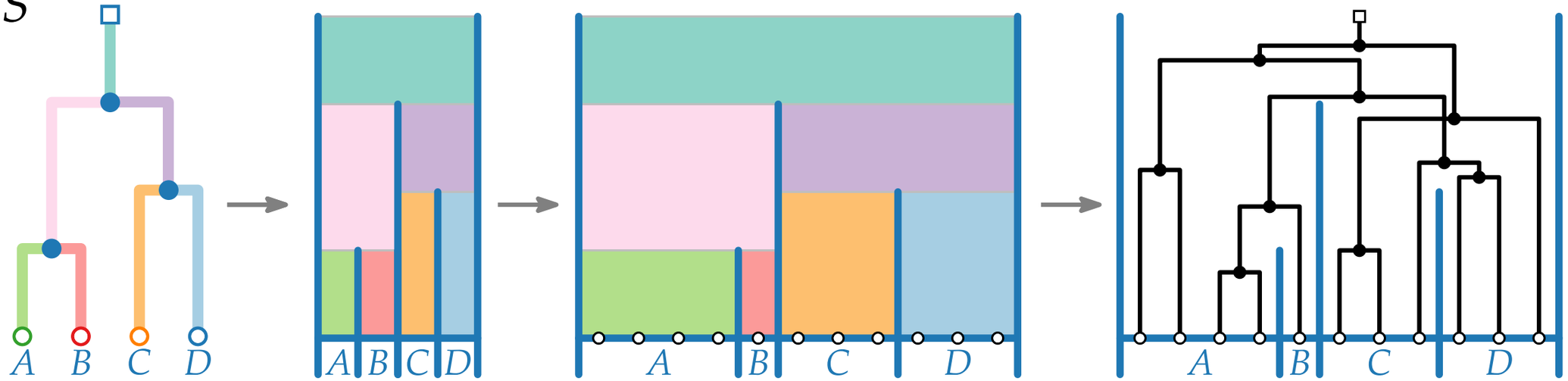

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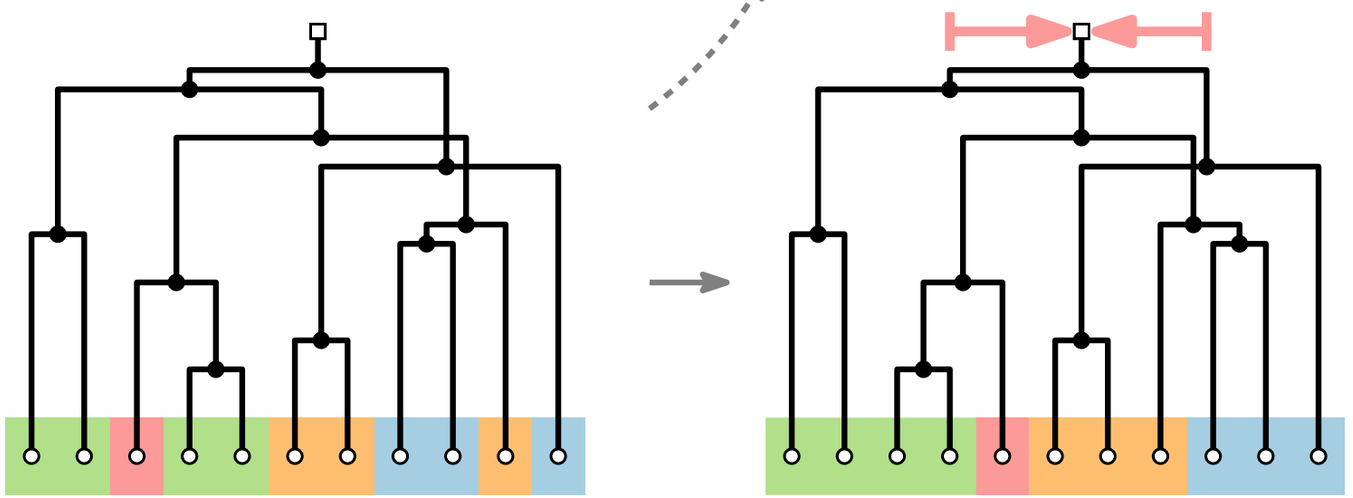

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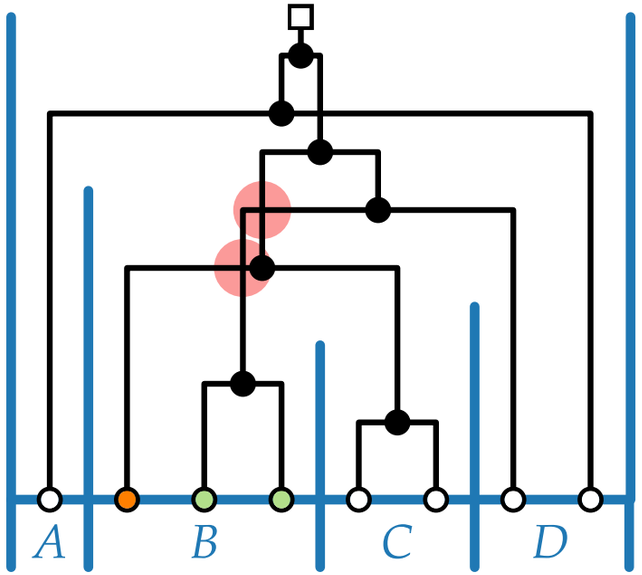
Crossing minimization

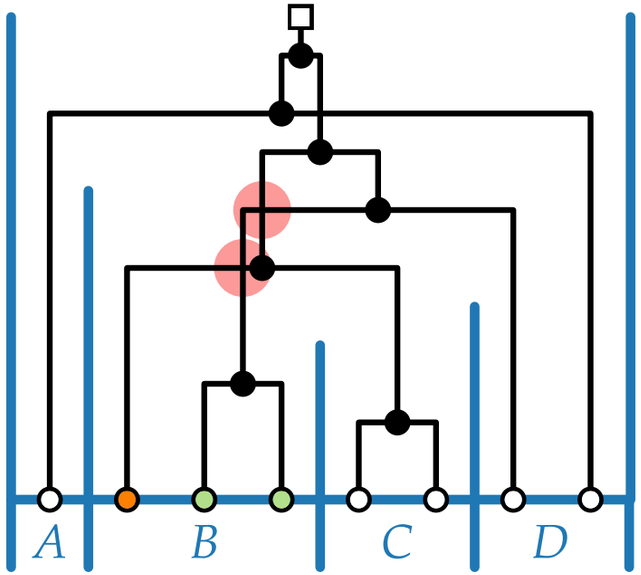
Minimize the number of crossings by...

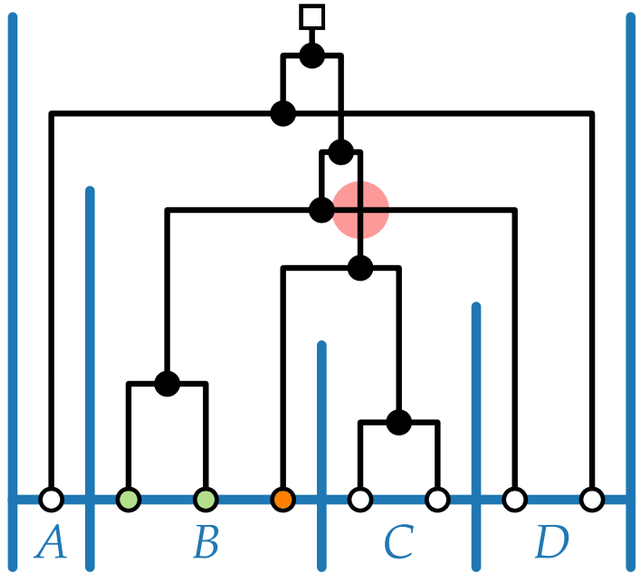


Crossing minimization

Minimize the number of crossings by...

changing gene order





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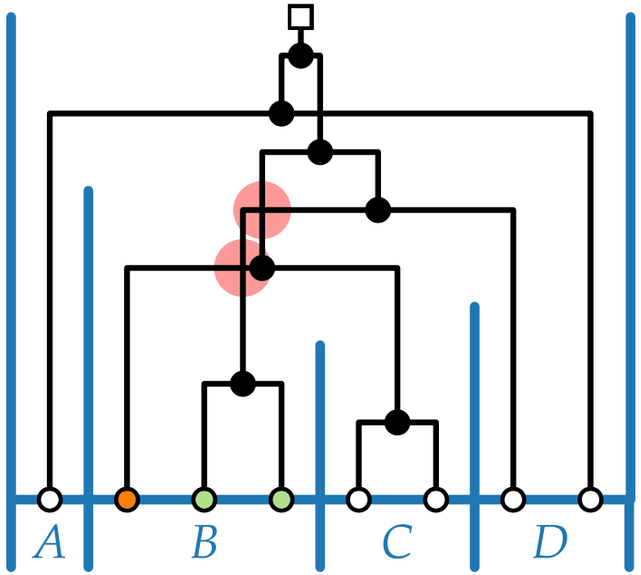
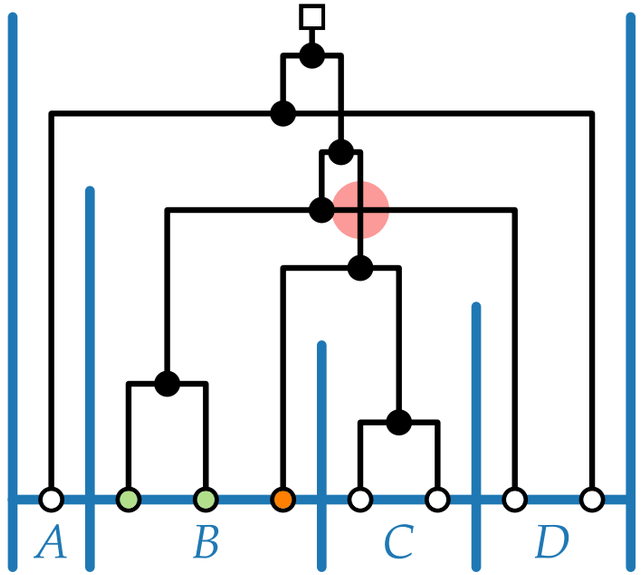


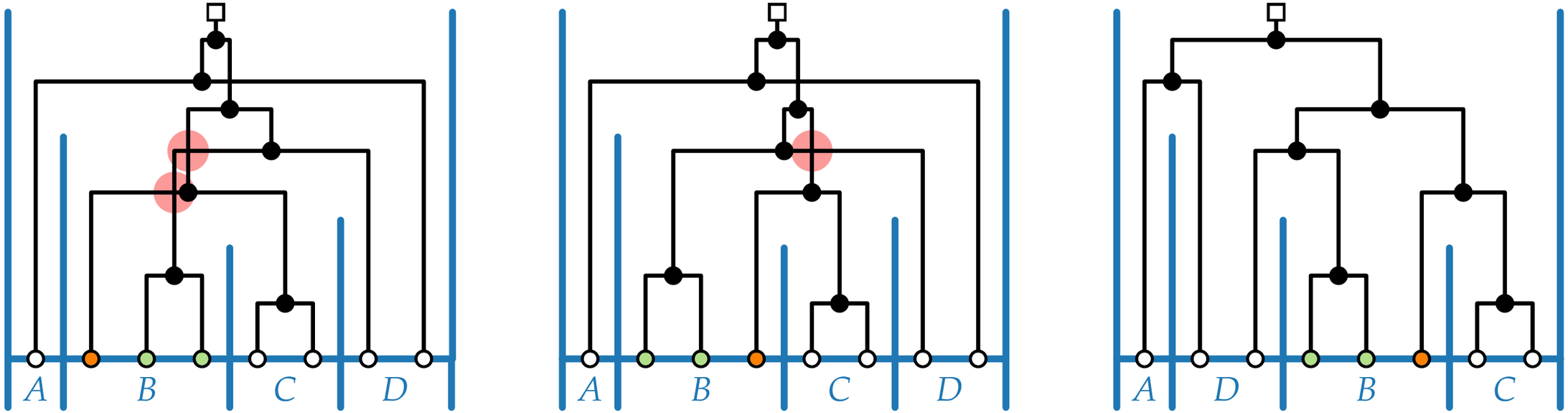


■ **fixed** species order

Crossing minimization

Minimize the number of crossings by...

changing gene order + changing species order



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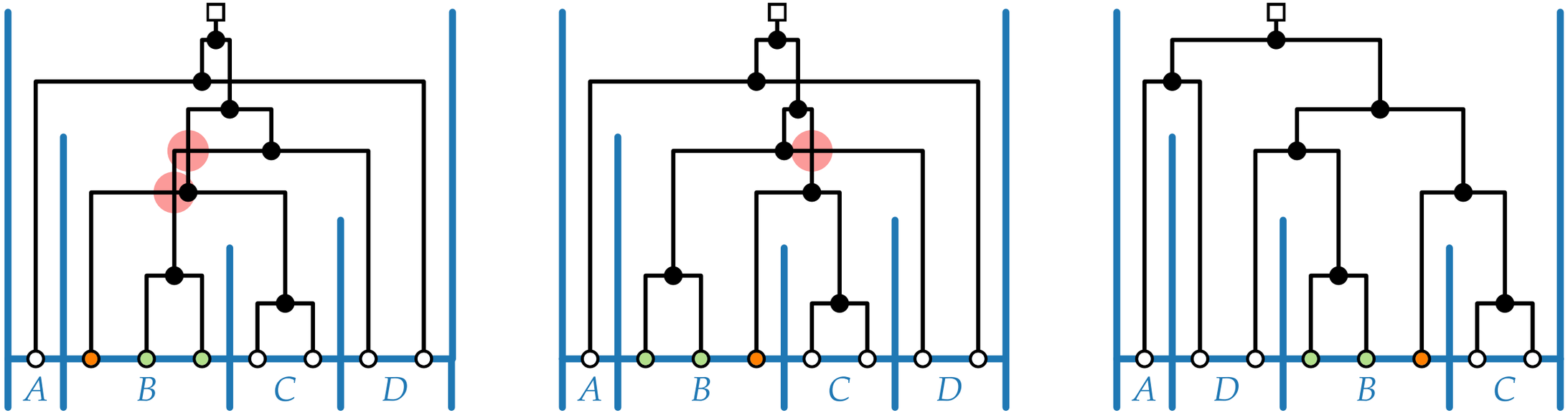

- **fixed** species order
- **variable** species order

Related work

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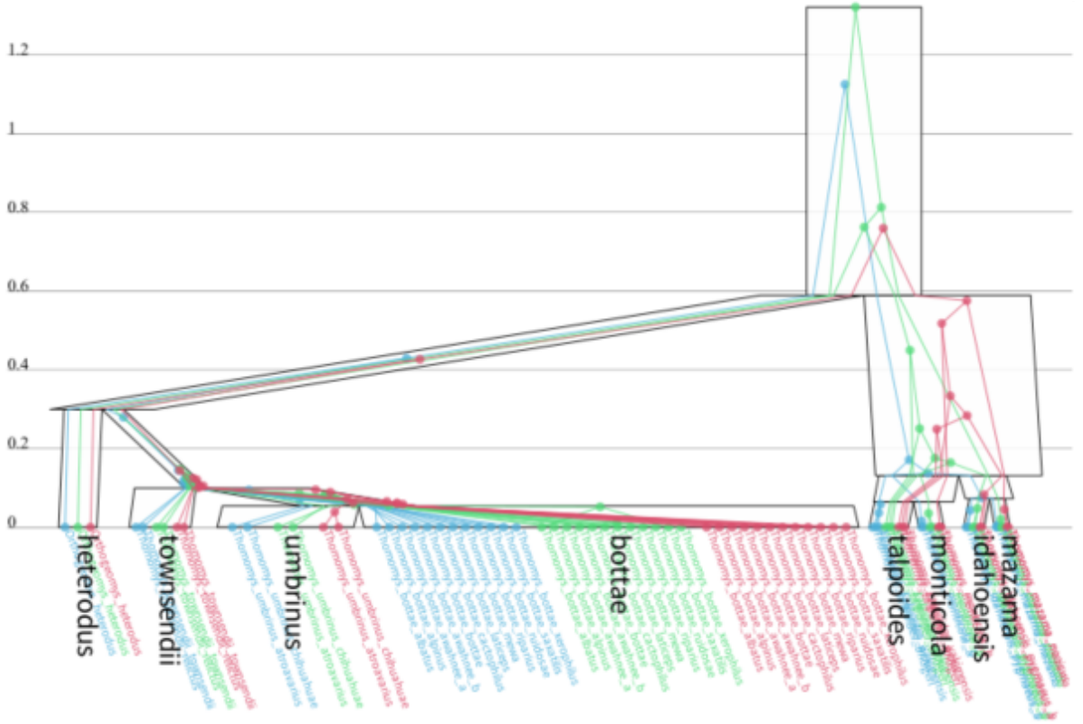

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  - Parasite vertex heights not given
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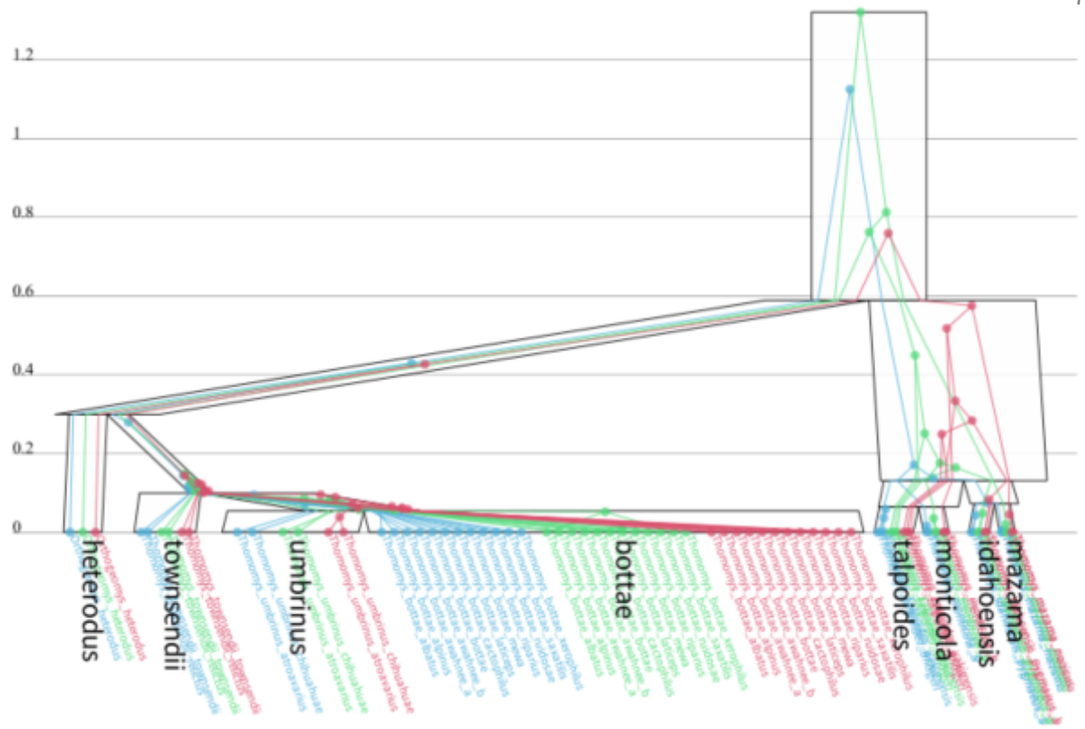

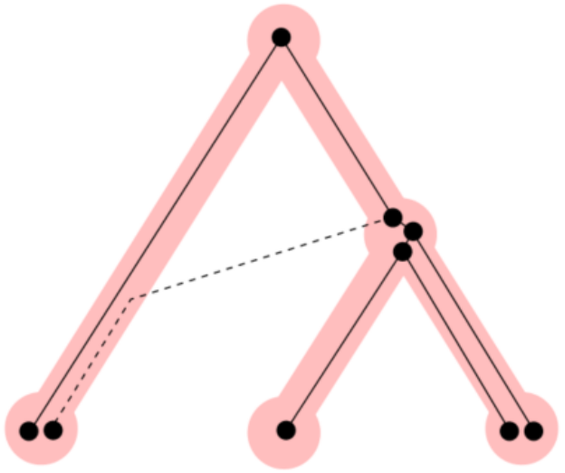

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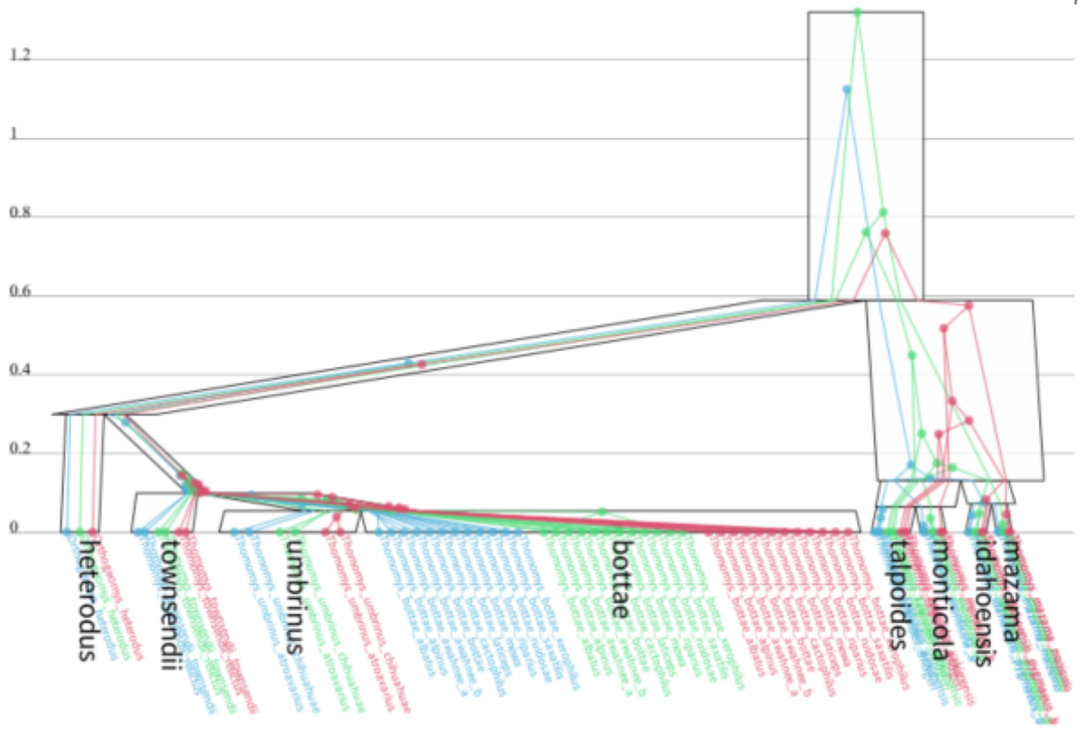

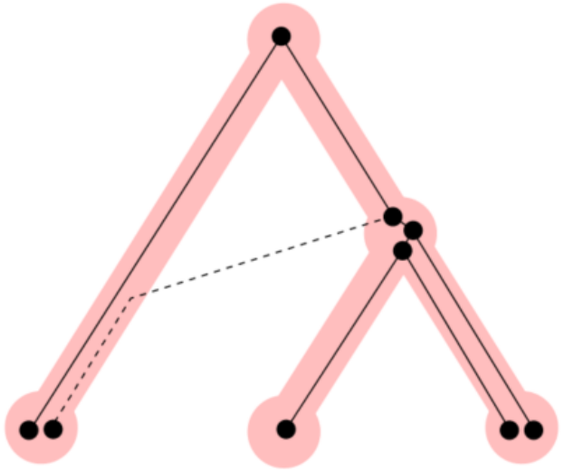

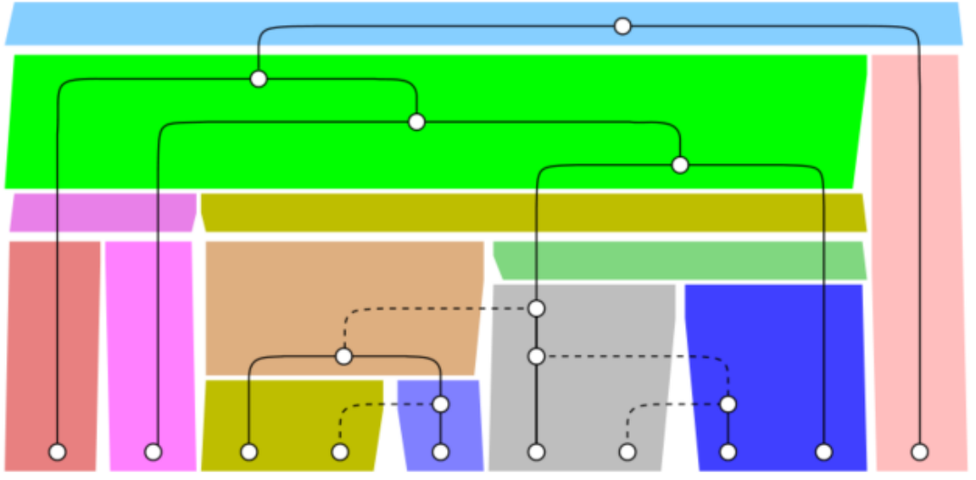

Our contribution

- We have defined drawing style for MSC trees.
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- Crossing minimisation is NP-hard (for fixed & variable species order).
- We present two simple heuristics and an integer linear program (ILP).
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variable species order

fixed species order

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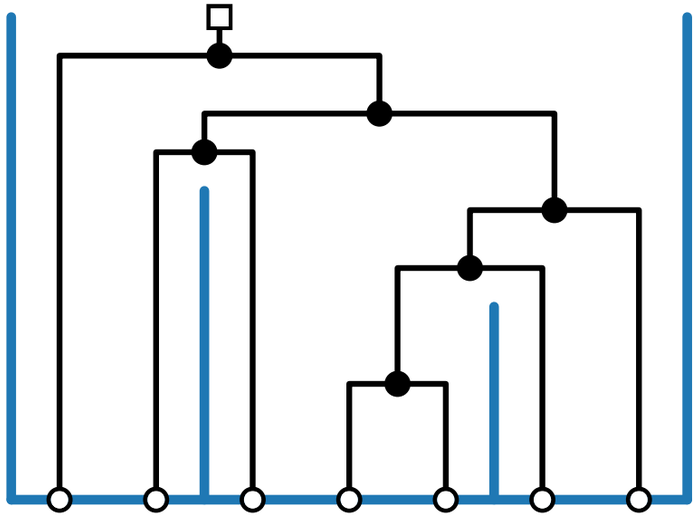

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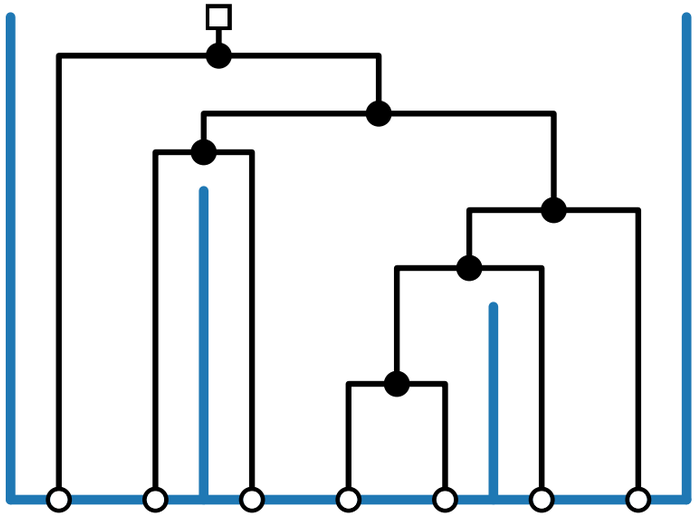

