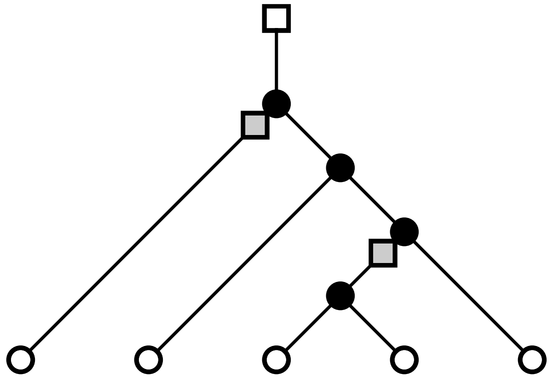
Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

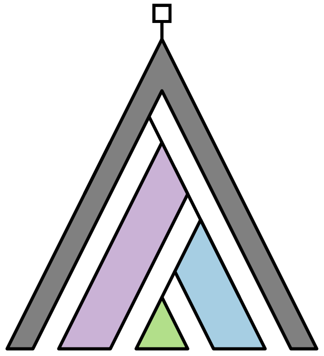
# Advanced Algorithms

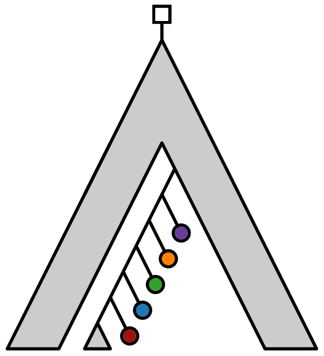
## Rearrangement Distance of Phylogenetic Trees