Planar instances

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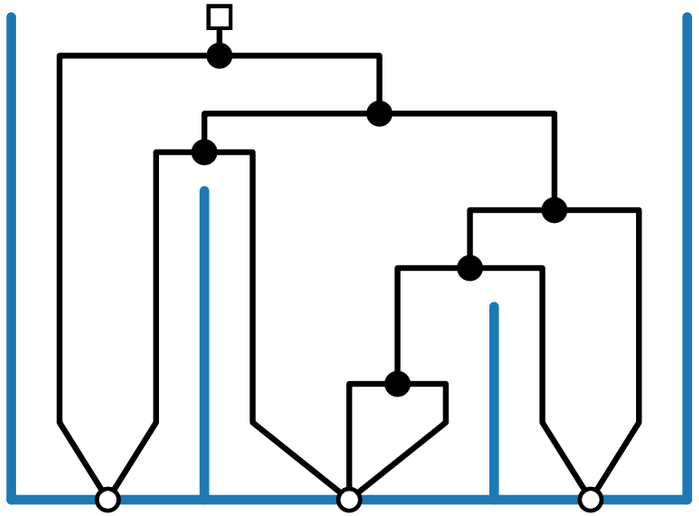

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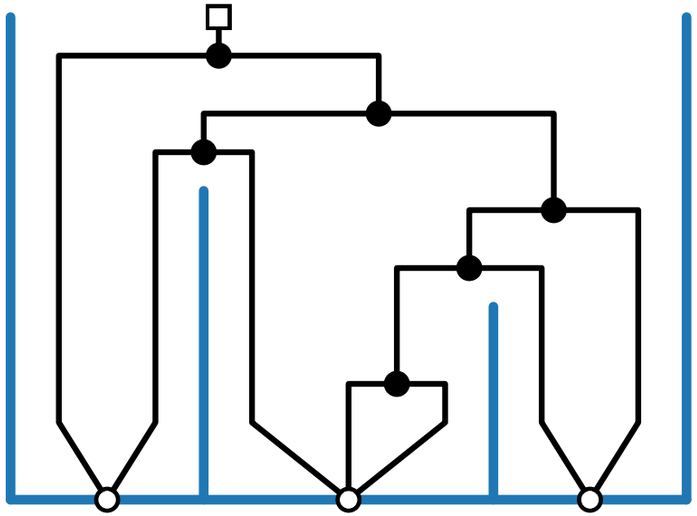

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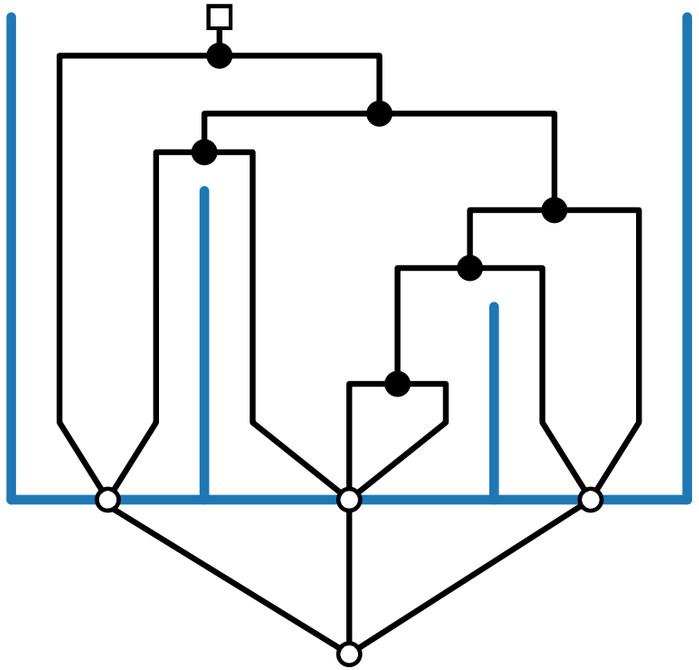

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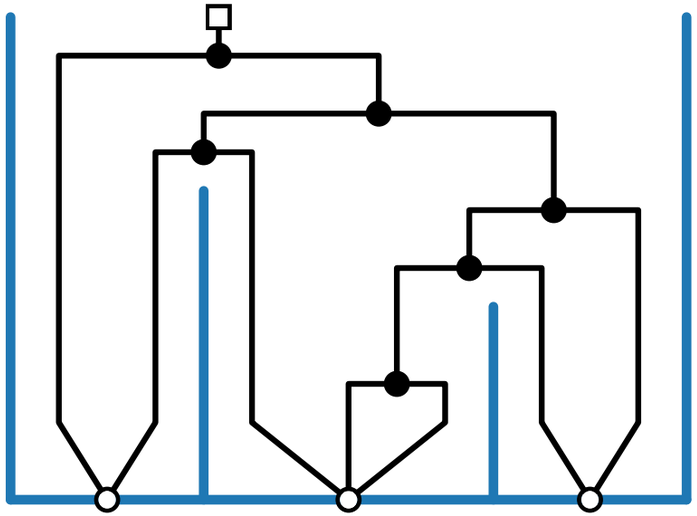

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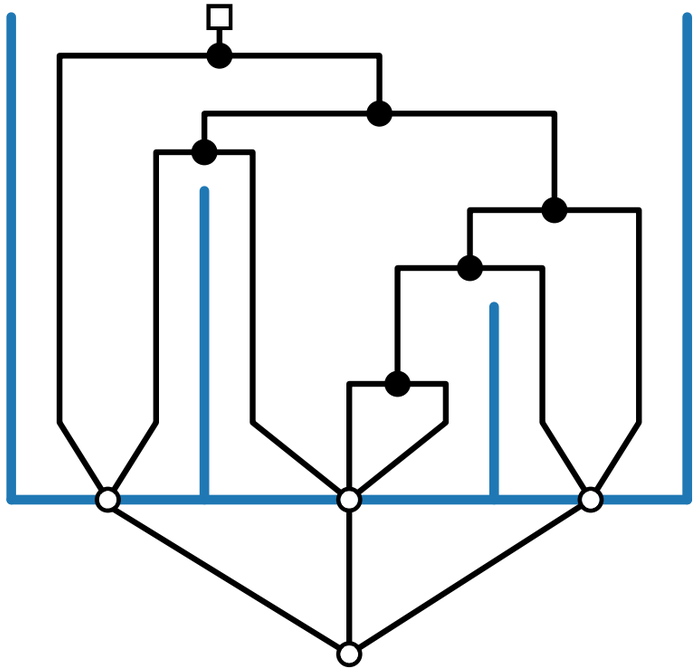

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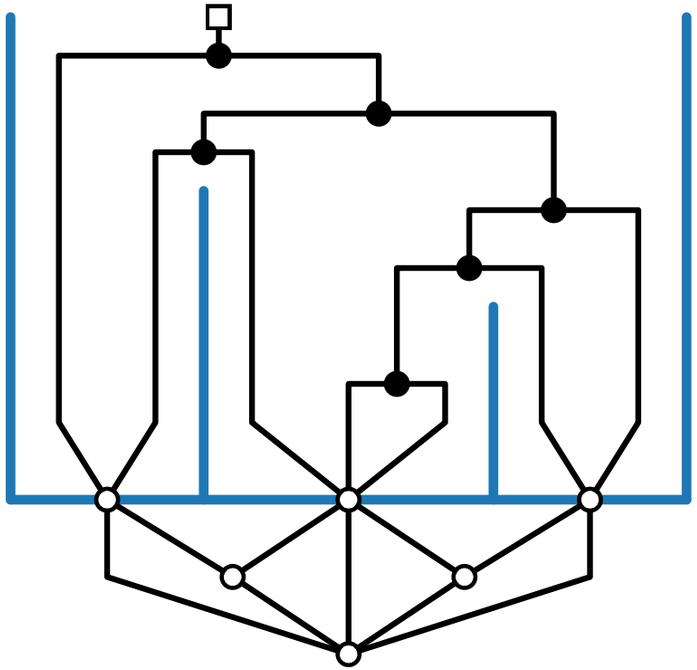

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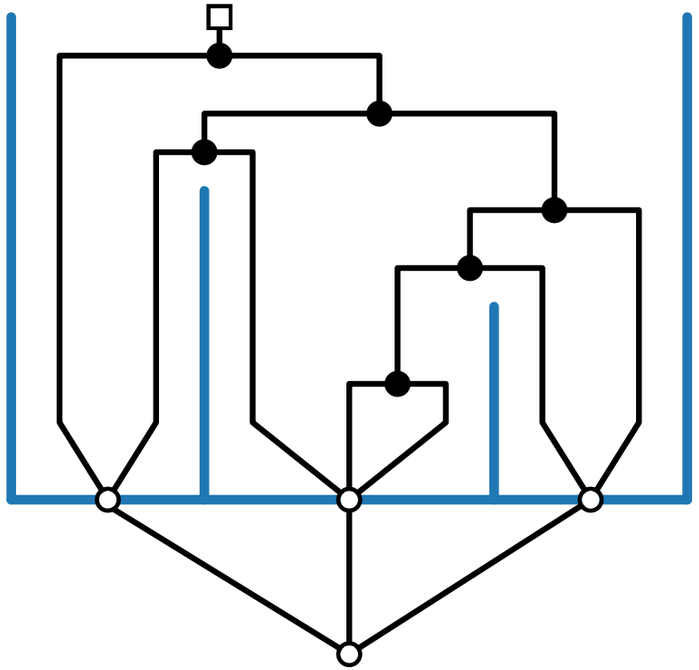

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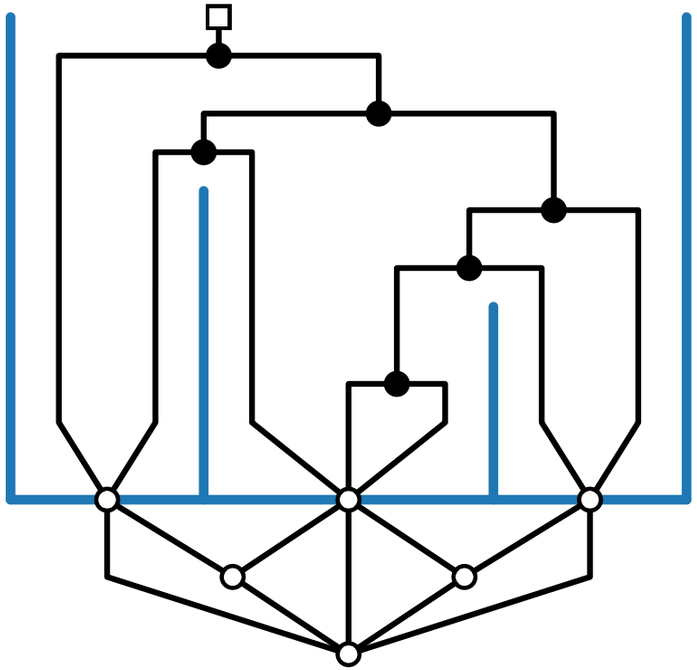
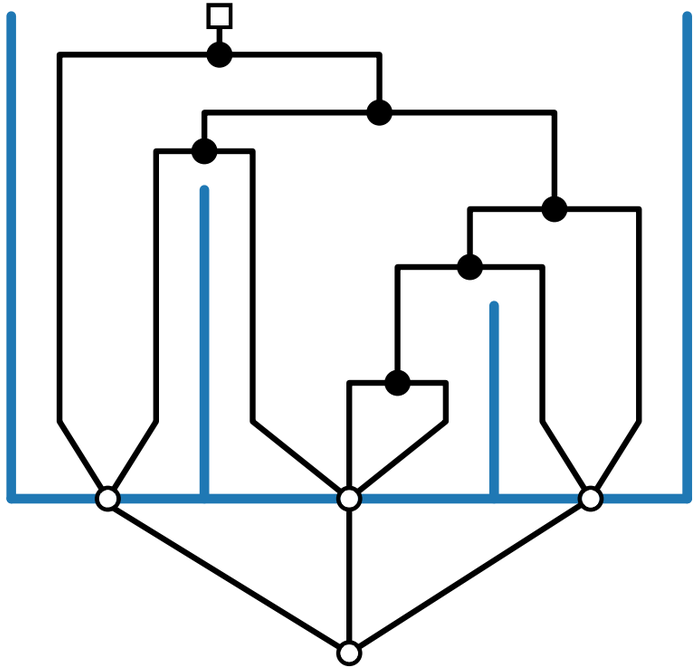


Upward planar!

Planar instances

variable species order



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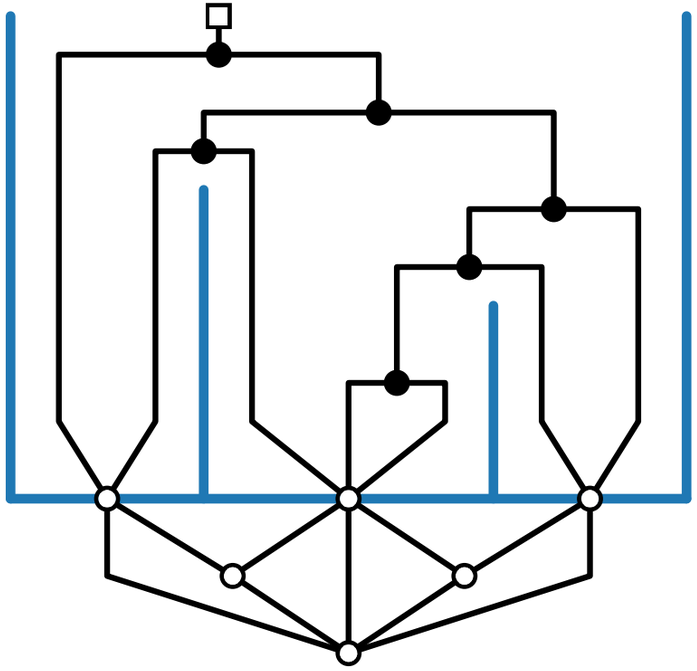

Upward planar! → Testing upward planarity of single-source digraphs can be done in linear time.

[Bertolazzi, Di Battista, Mannino, Tamassia: SIAM J. Comput. '98]

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Theorem.
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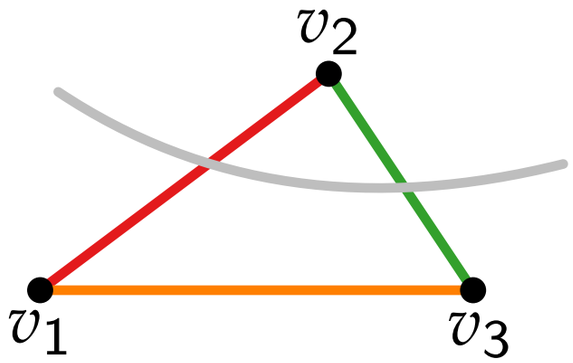
NP-Hardness with variable species order

Reduction from MAX-CUT



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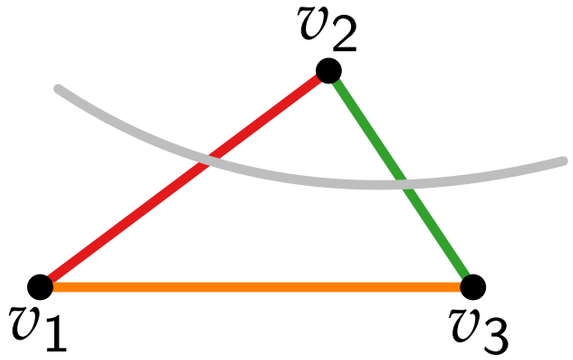

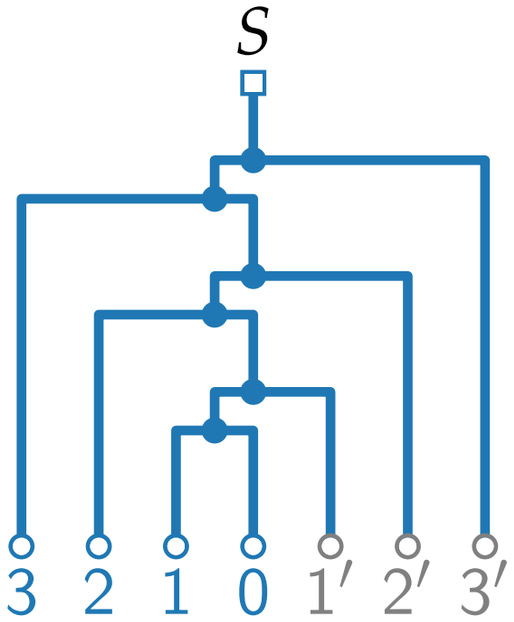

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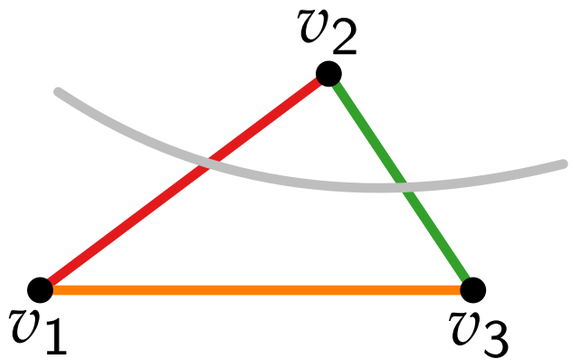

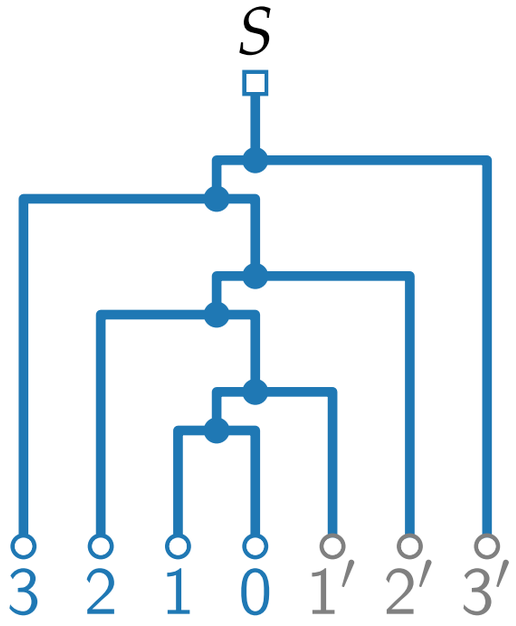

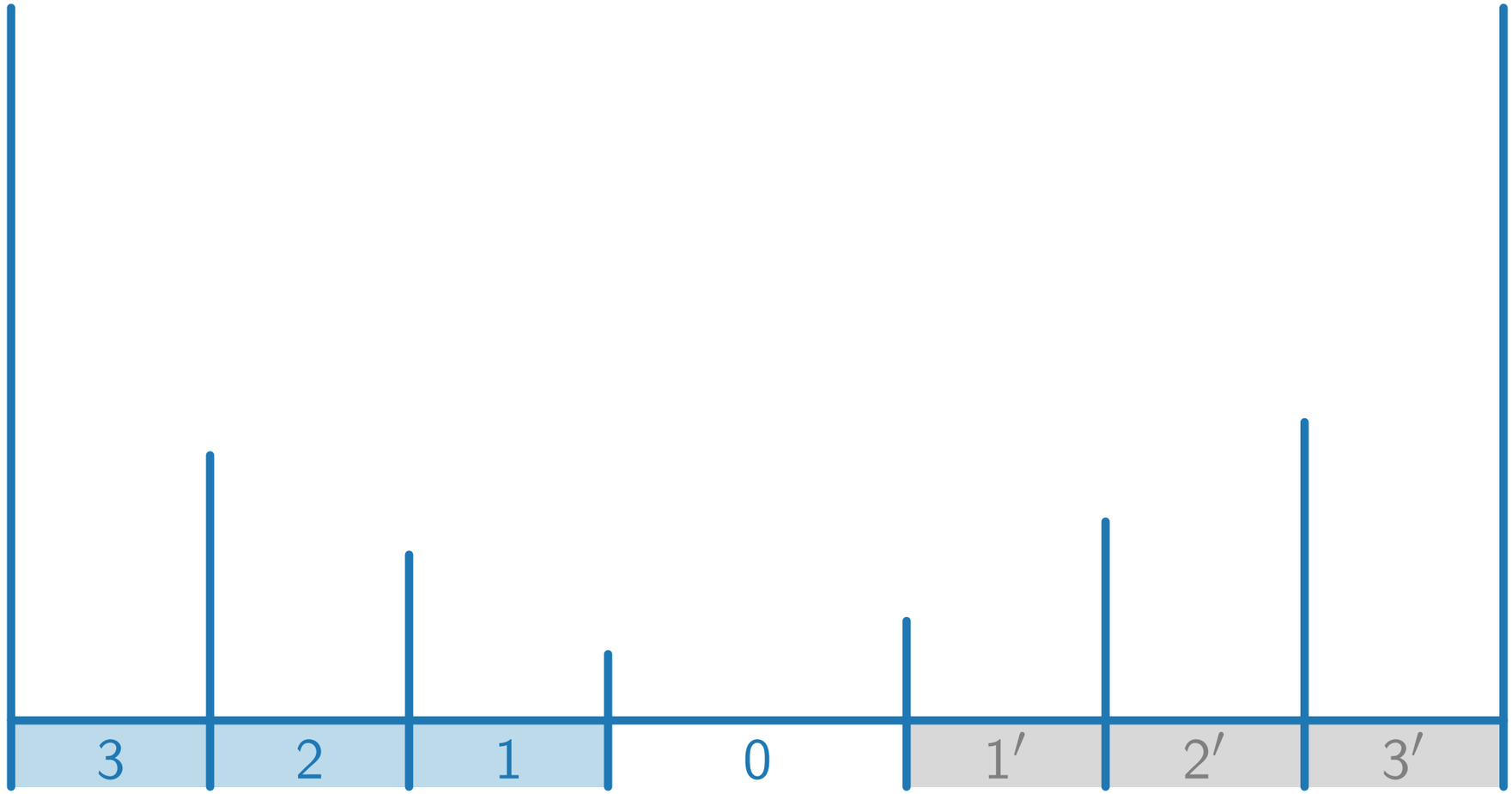

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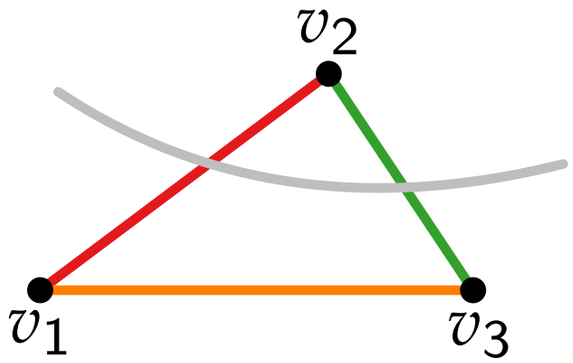

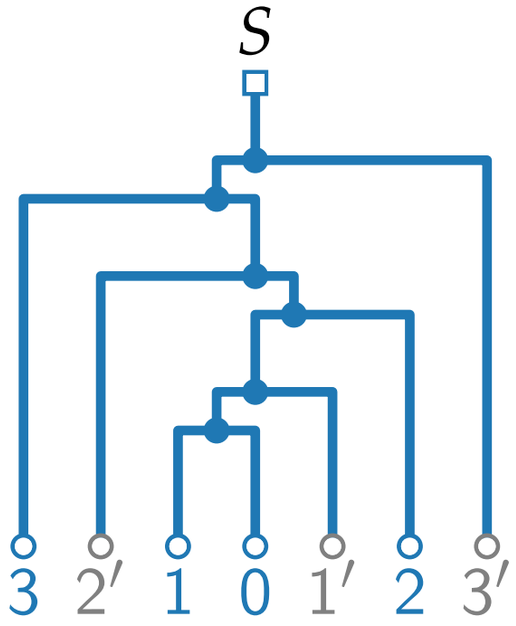

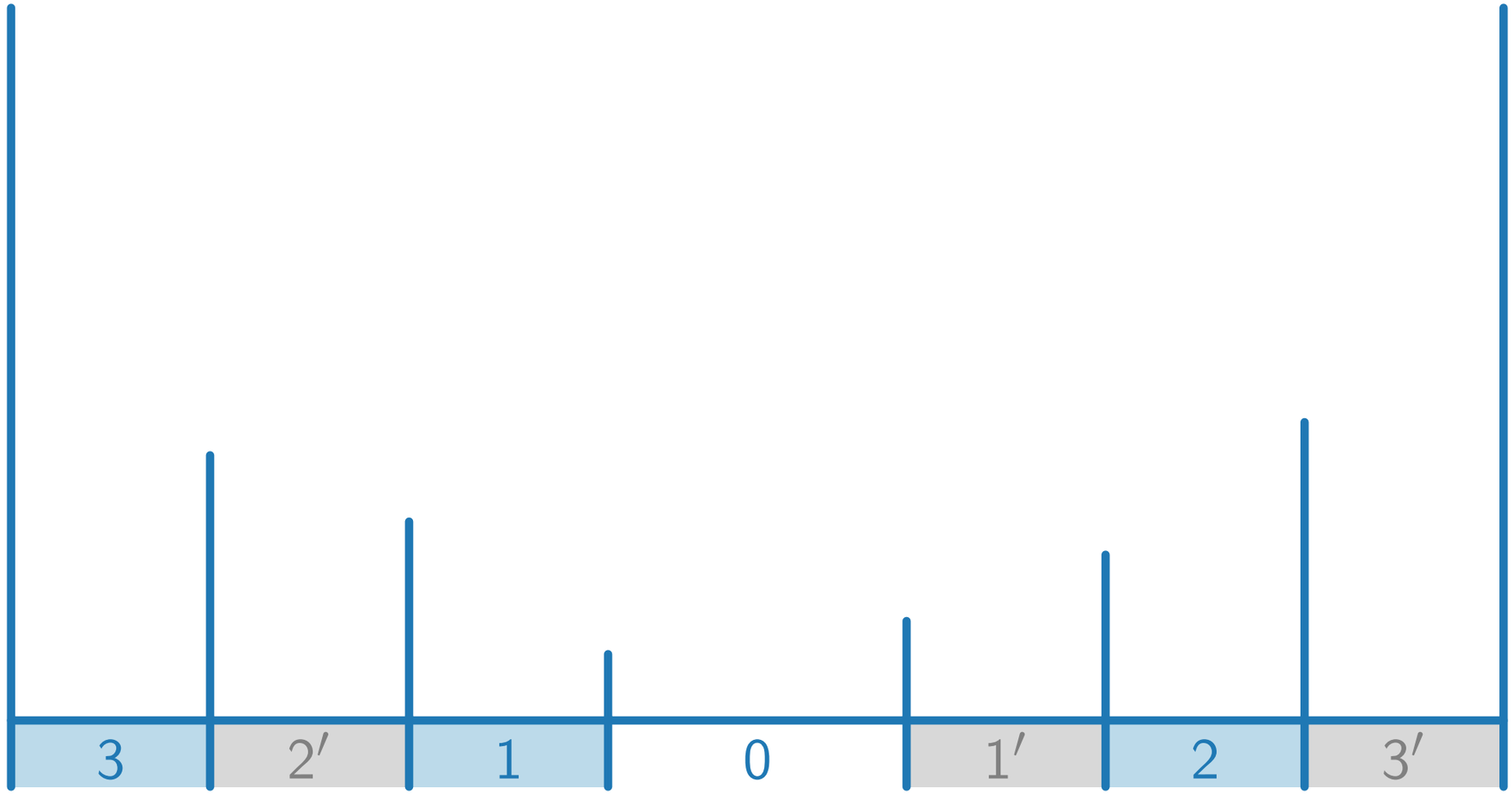

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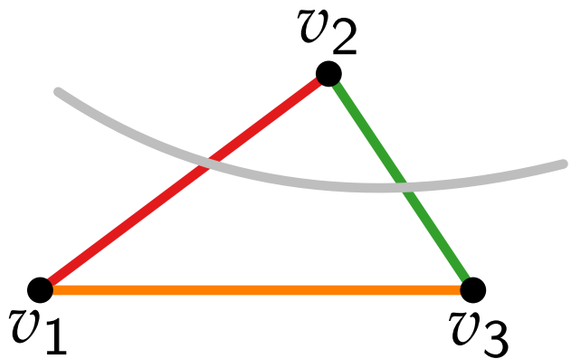

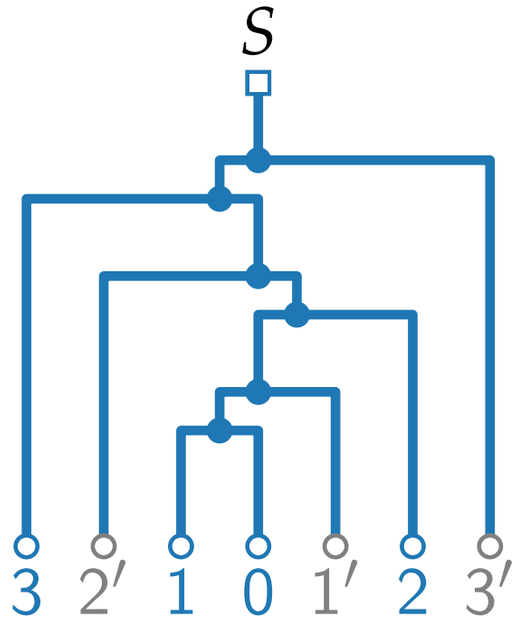

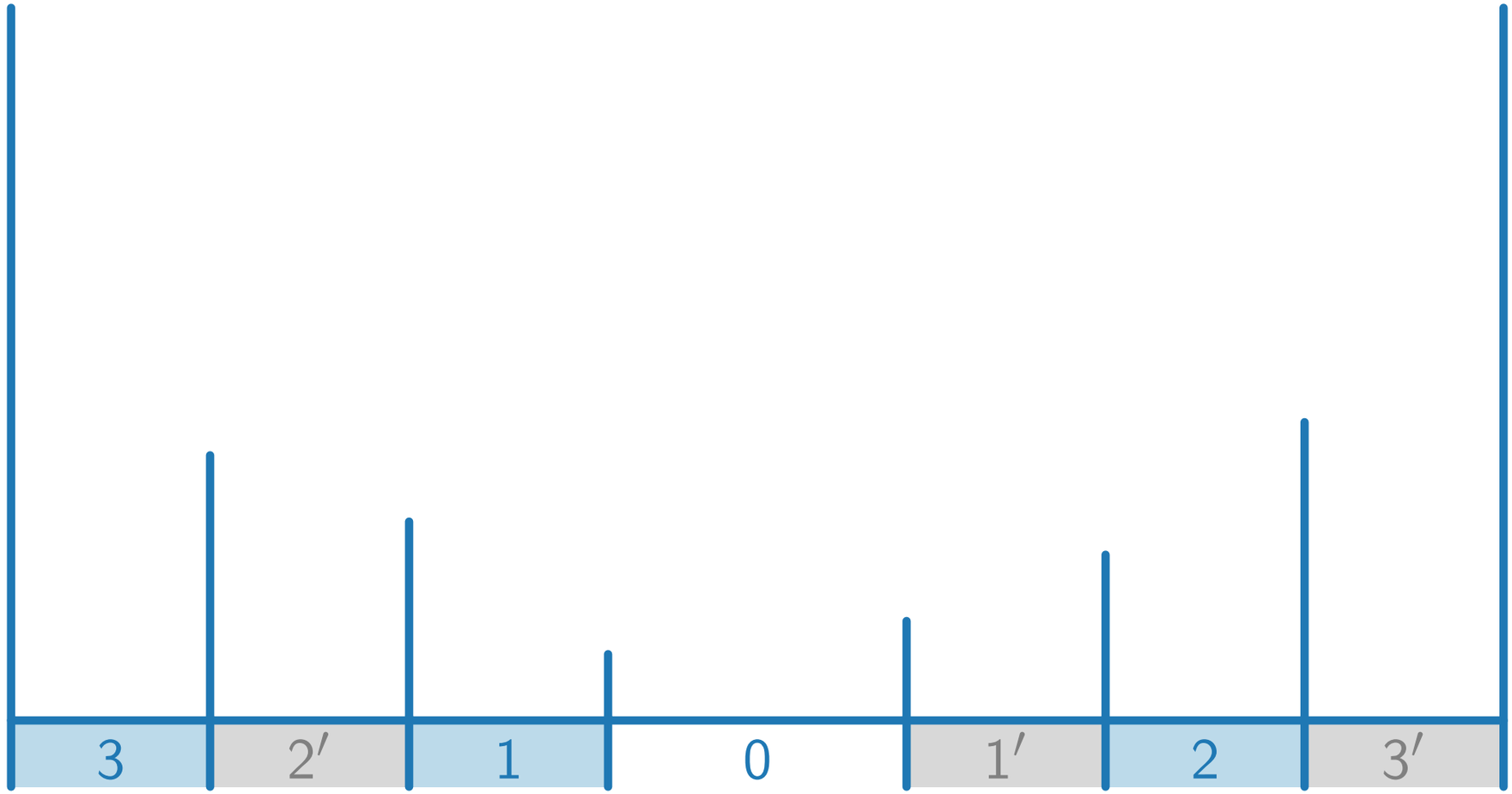

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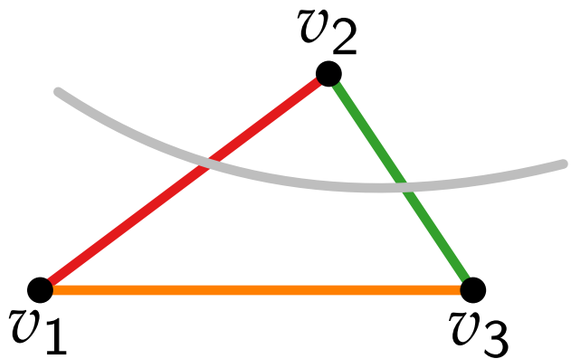

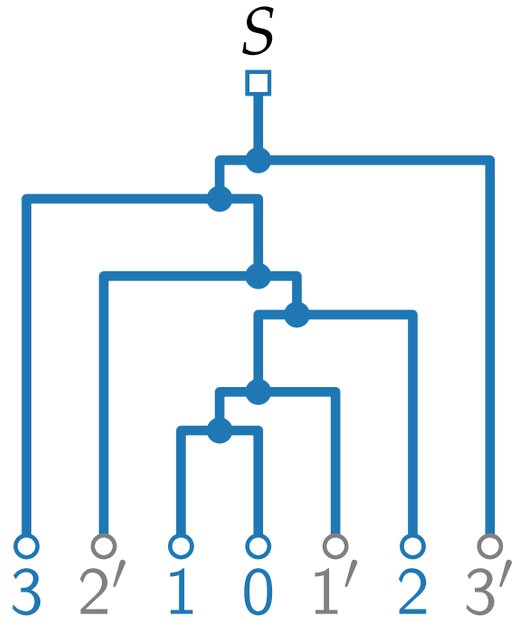

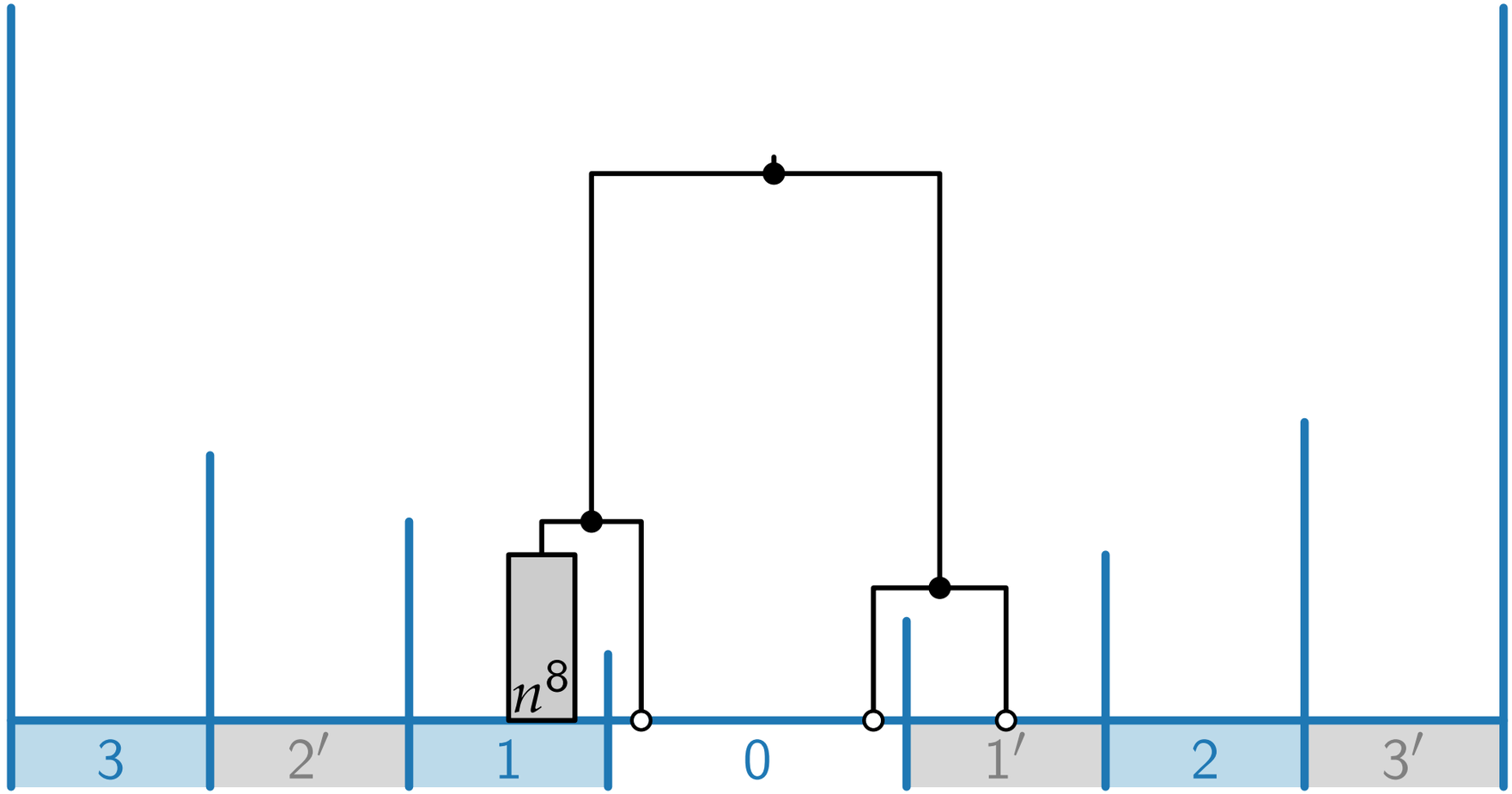

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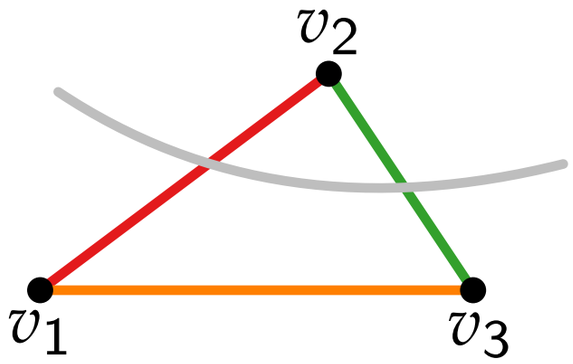

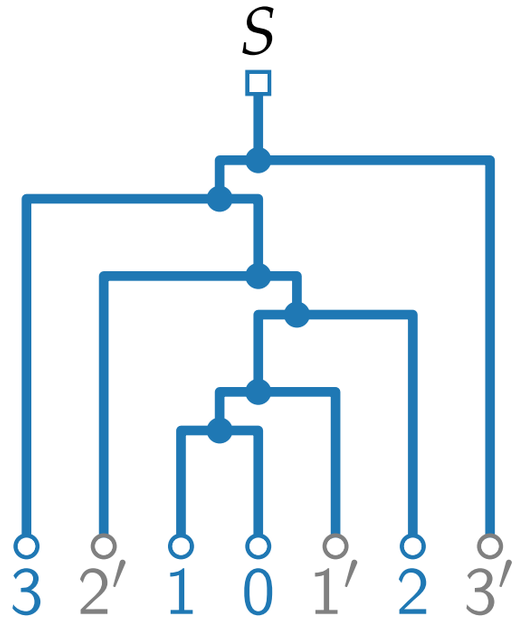

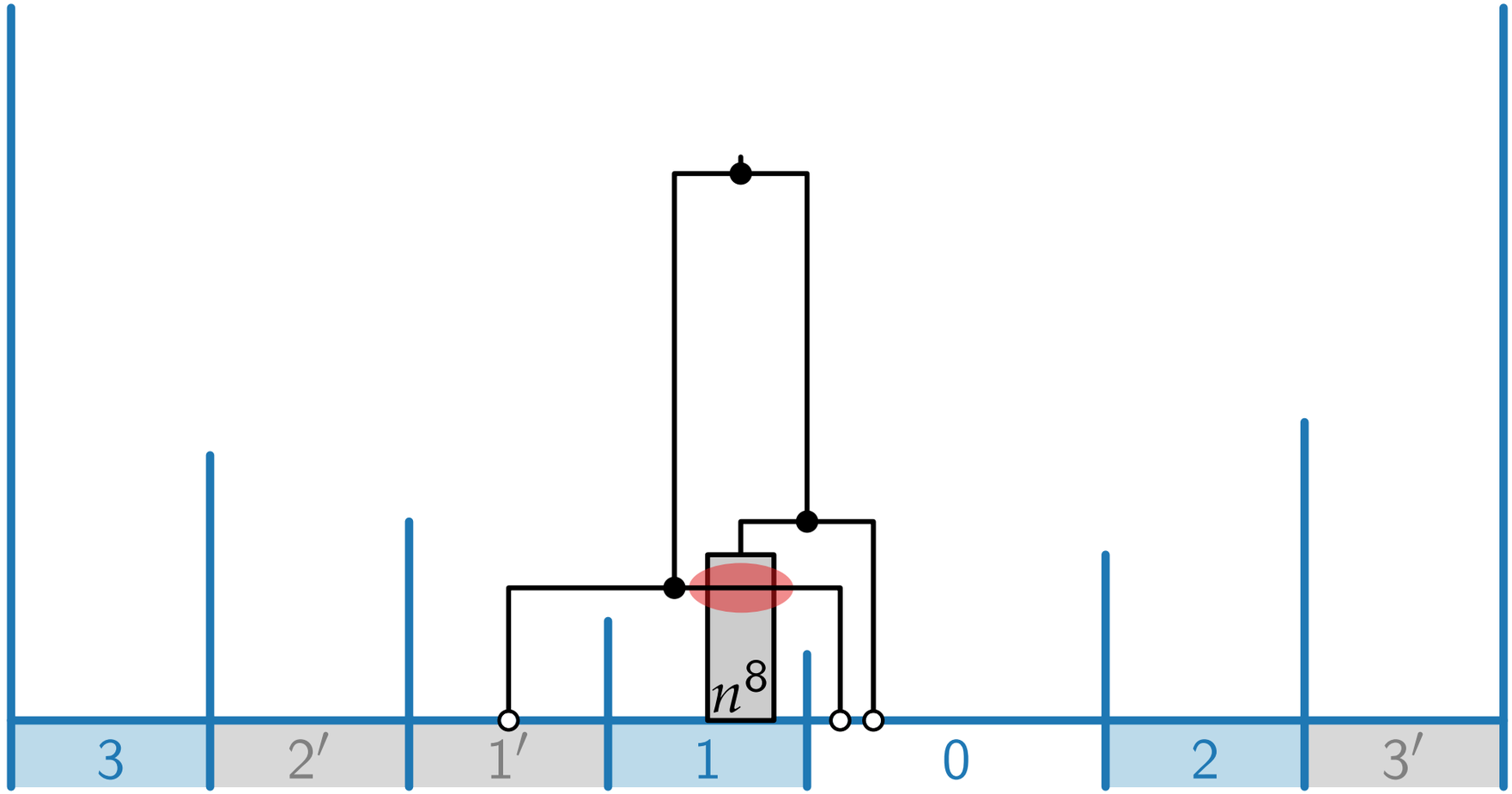

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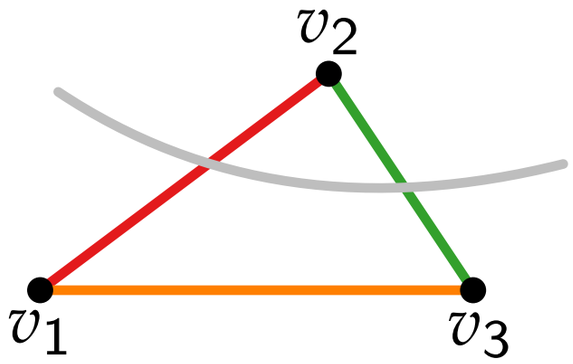

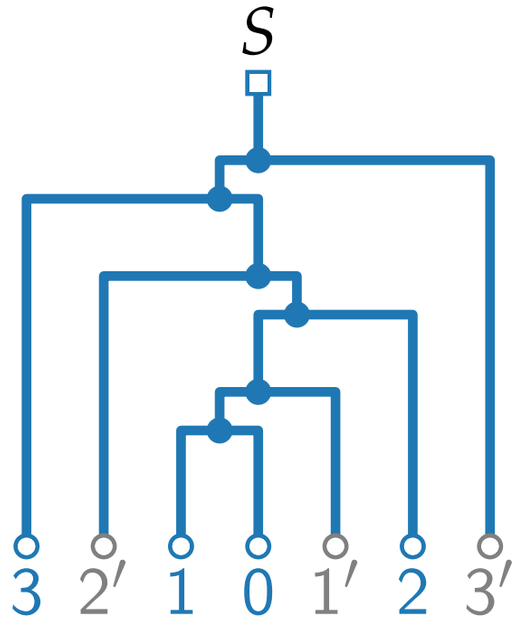

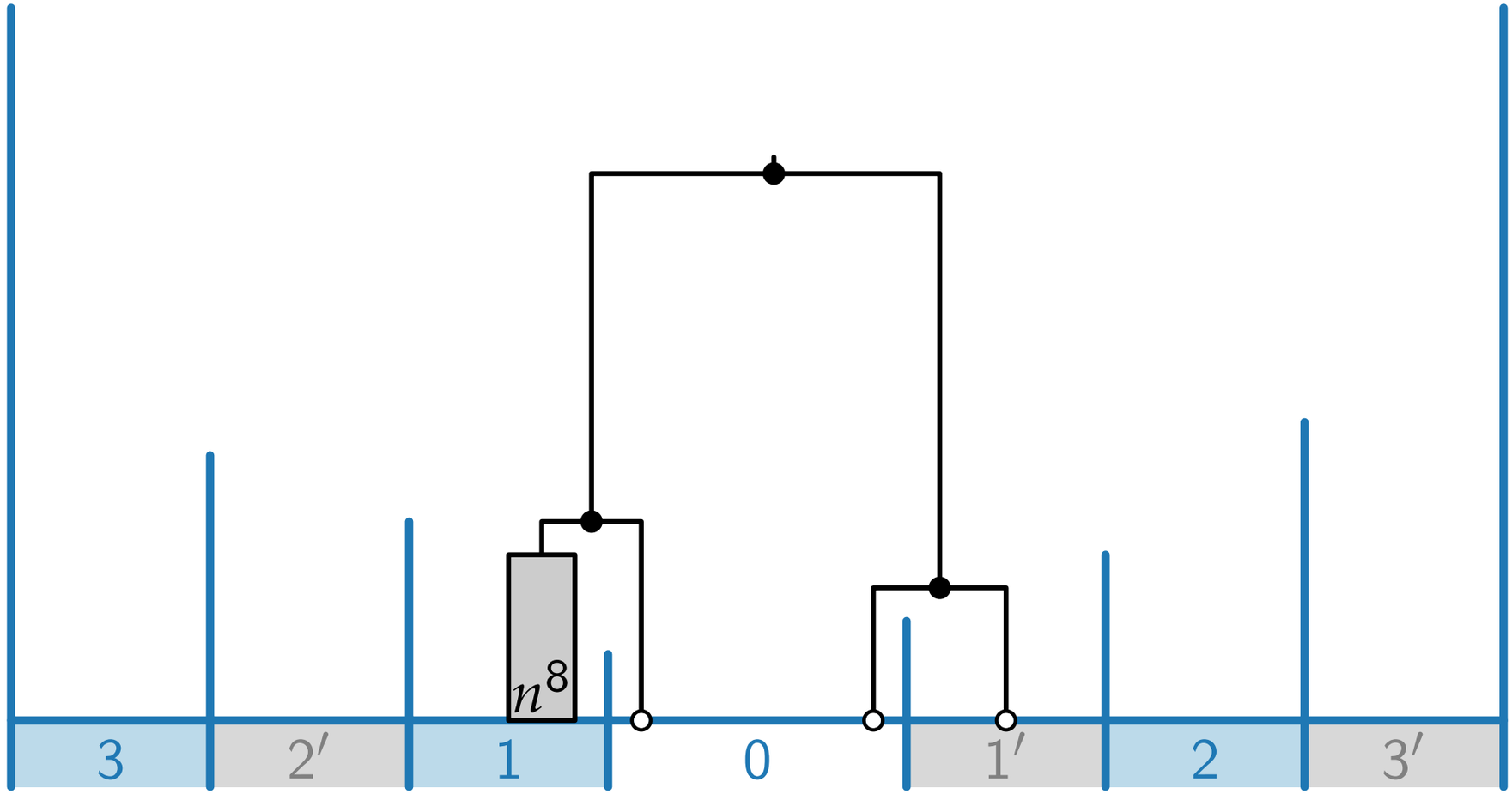

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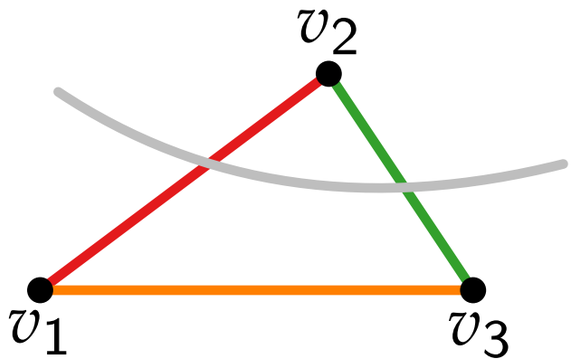

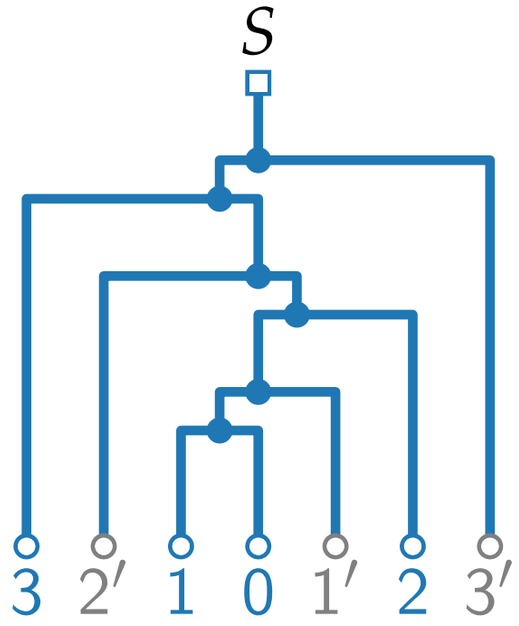

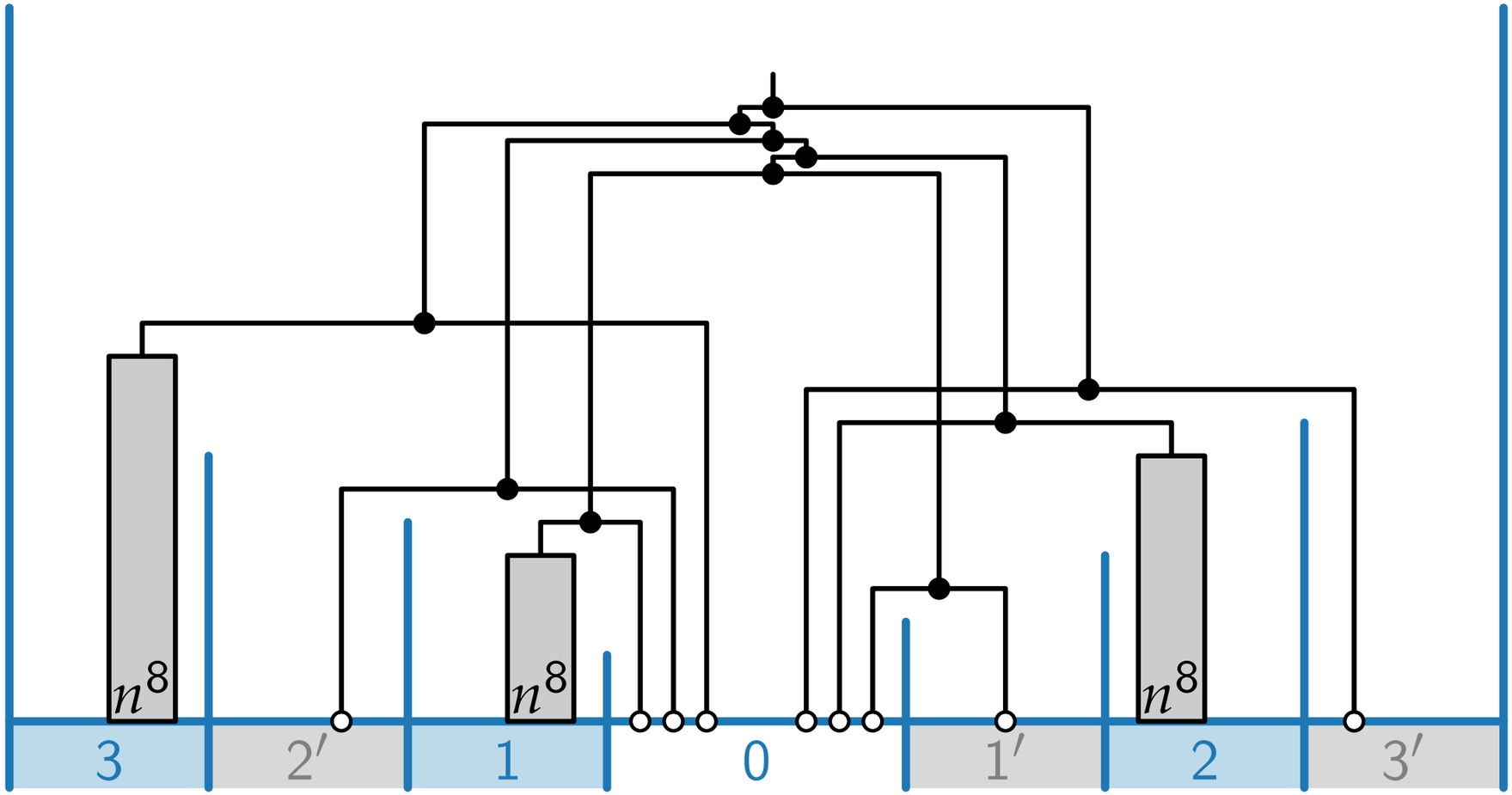

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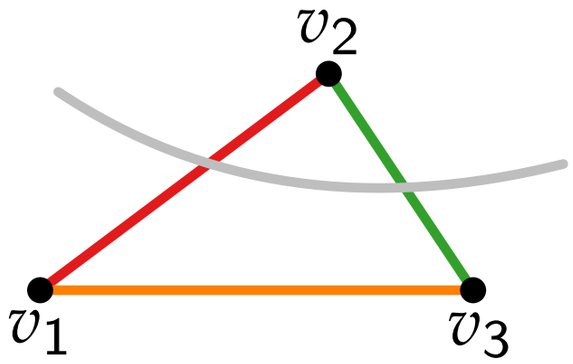

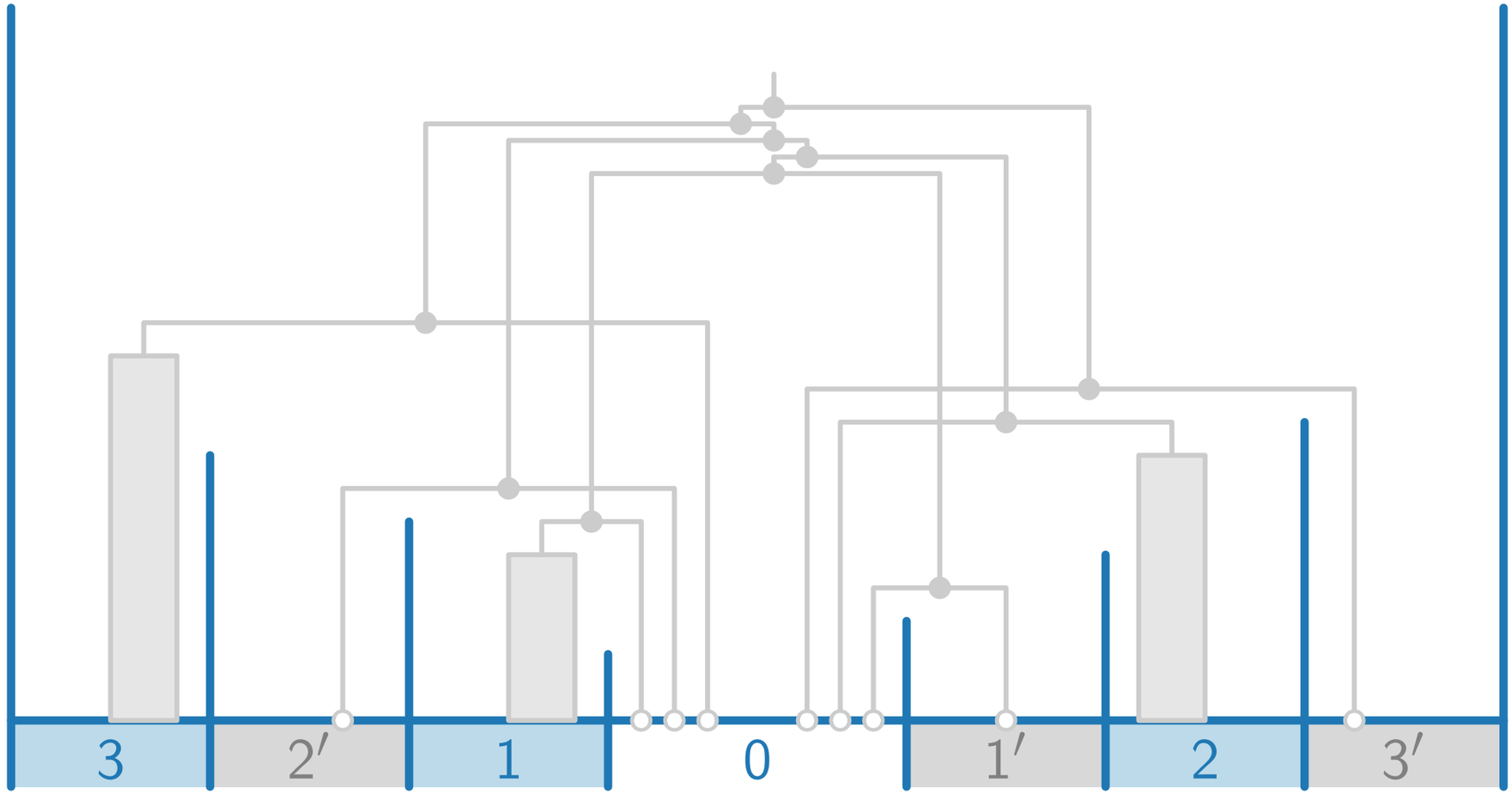

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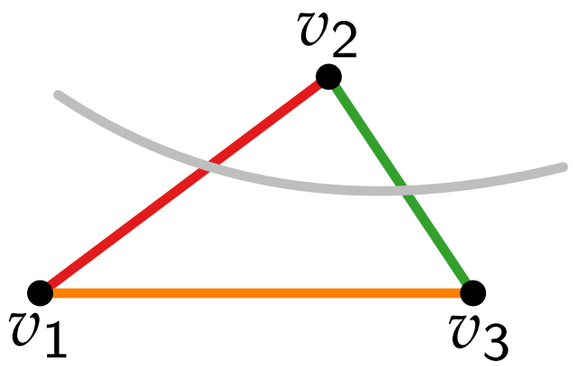

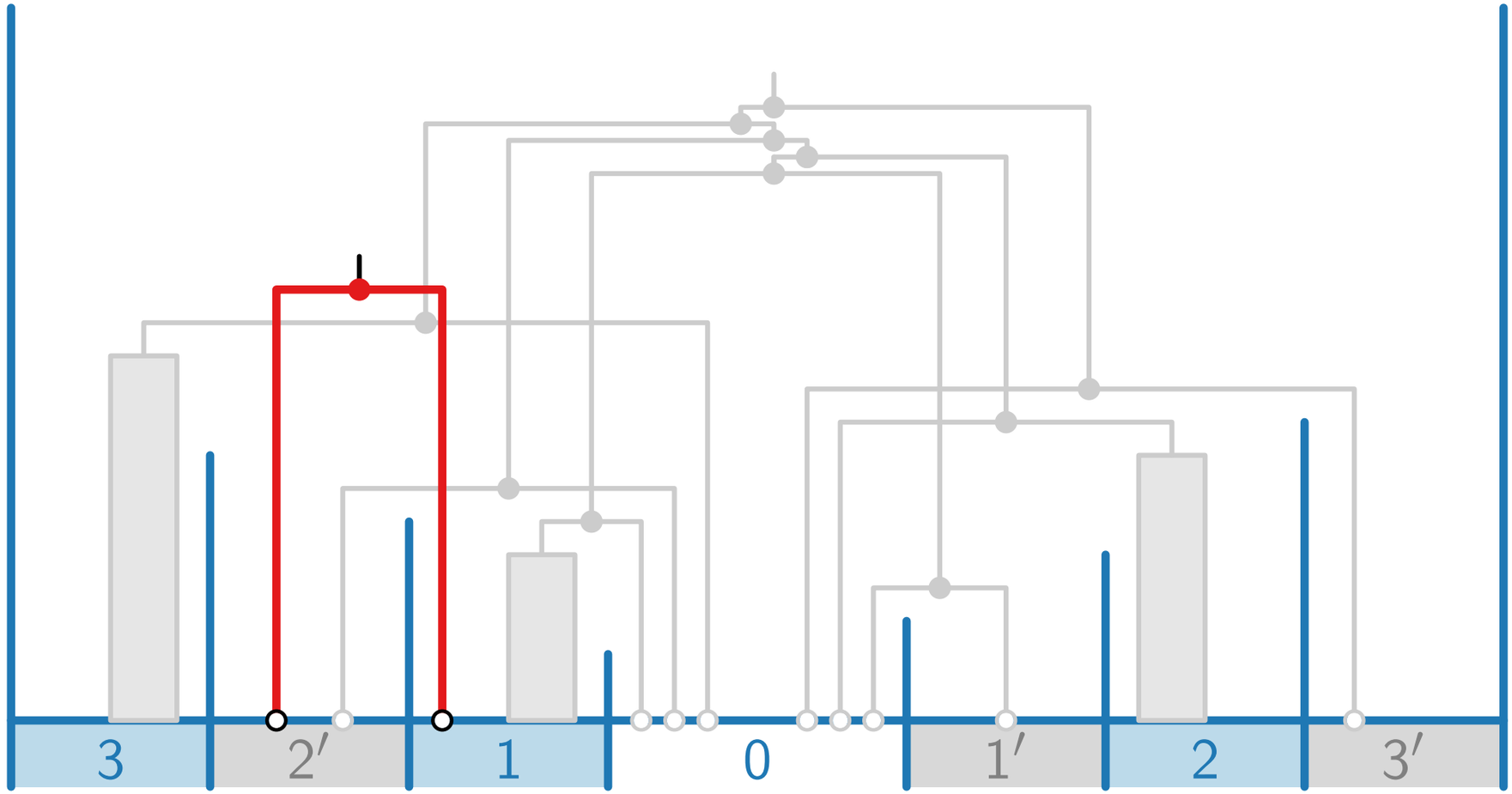

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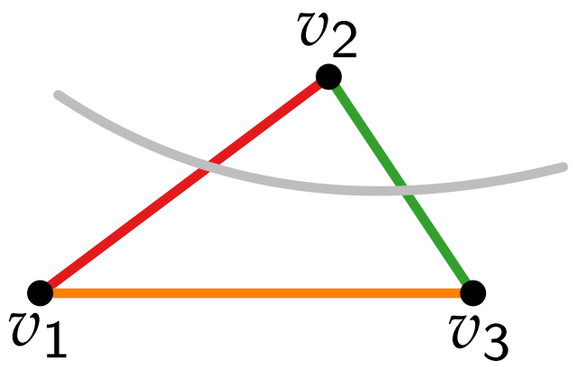

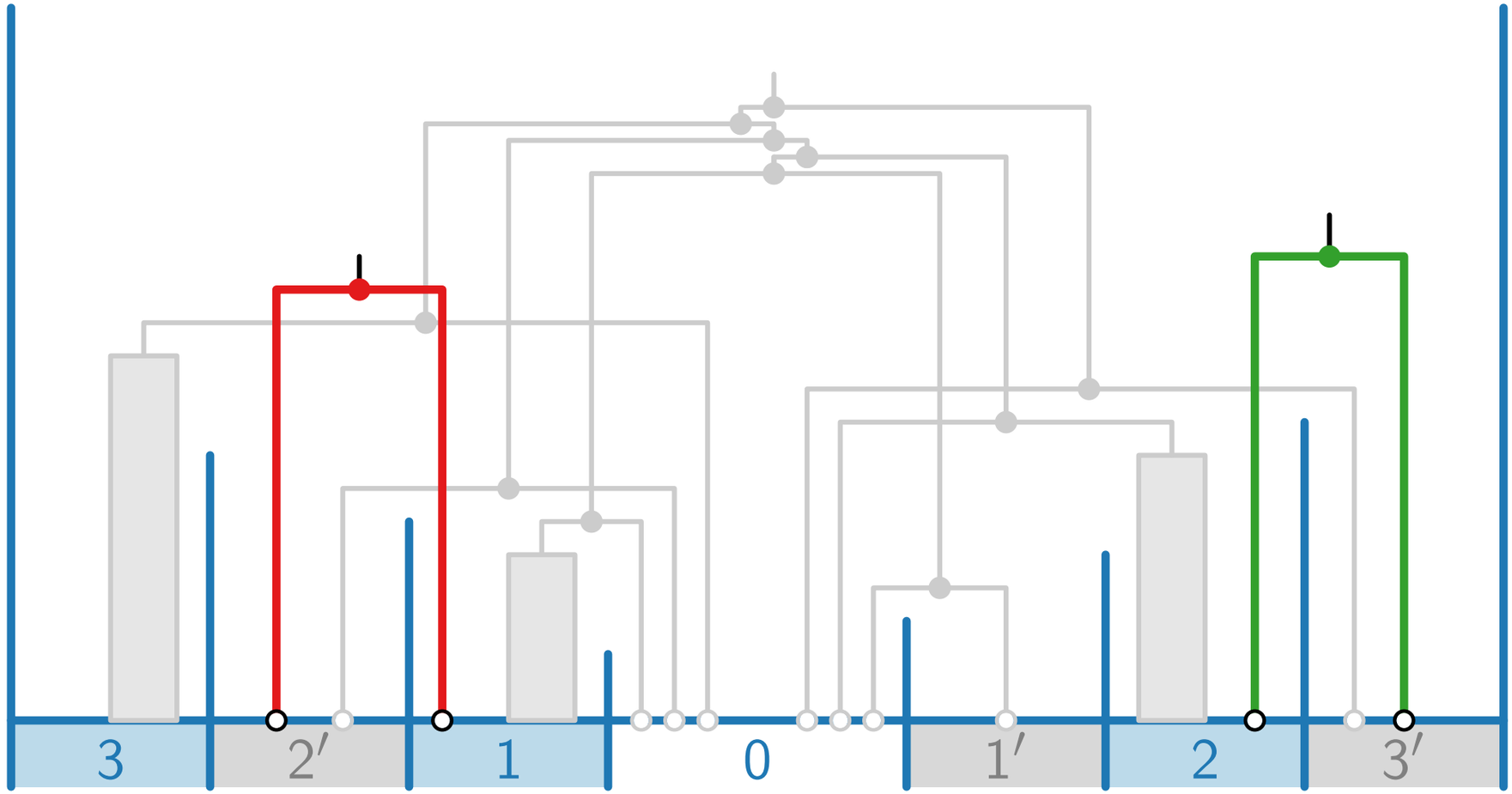

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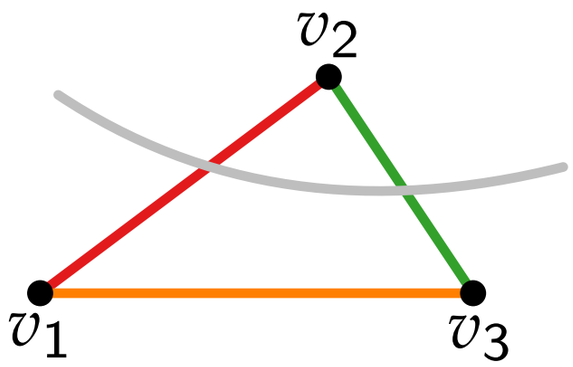

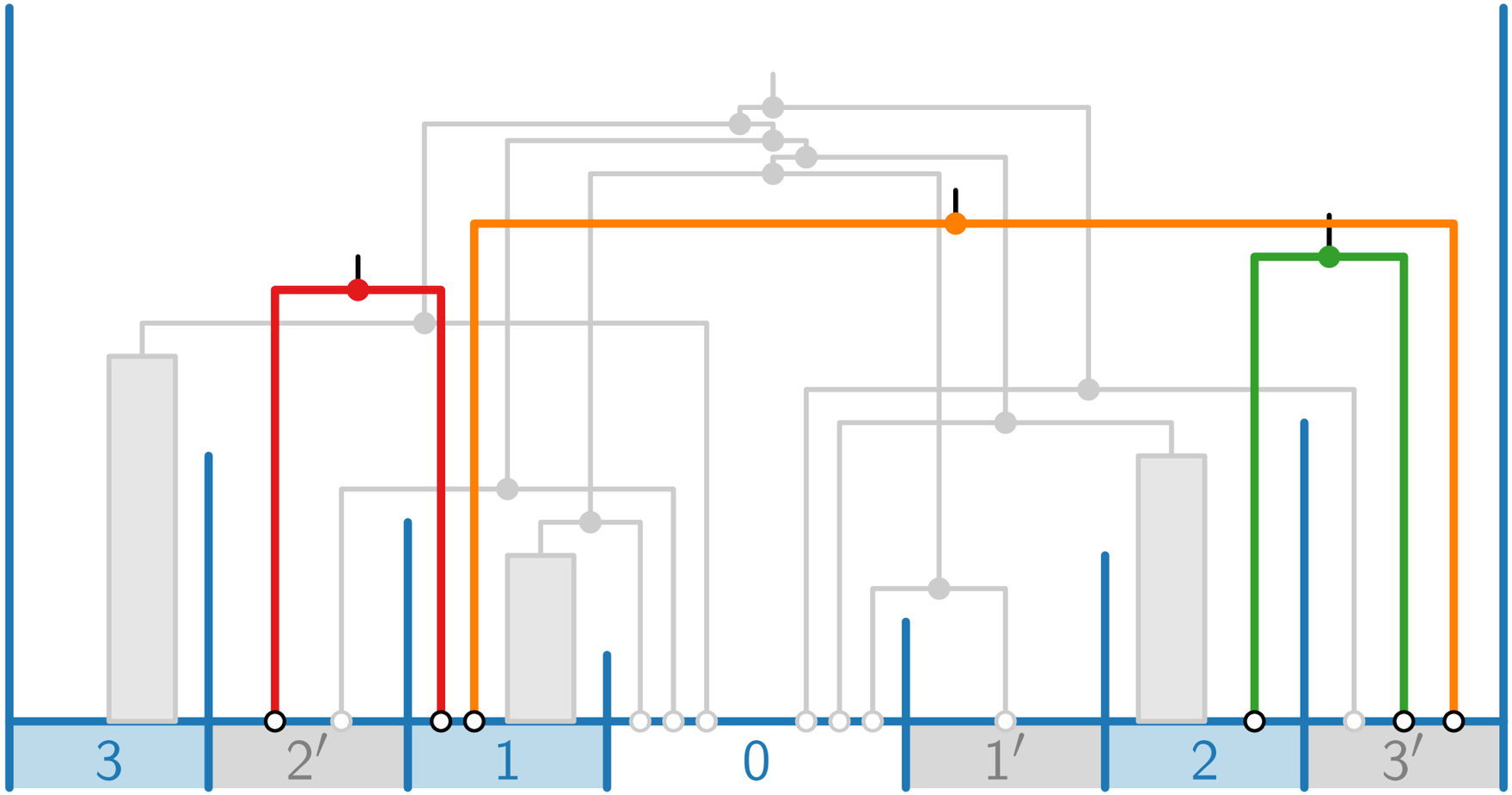

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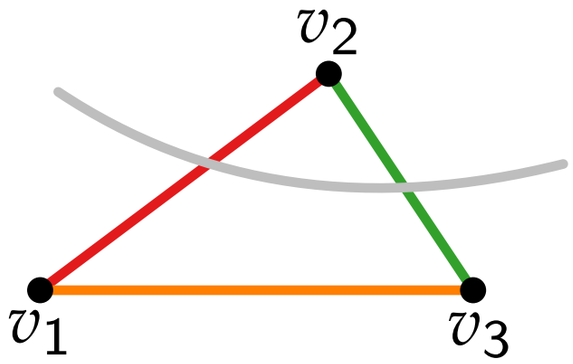

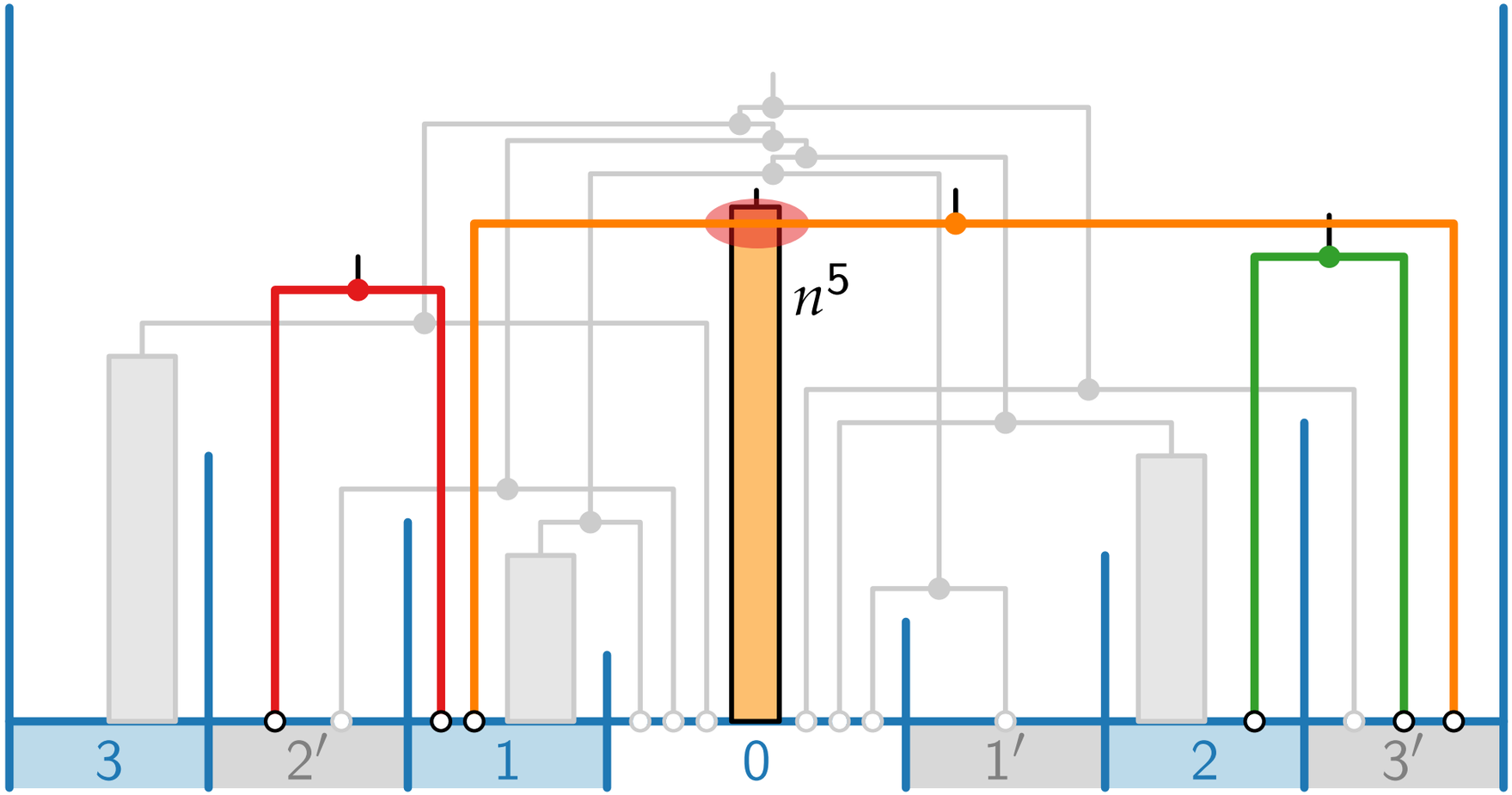

NP-Hardness with variable species order

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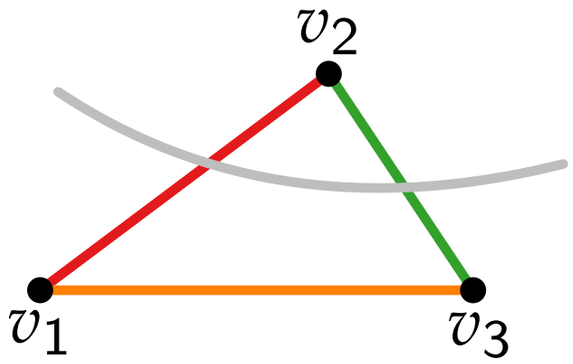

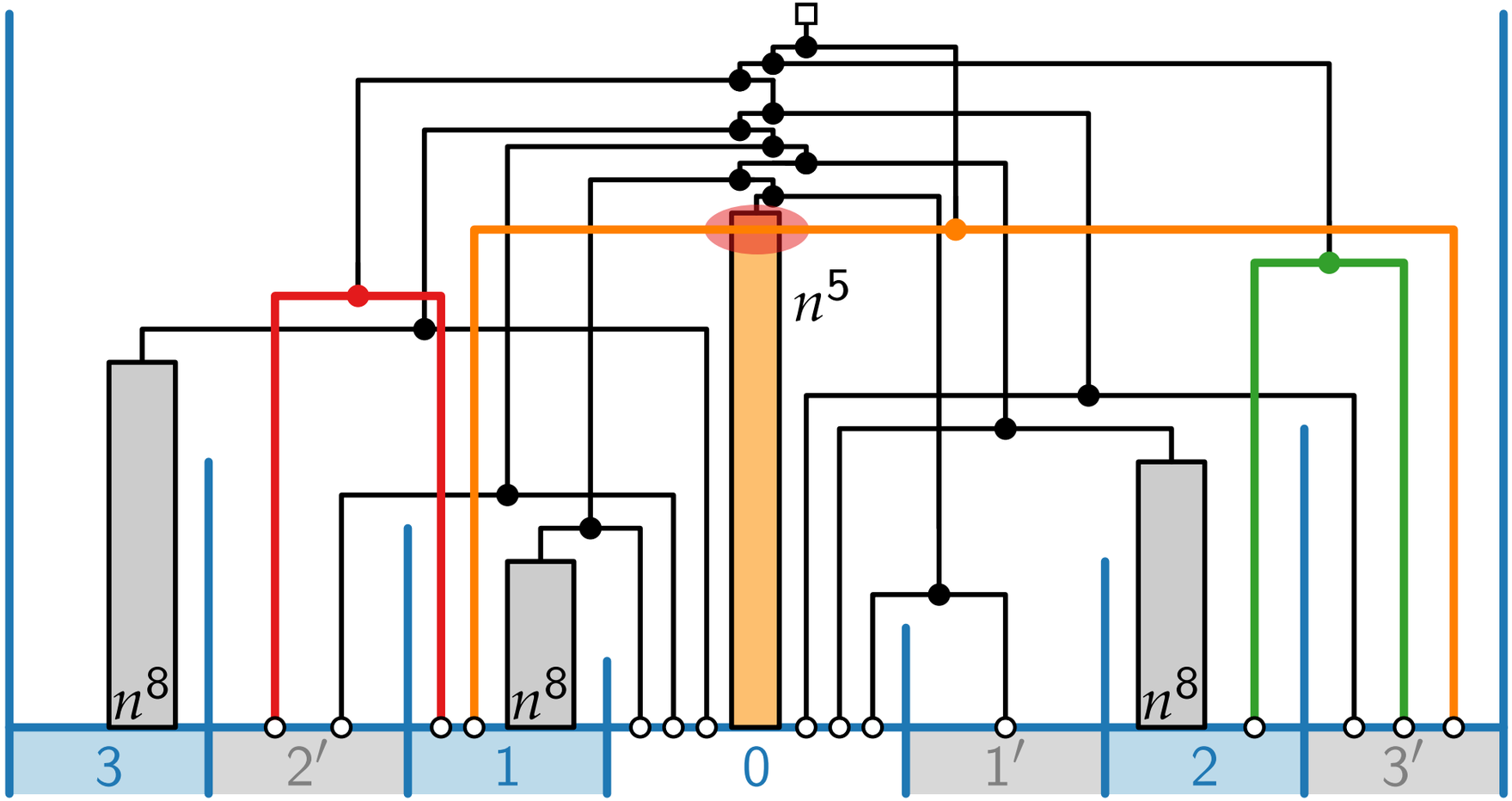

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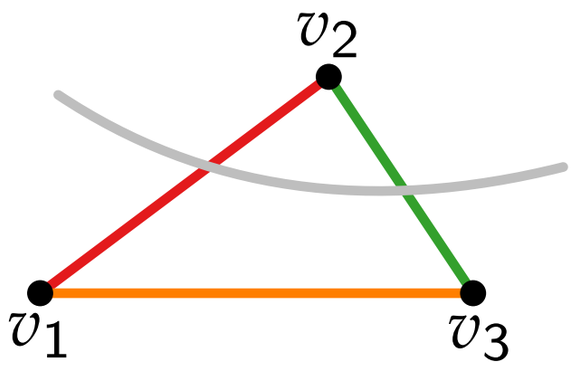

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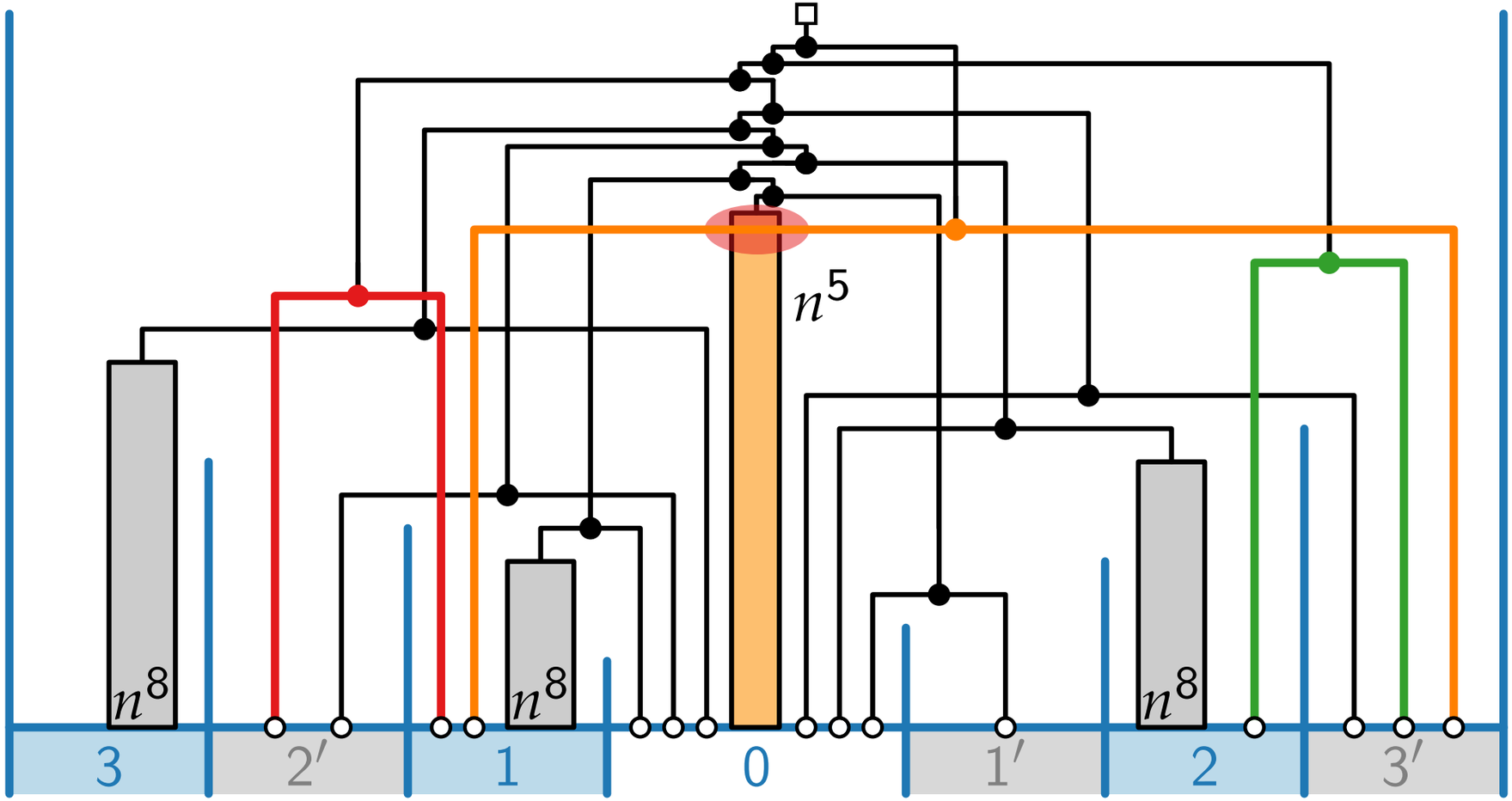

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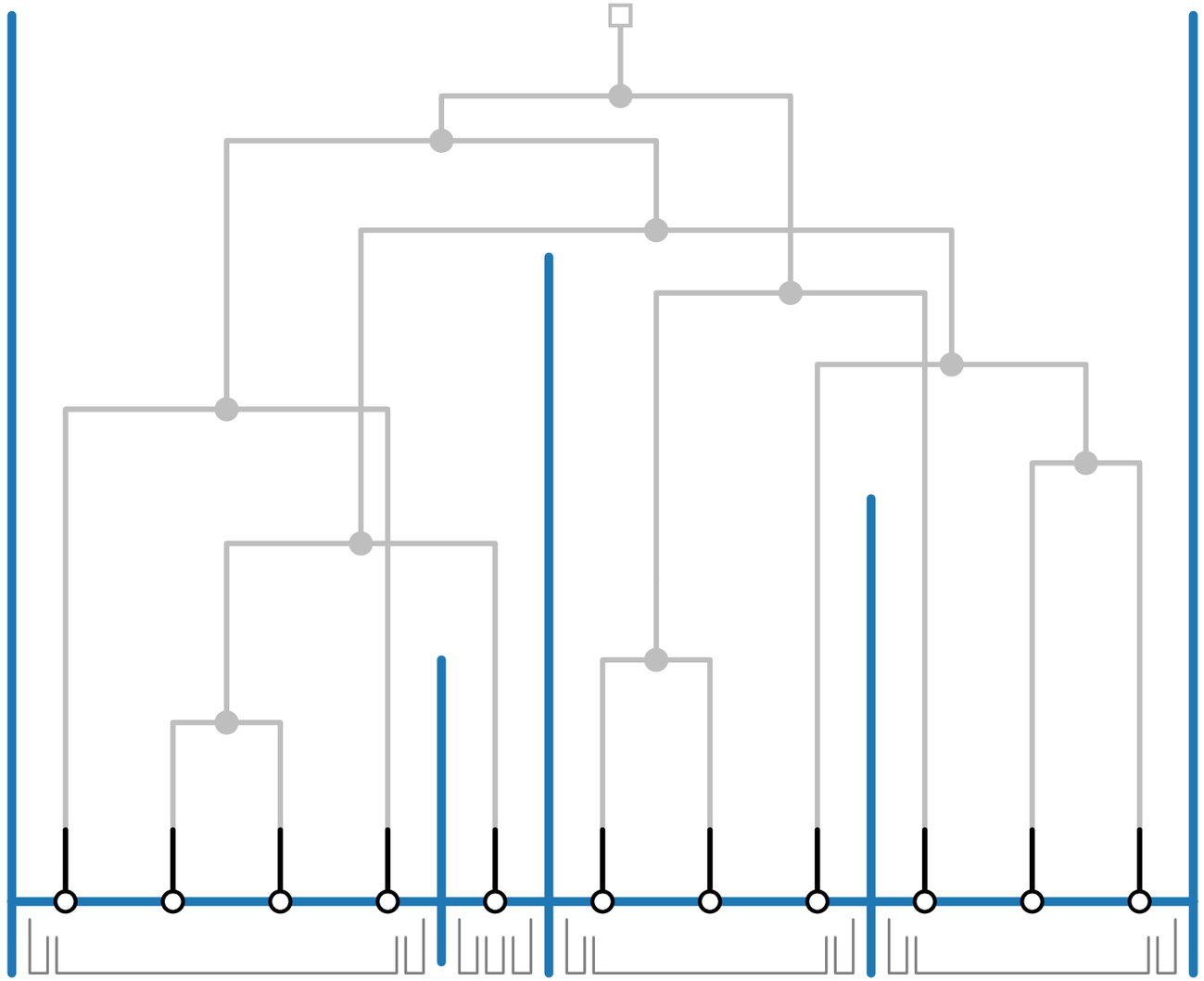

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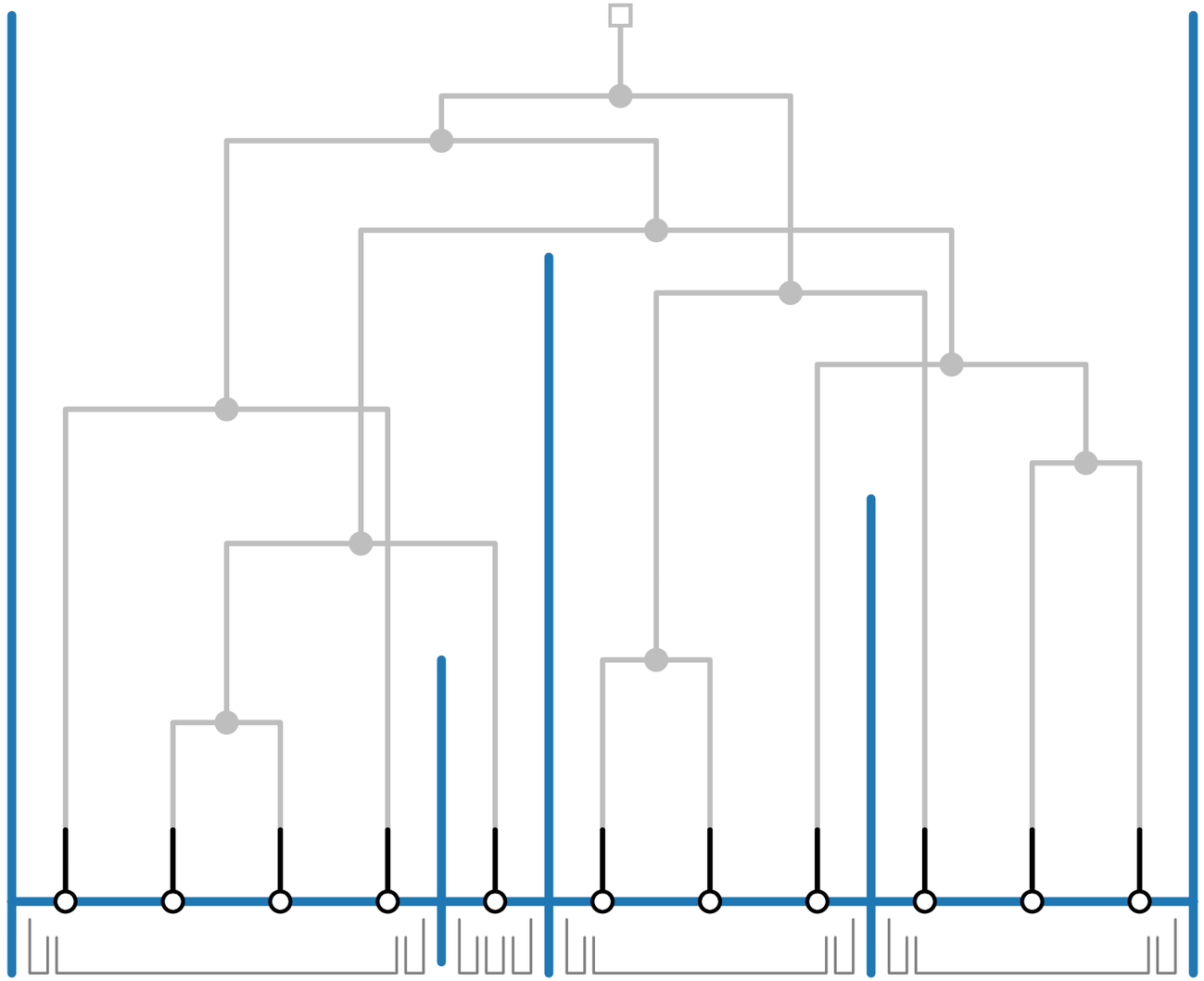

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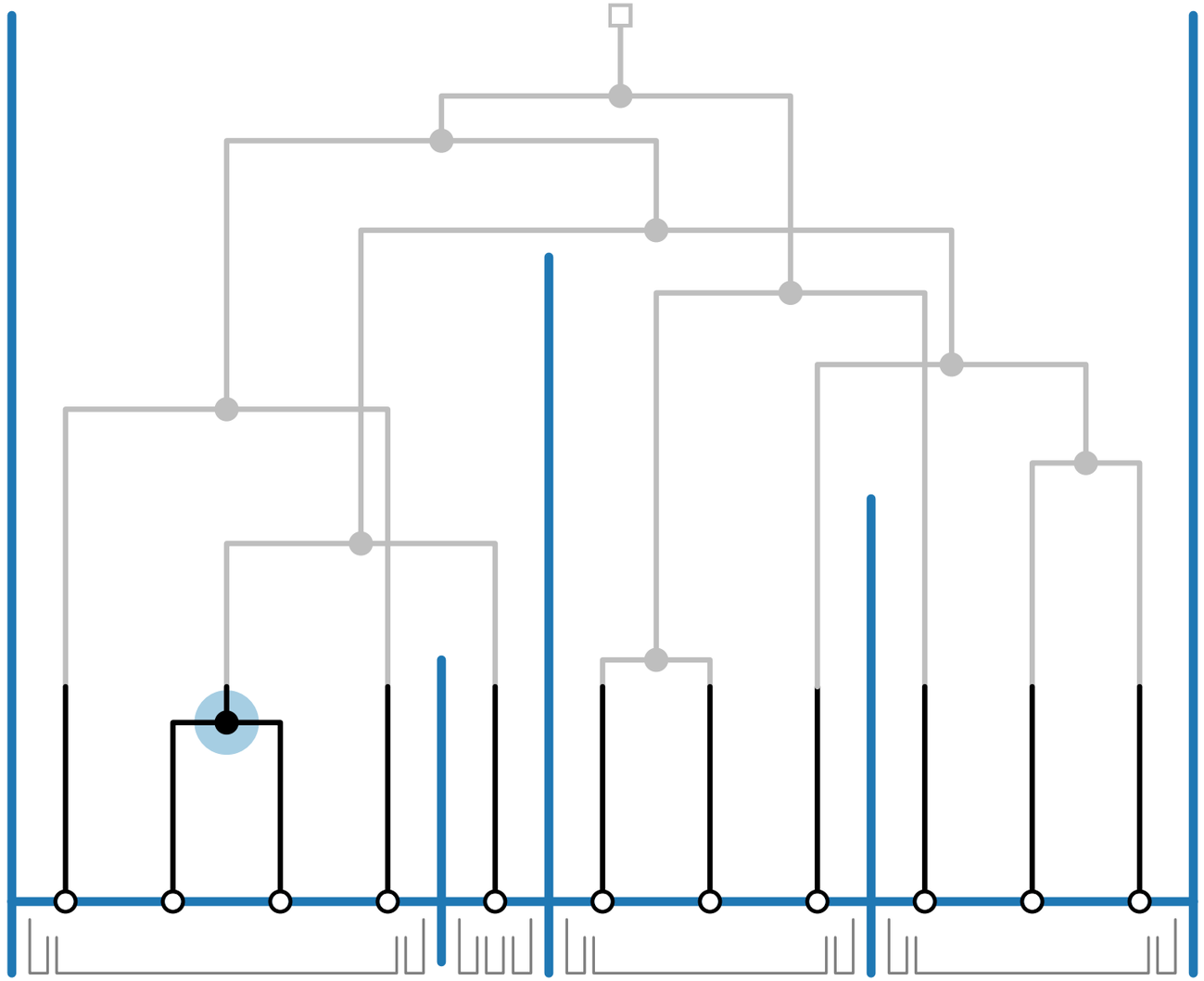

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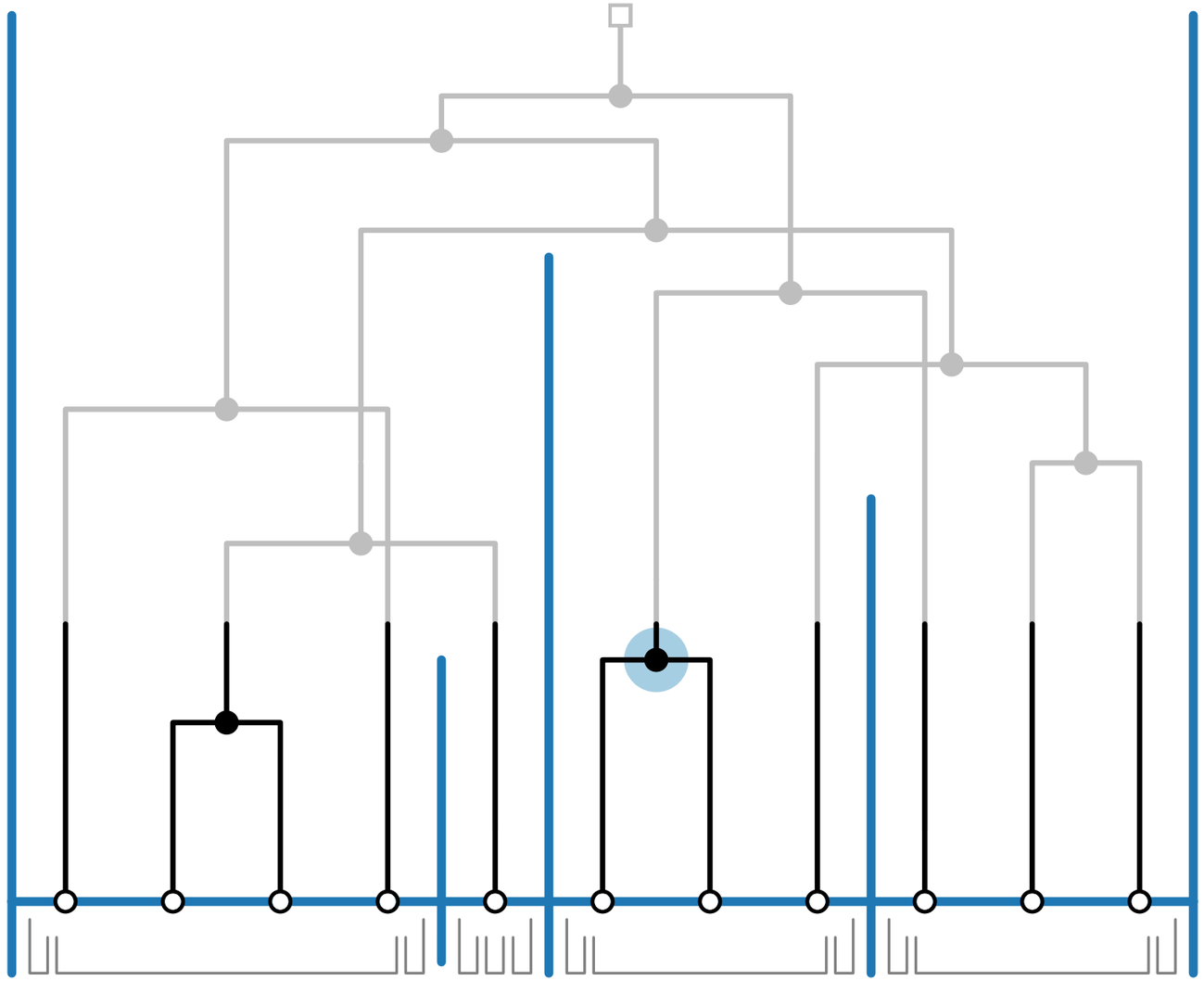

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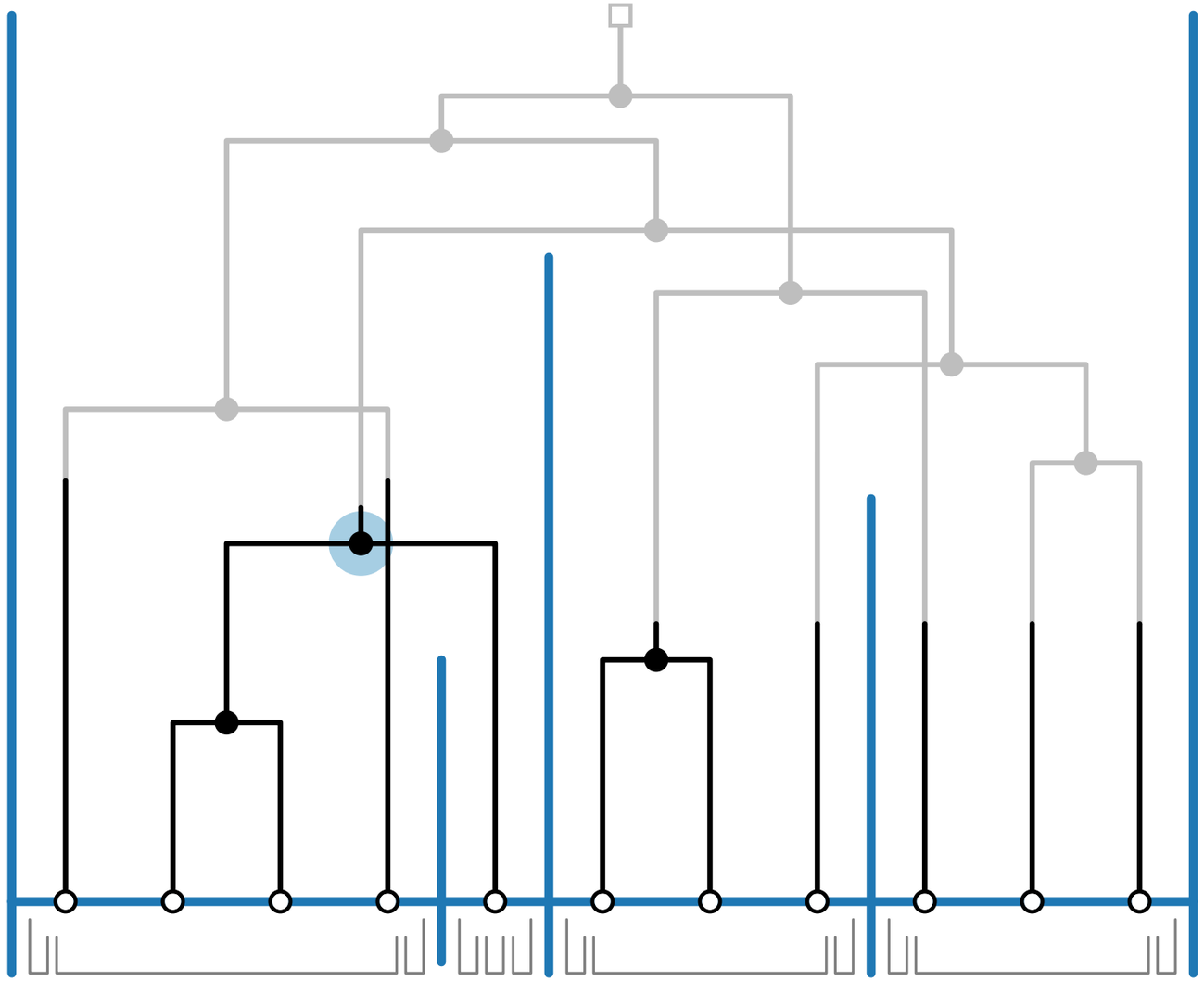

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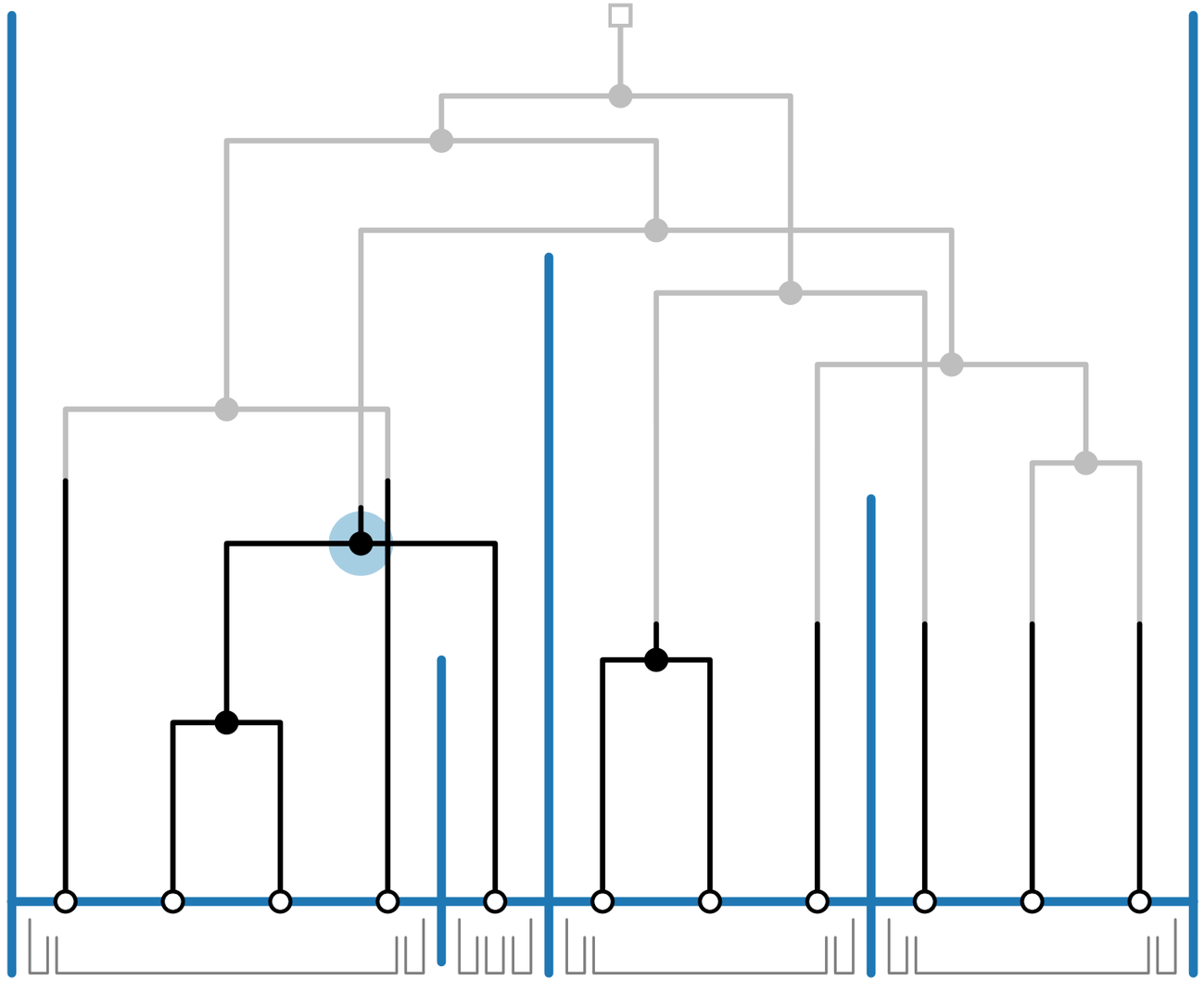

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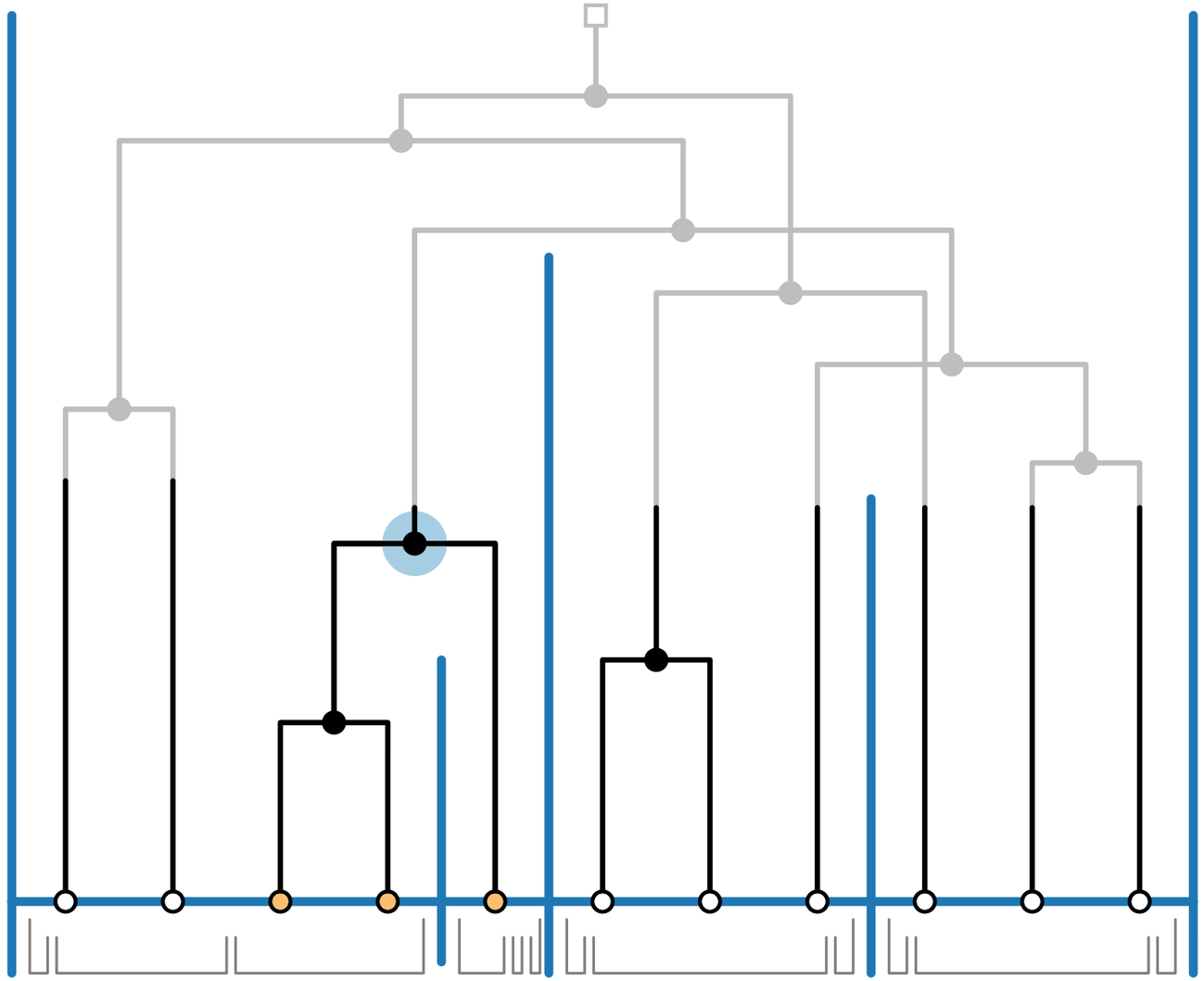

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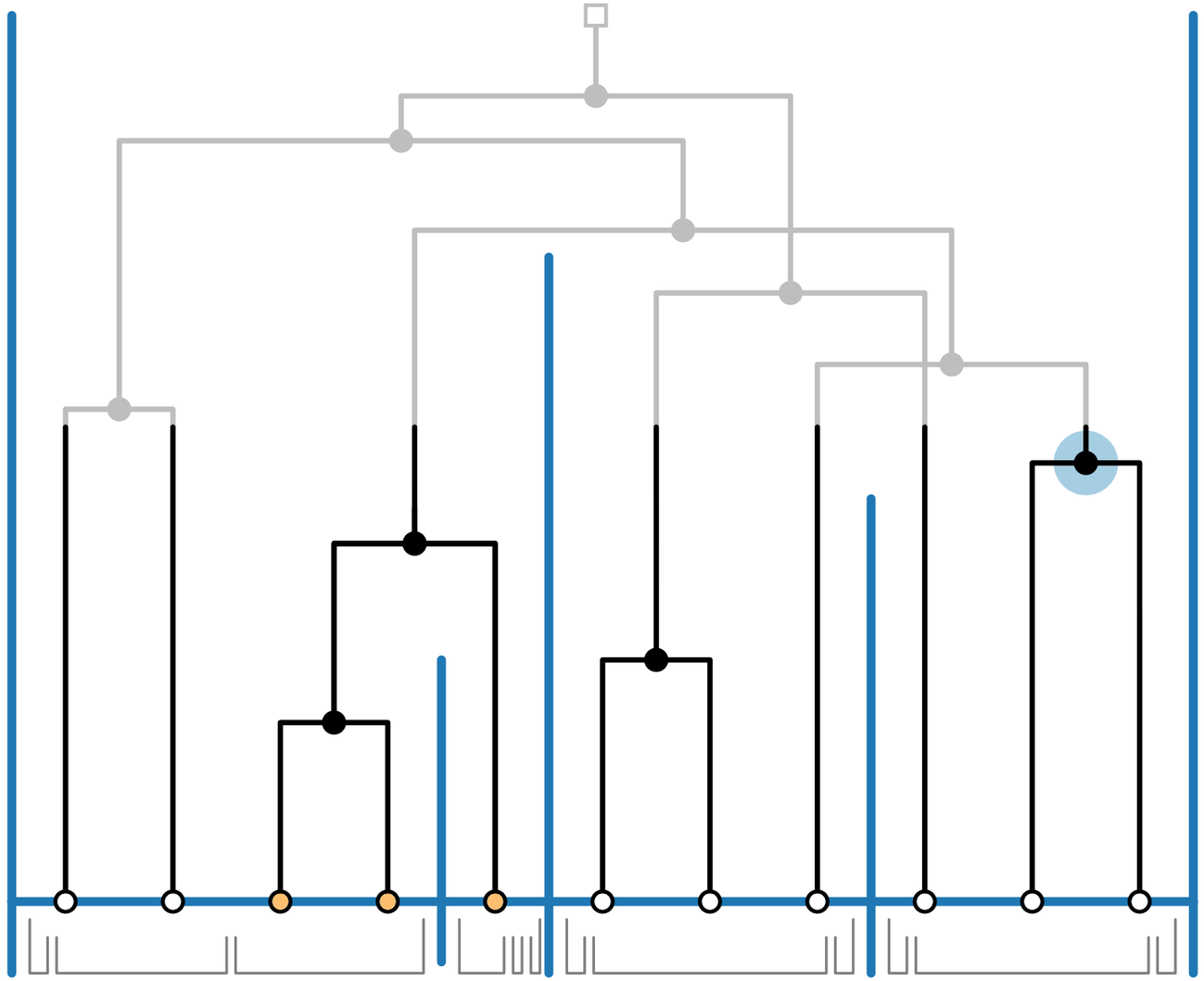

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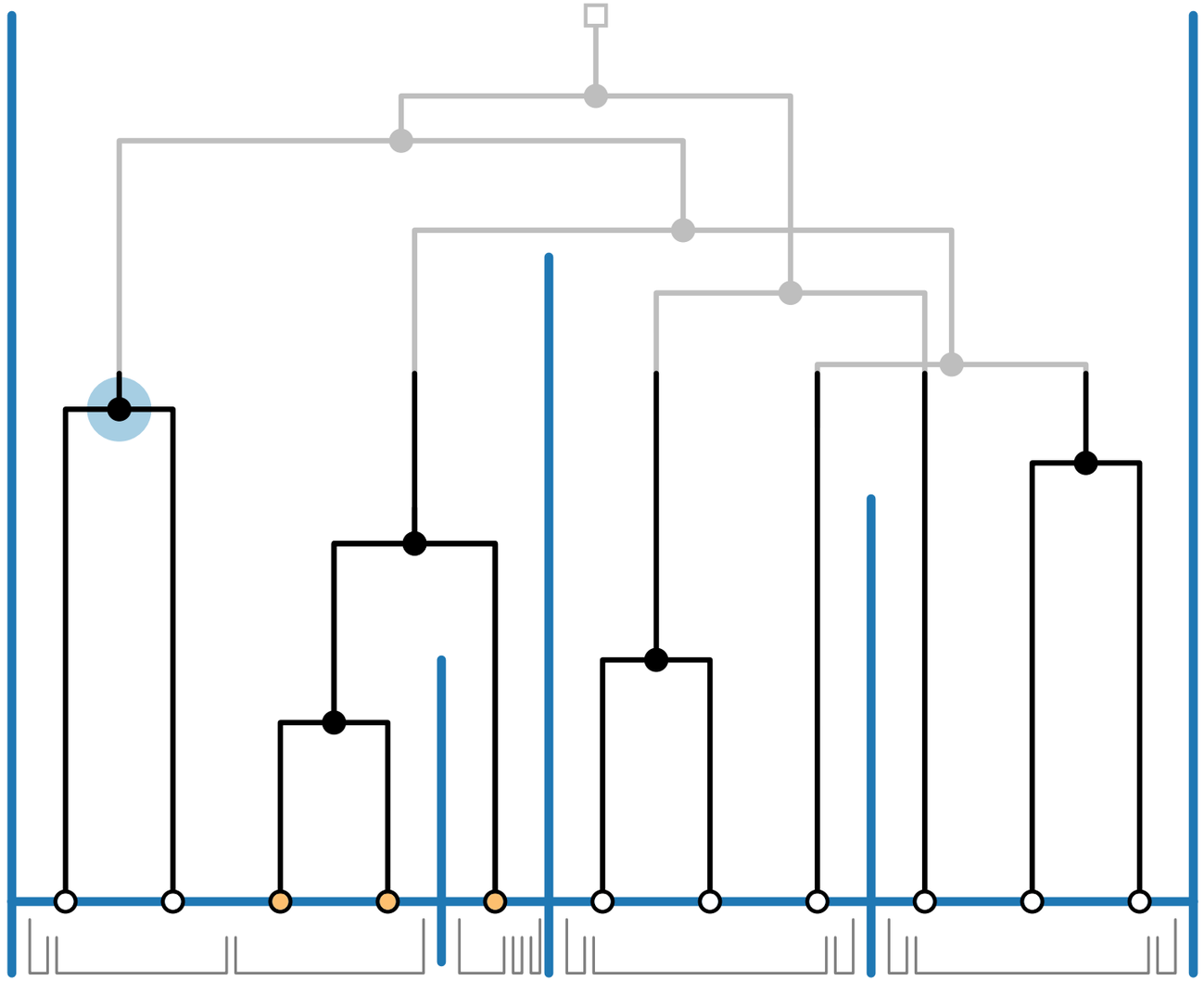

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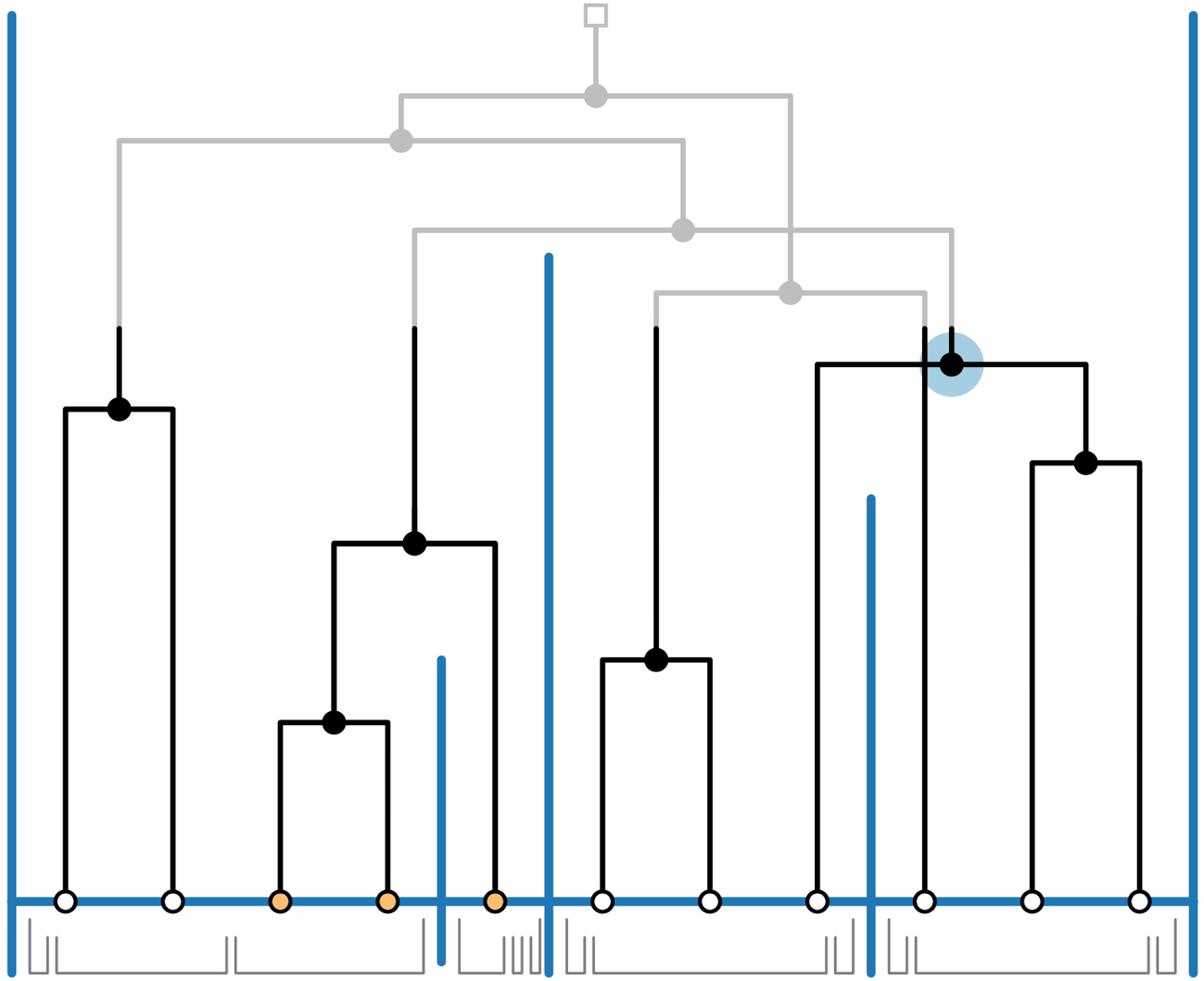

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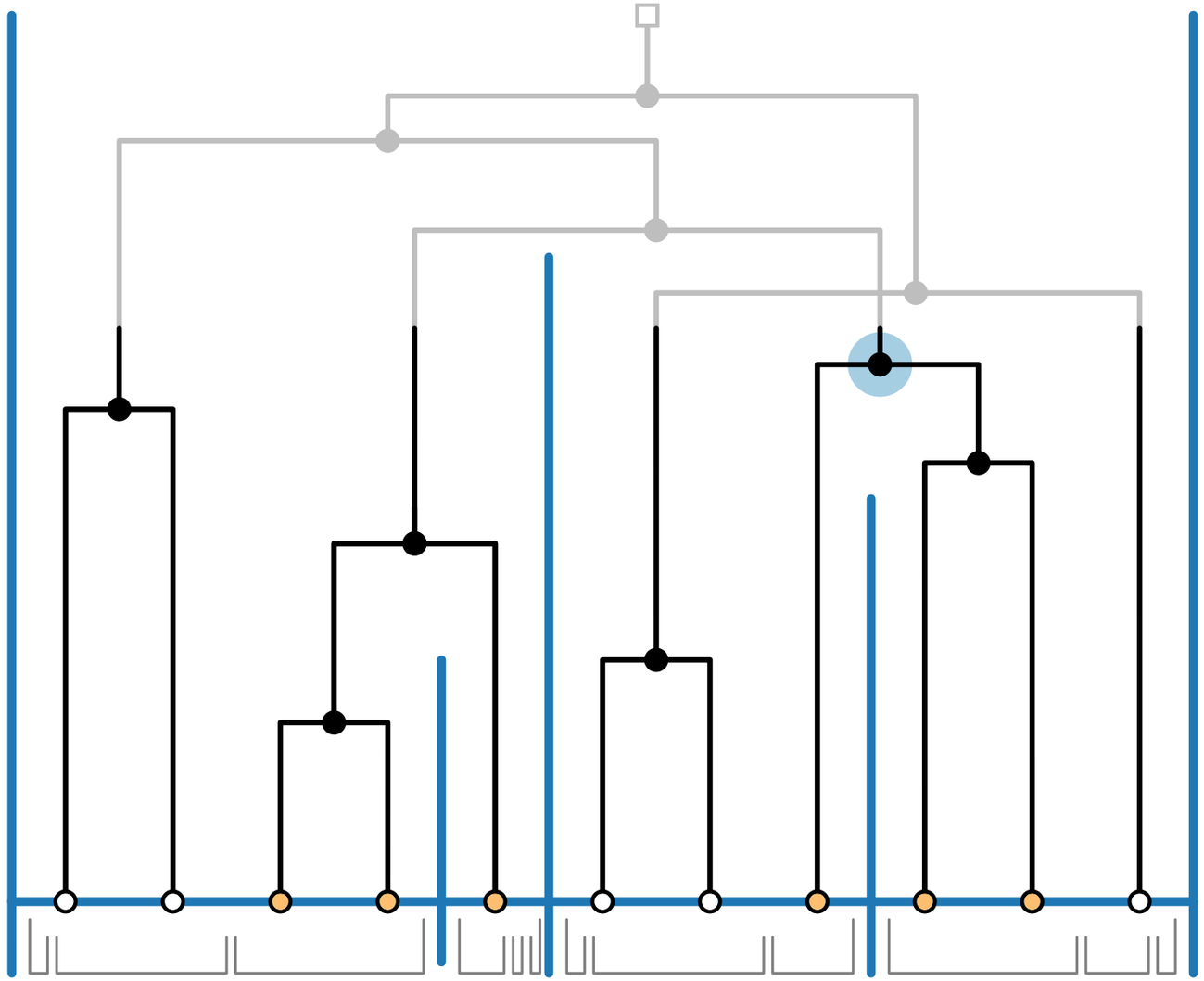

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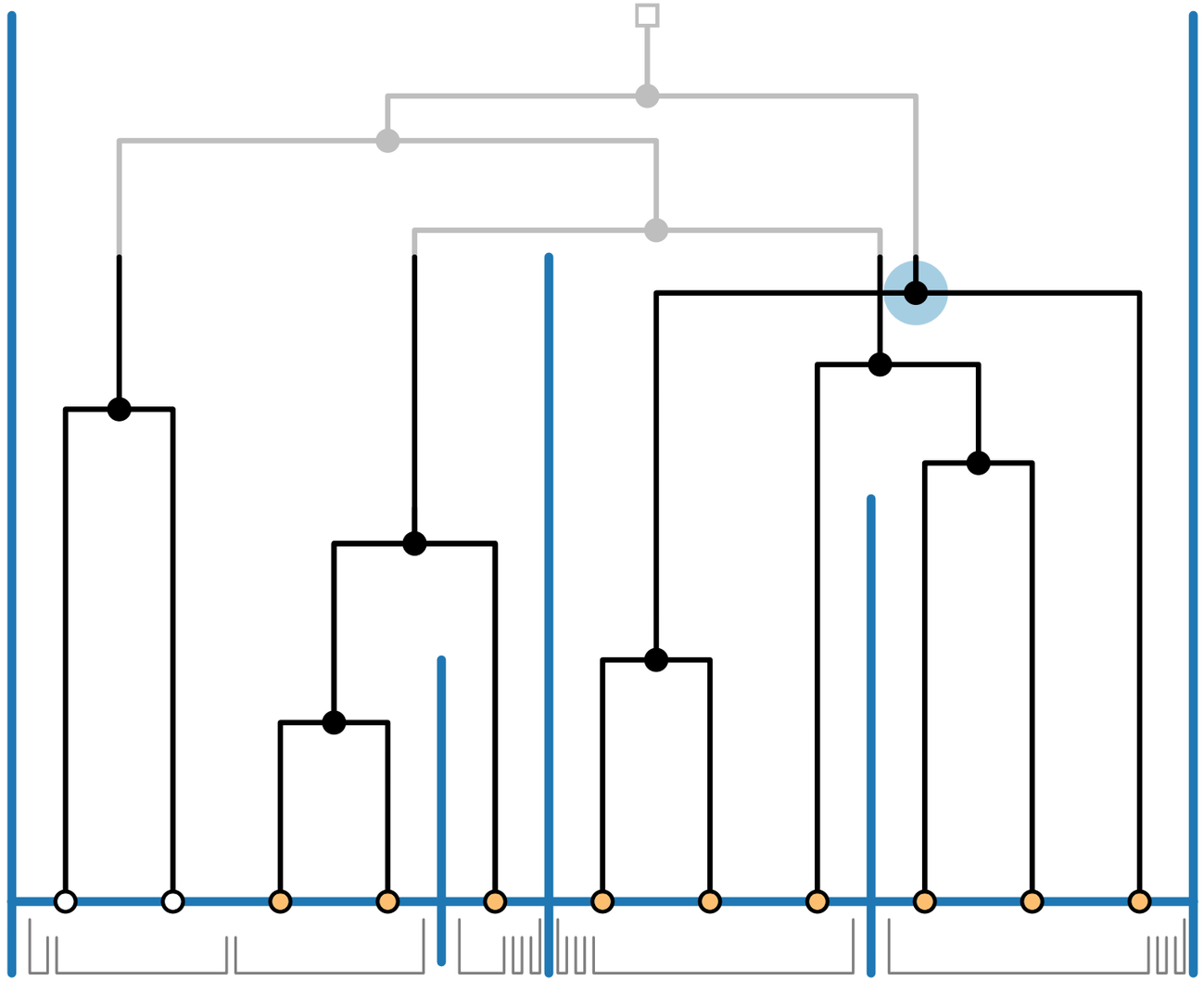

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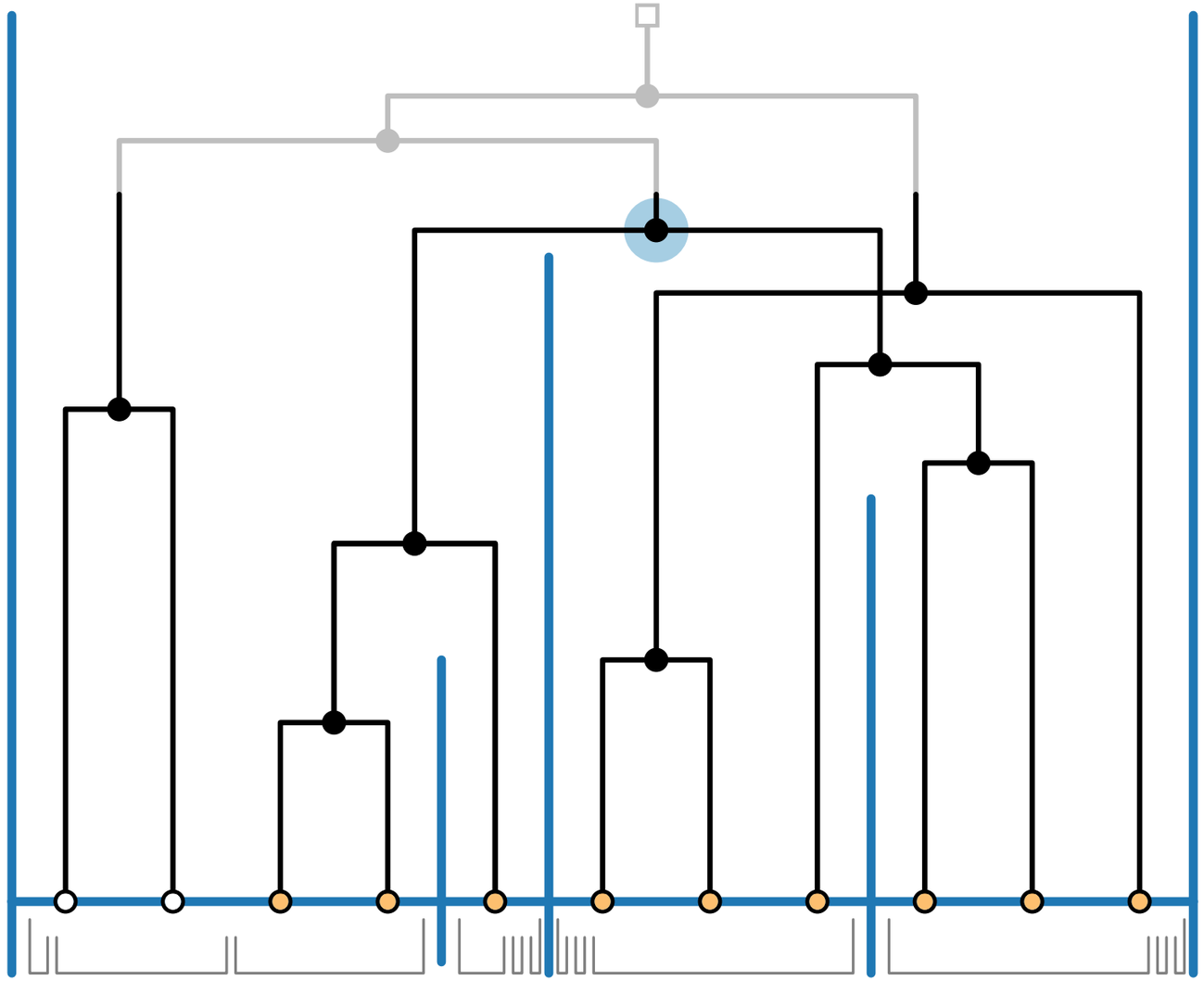

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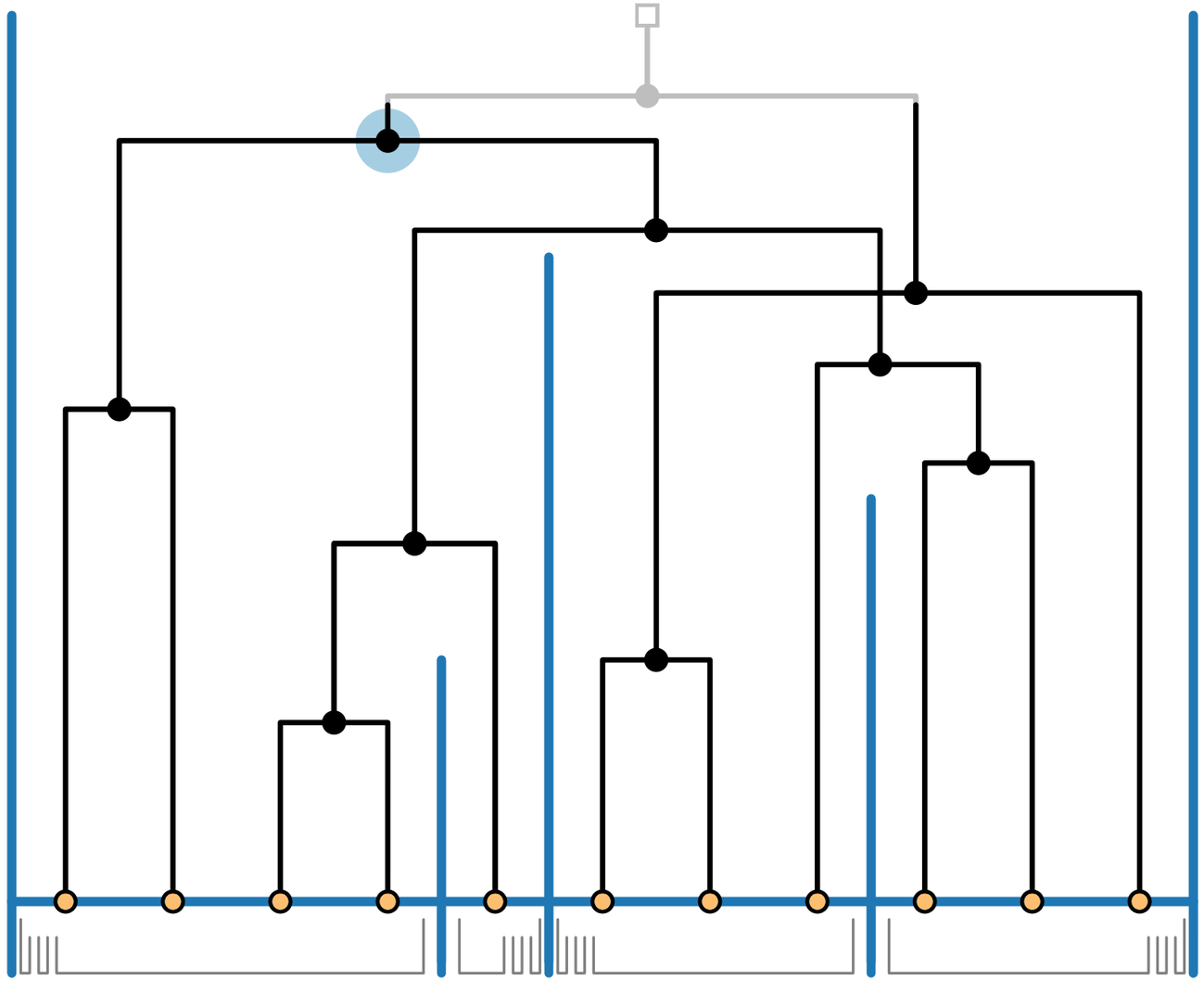

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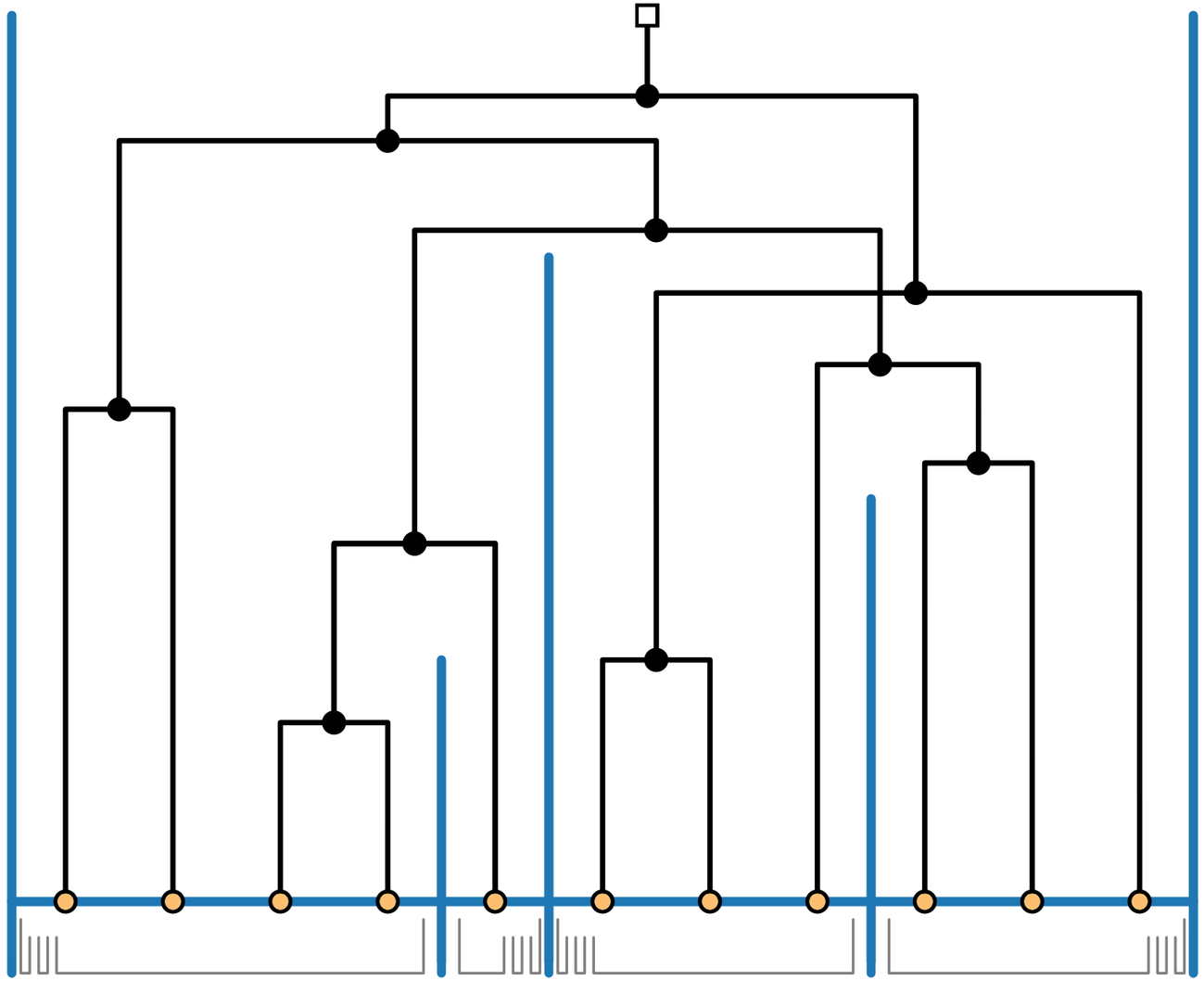

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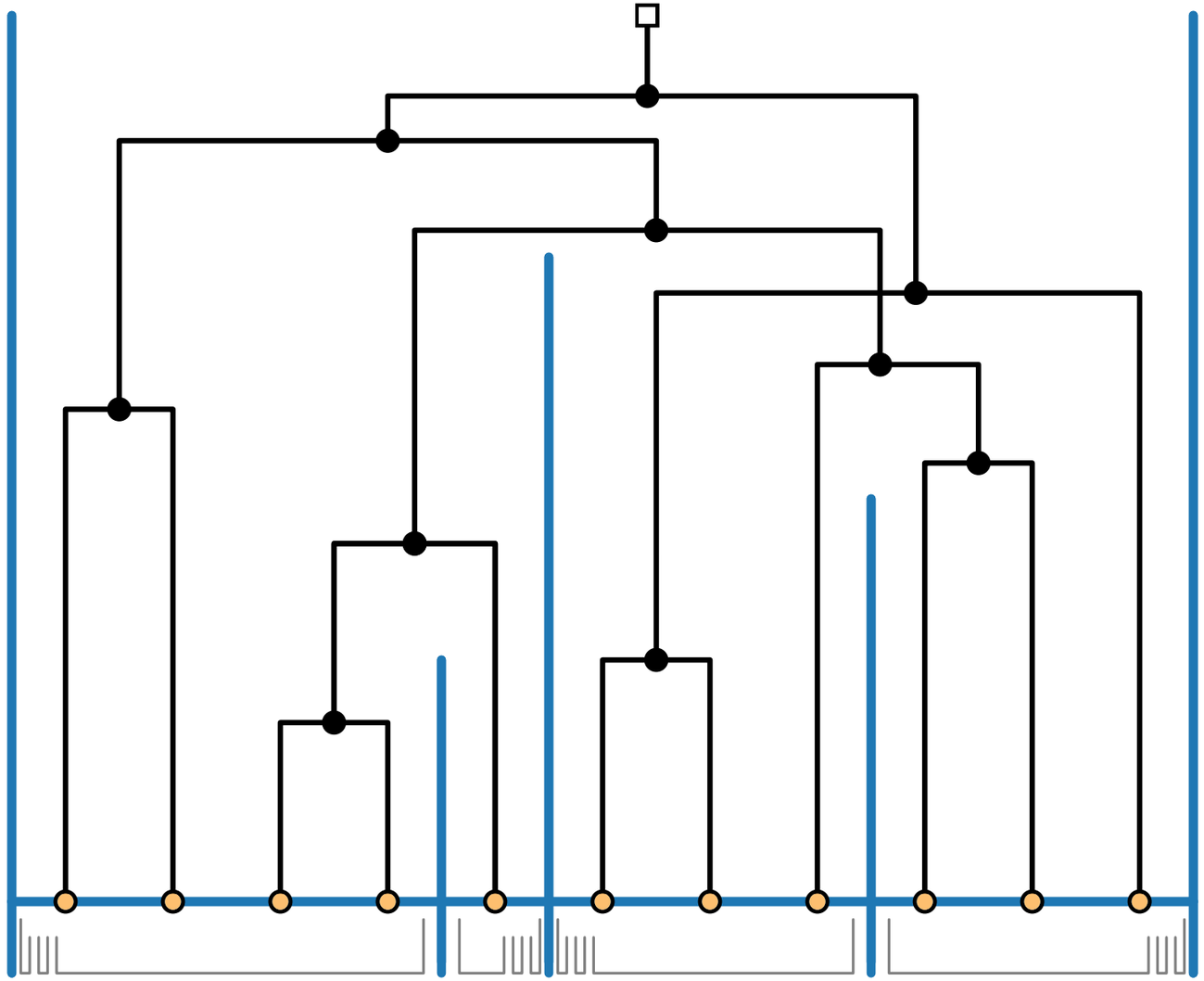

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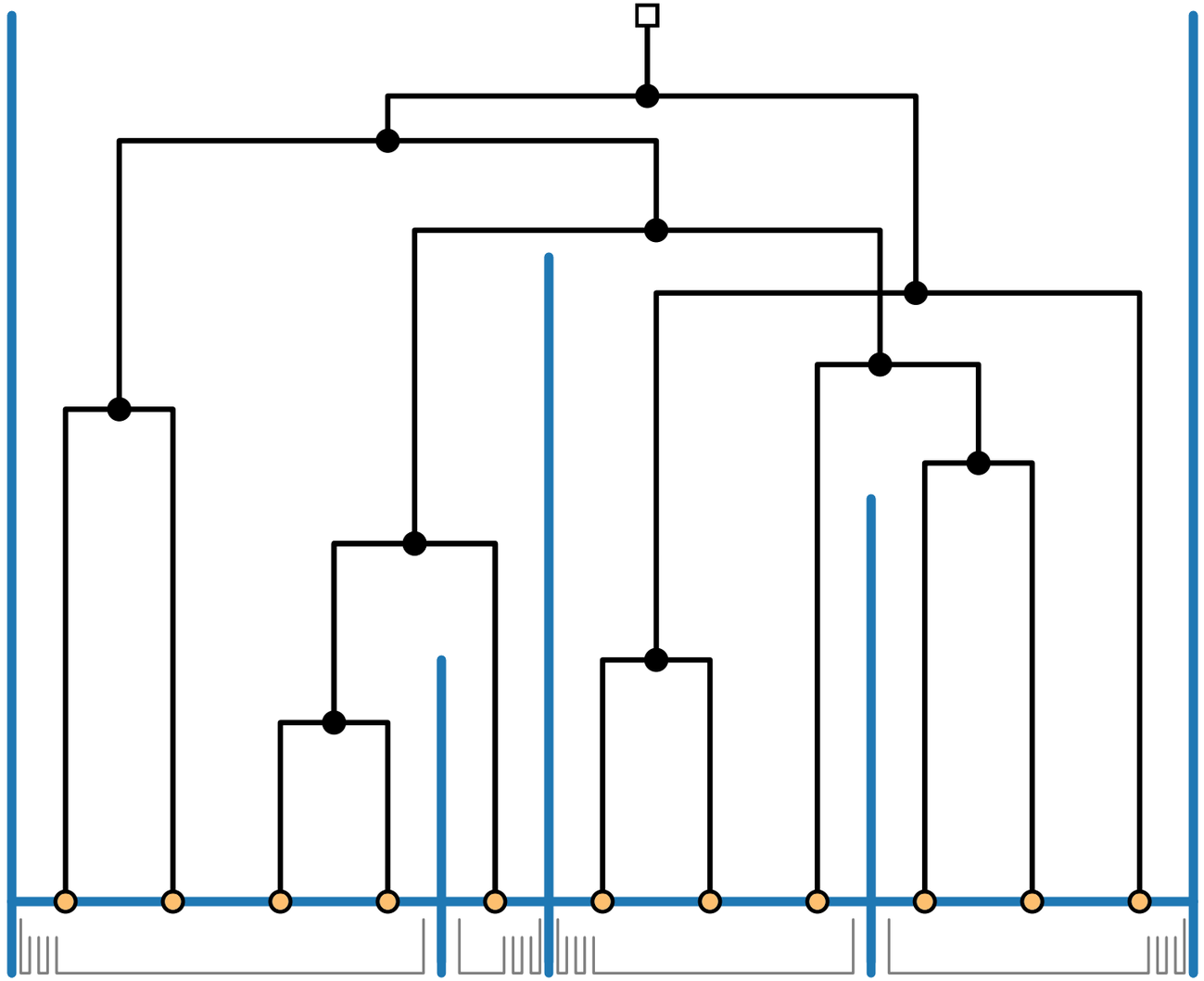

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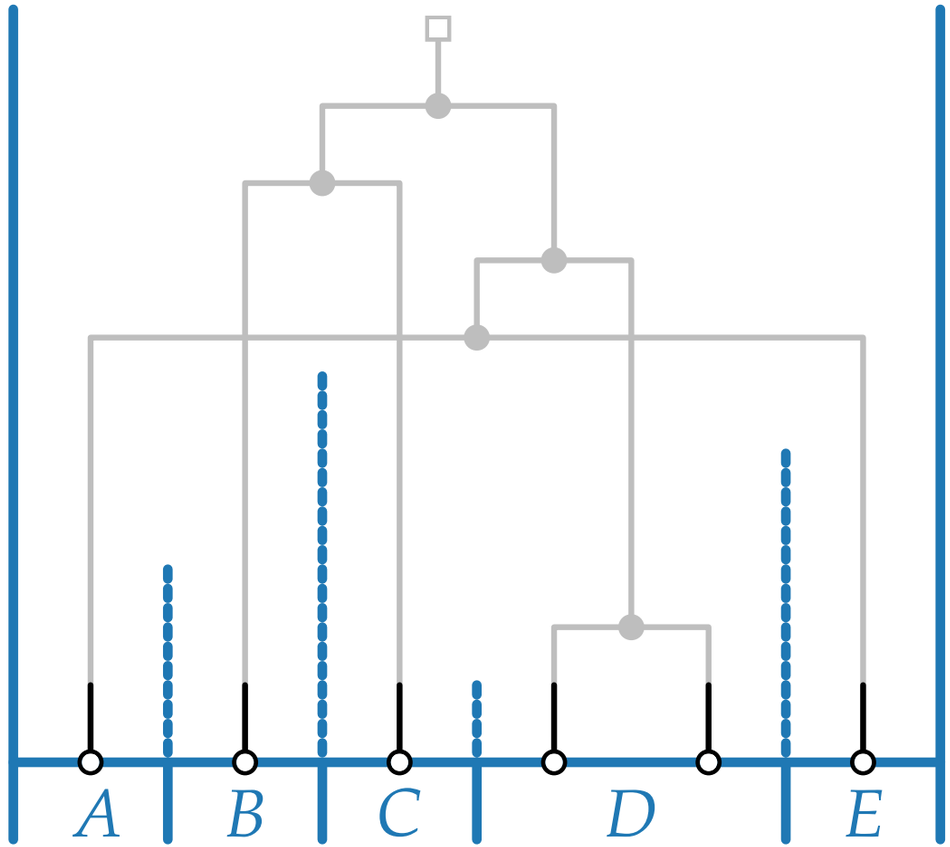

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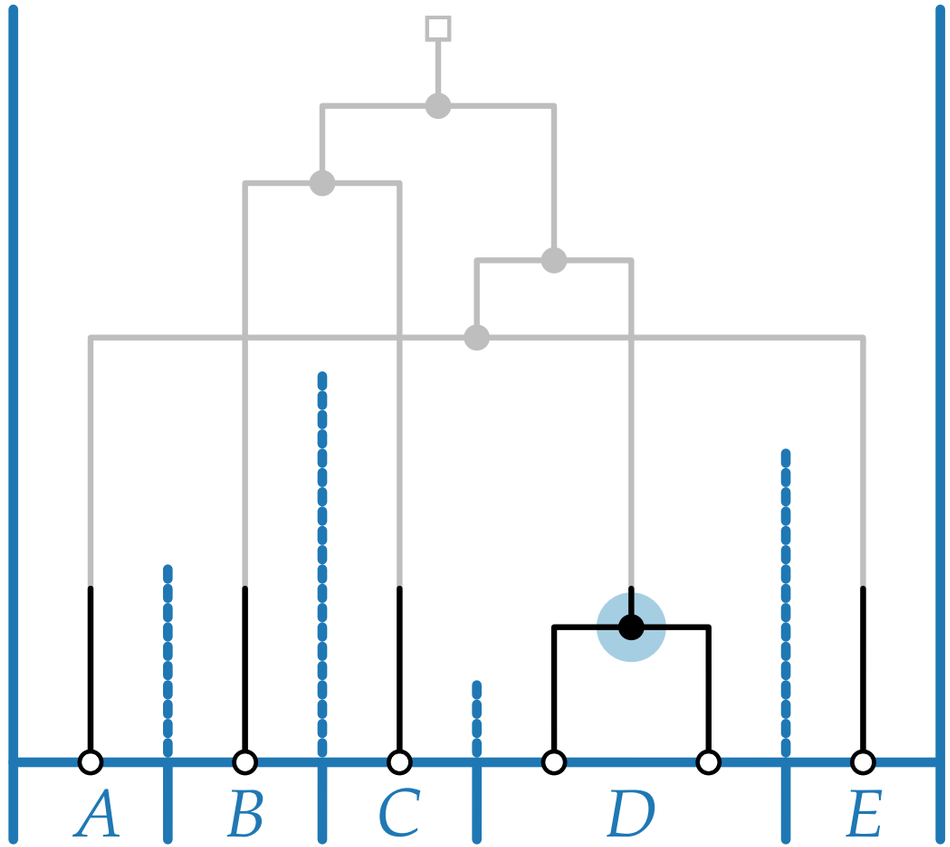

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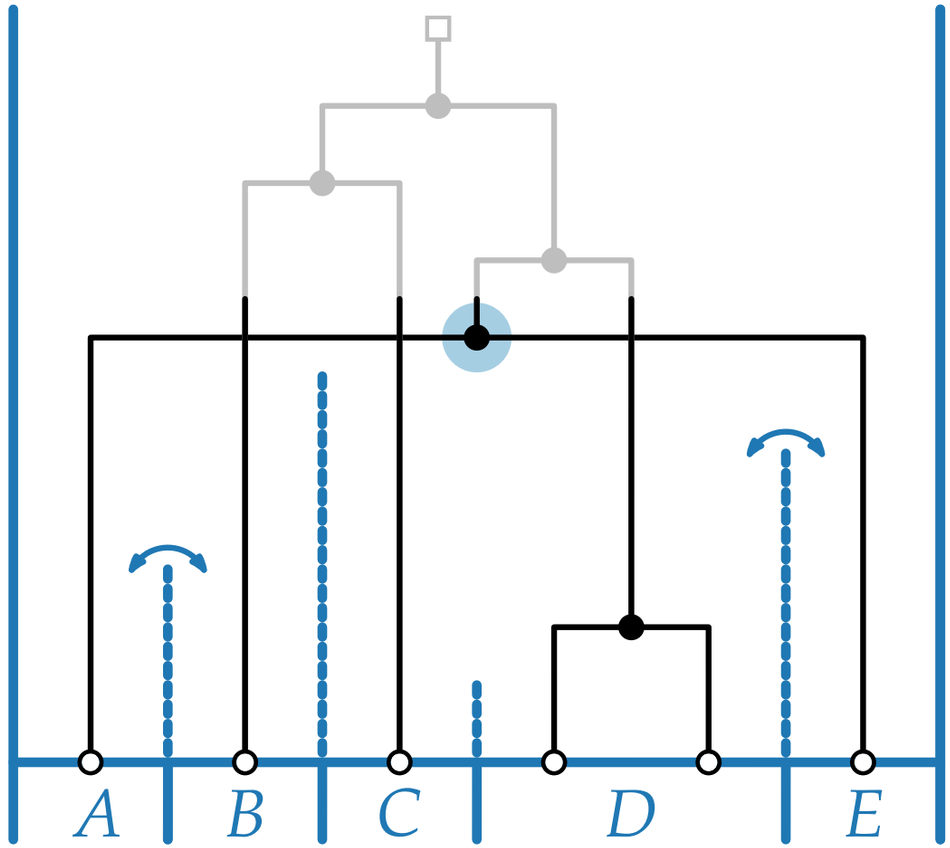

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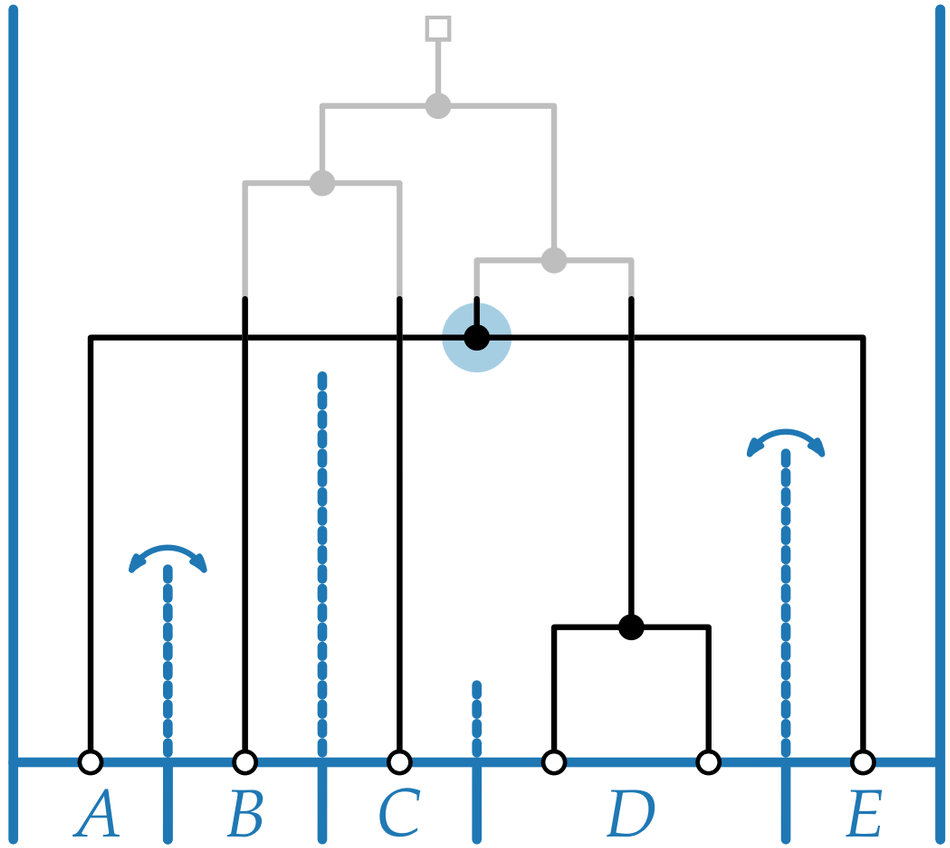

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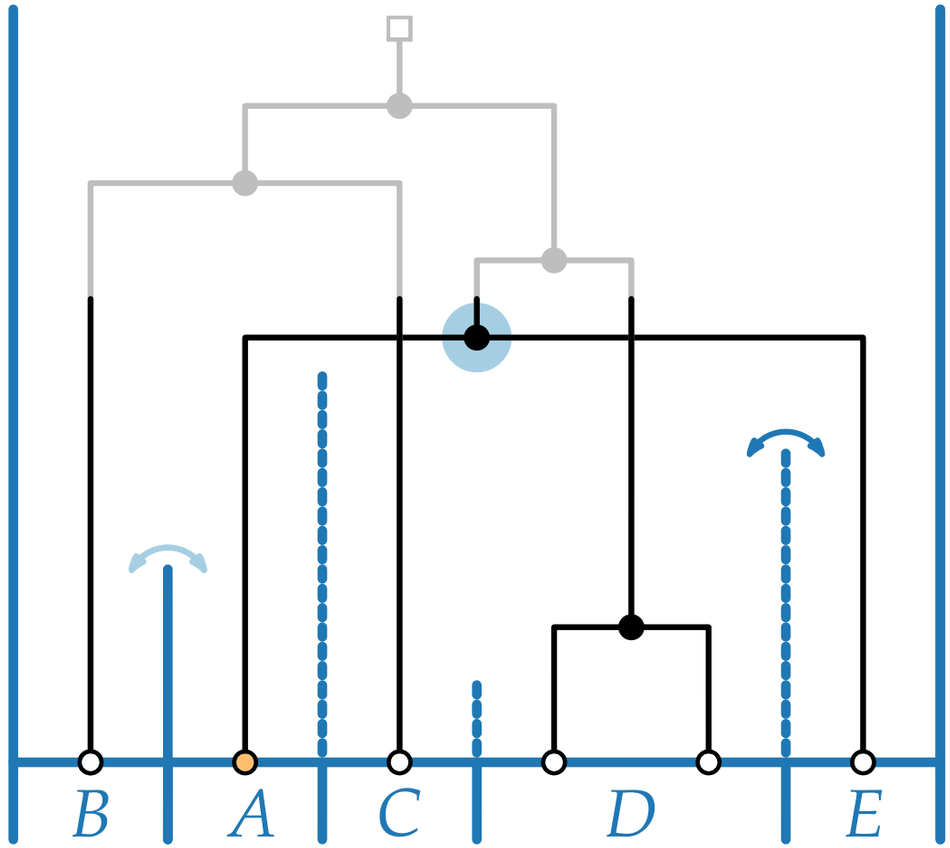

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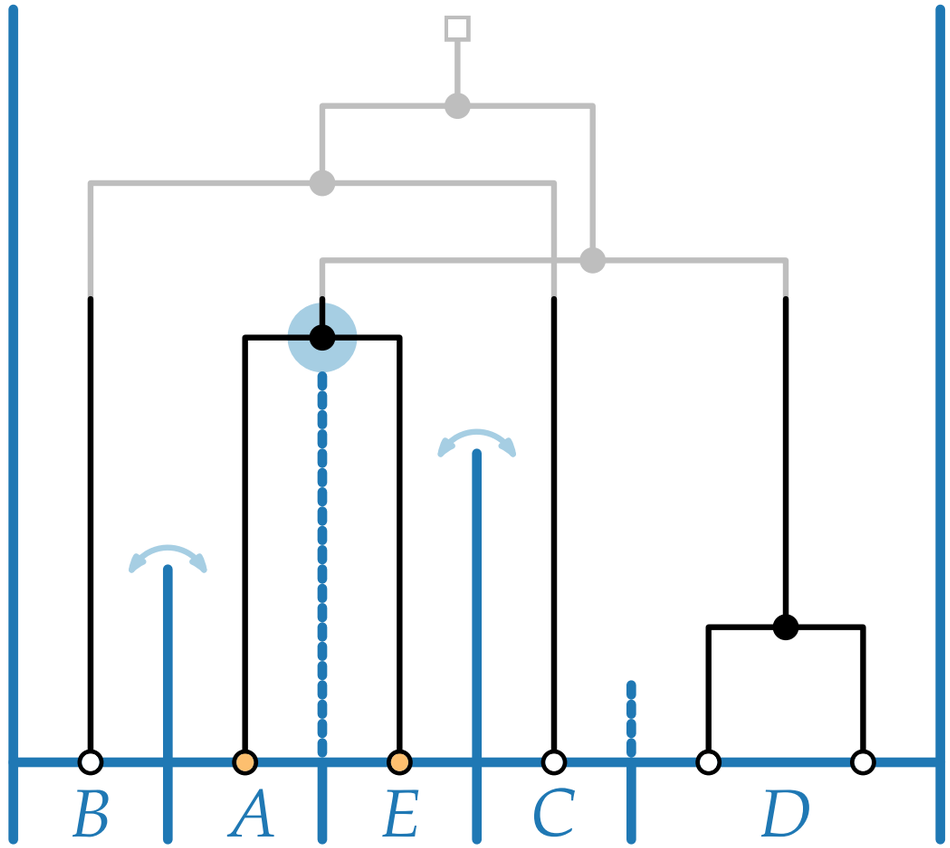

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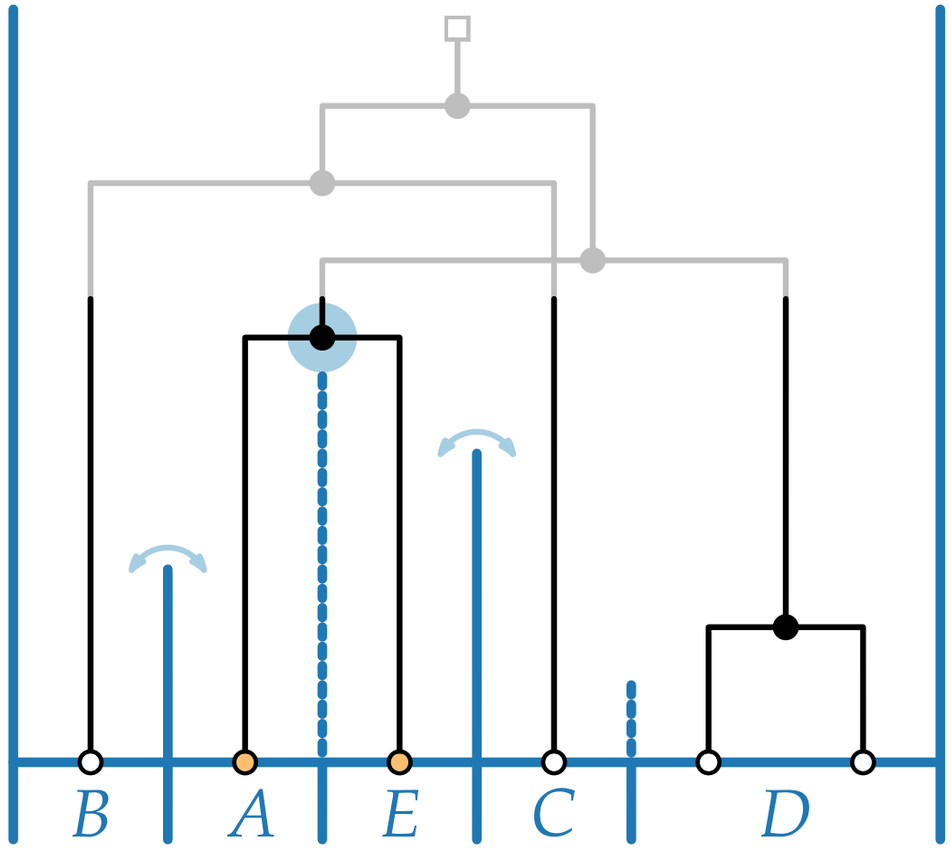

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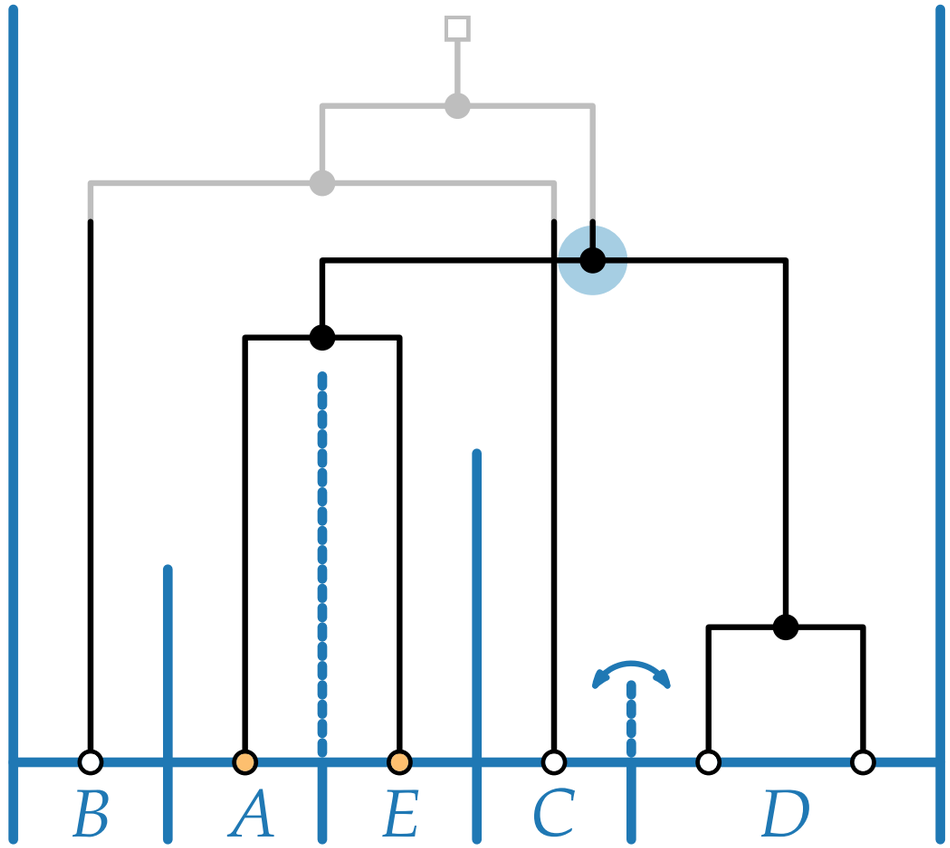

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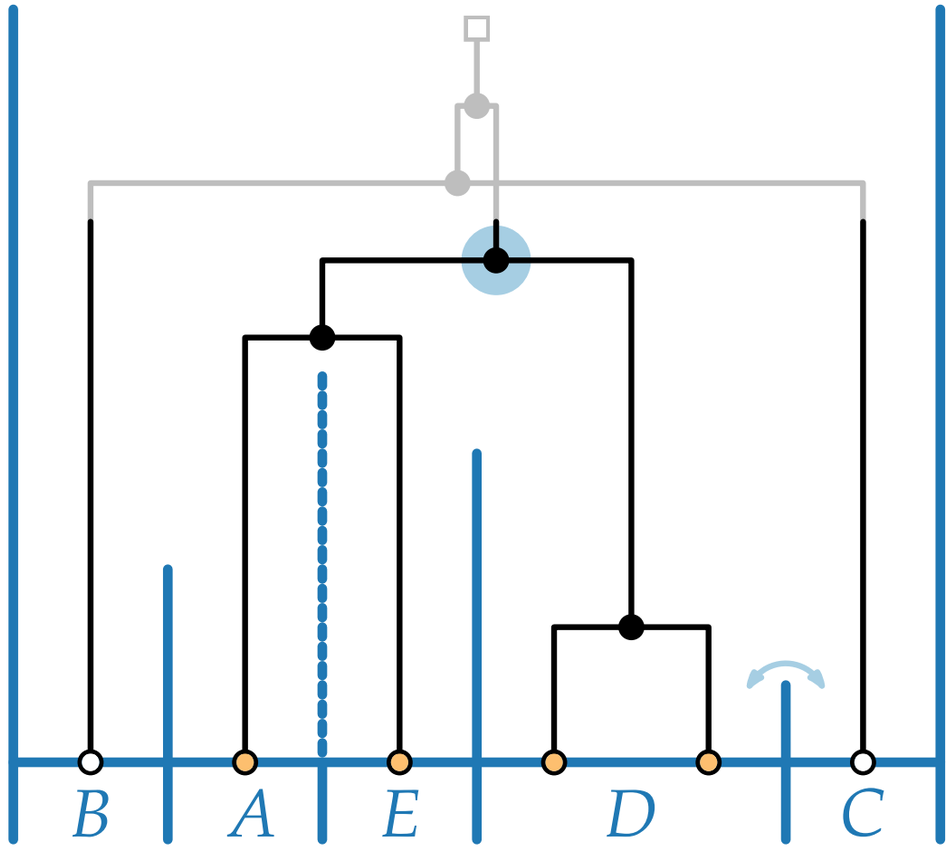

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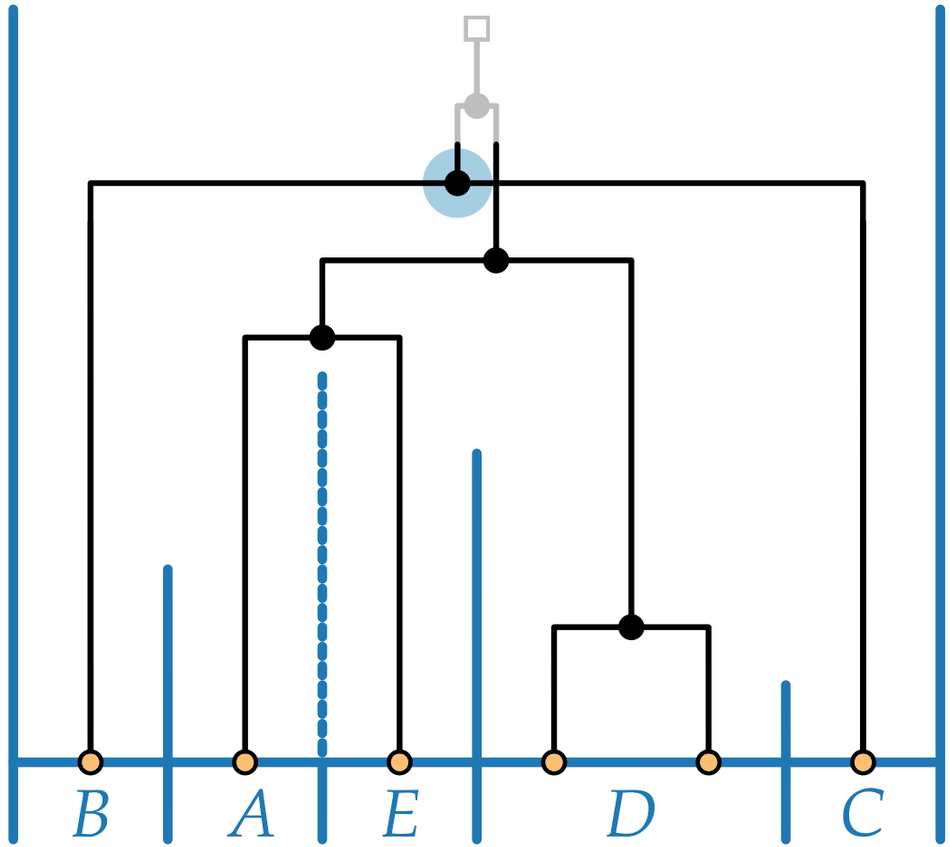

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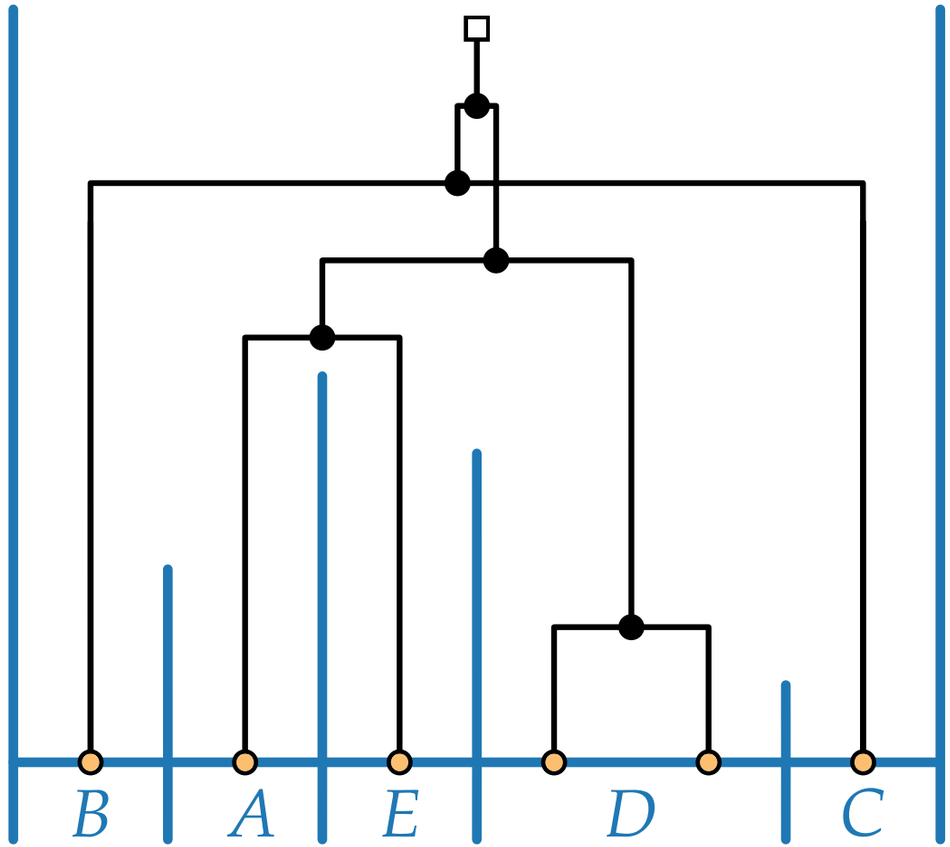

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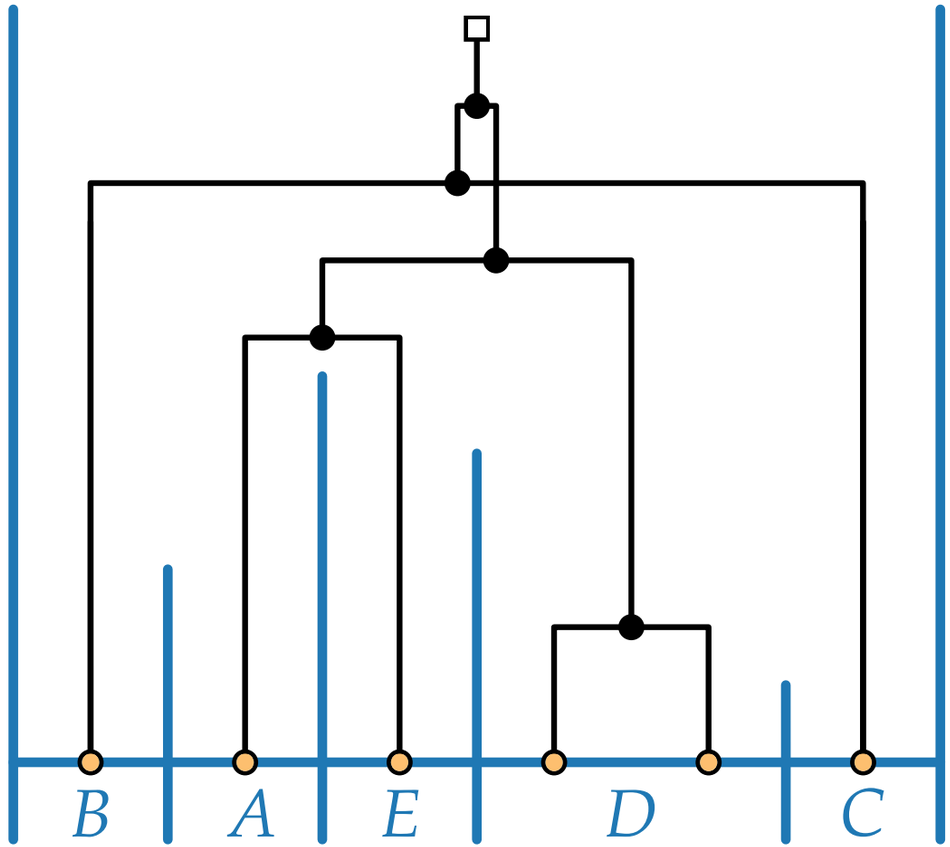

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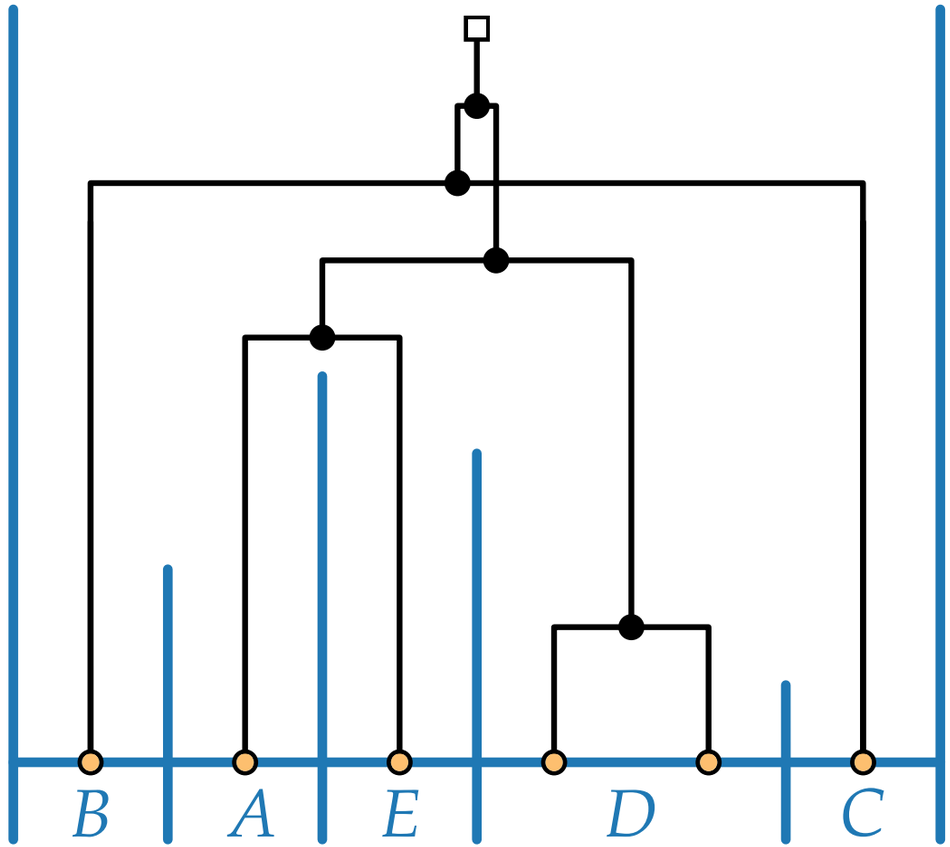
- quadratic running time



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- We need $O(n^2 + m)$ variables and $O(n^2 + n \cdot m)$ constraints, where $n = |V(T)|$ and $m = |V(S)|$

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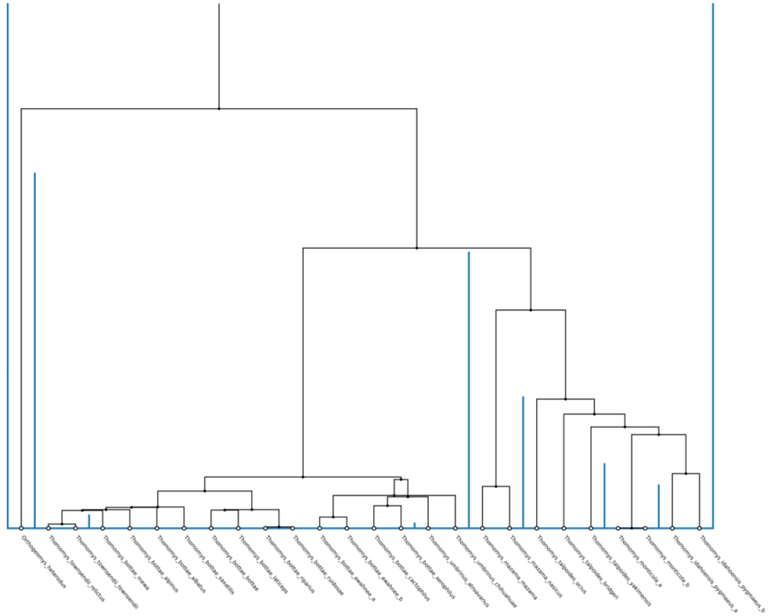

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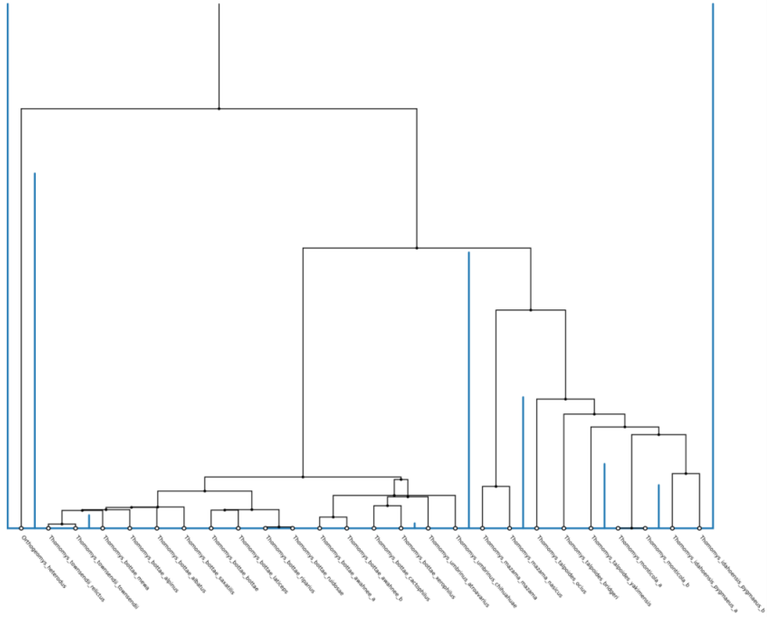

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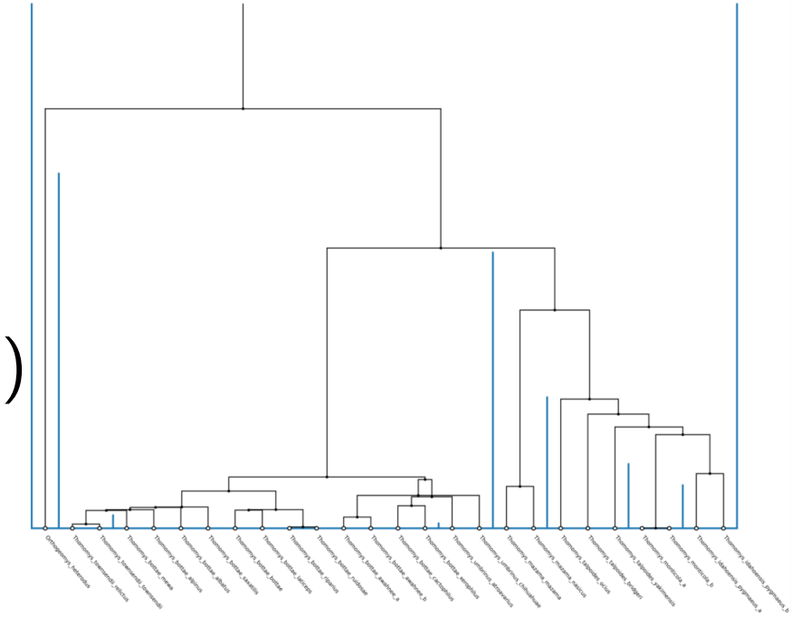

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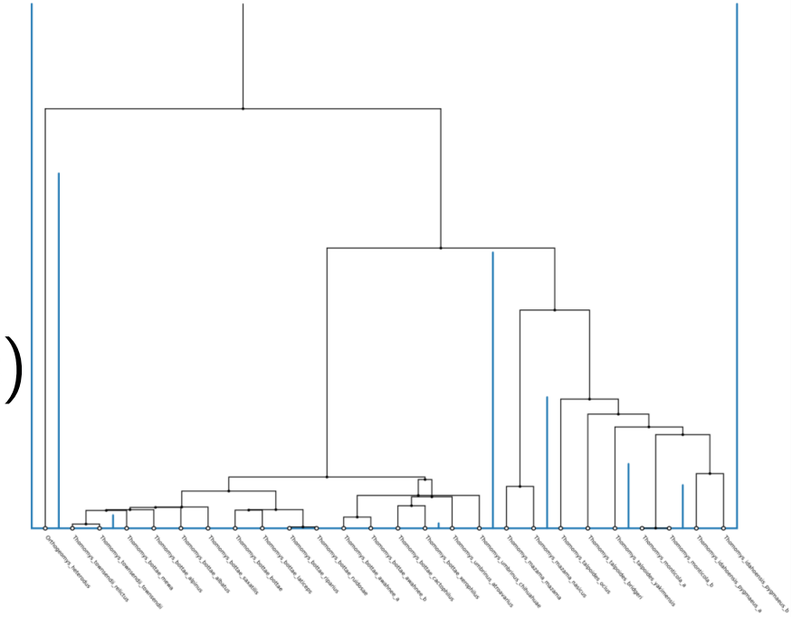

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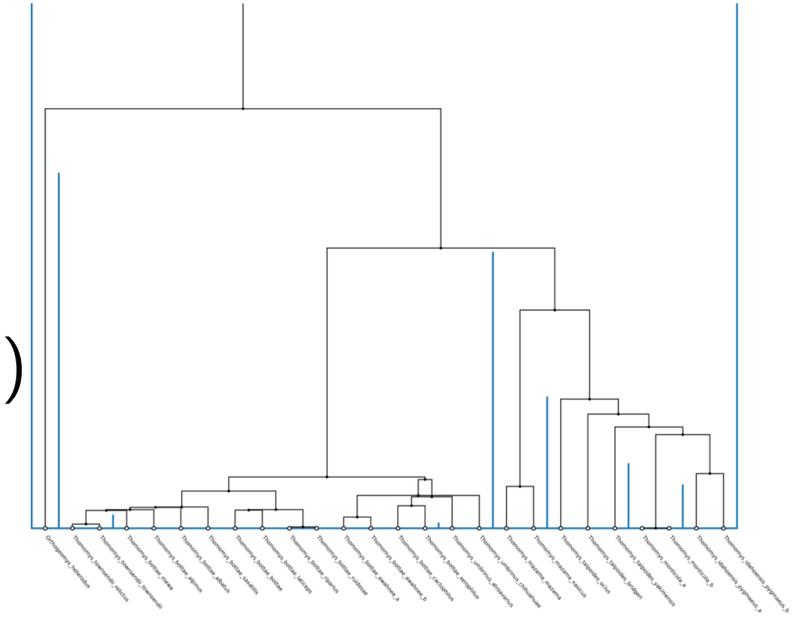

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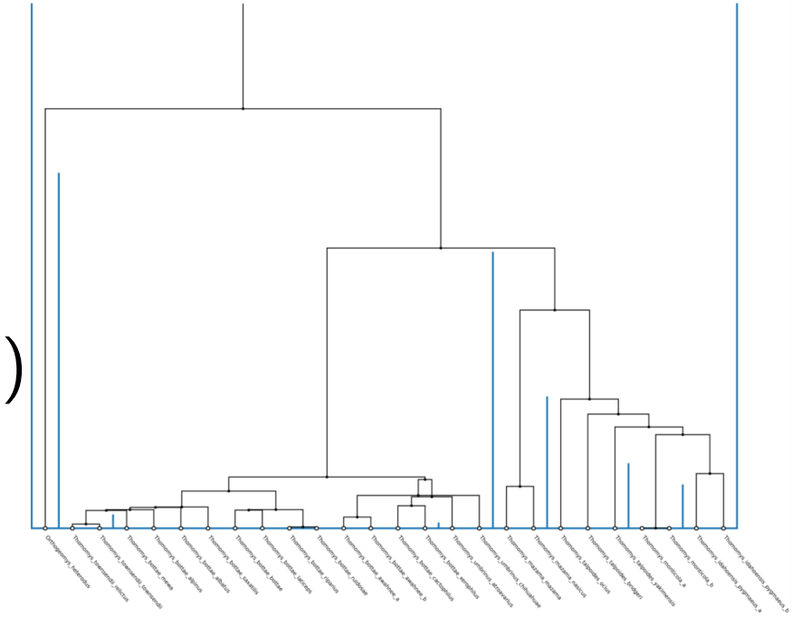

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Recommendation.
Try heuristics on random start embedding while improving; ILP only on small instances.

Summary

- Defined drawing style for multispecies coalescent trees.
- Planarity testing is easy.
- Crossing minimisation is NP-hard.
- Described simple heuristics and ILP.
- Recommend using heuristic on different start embeddings in practice.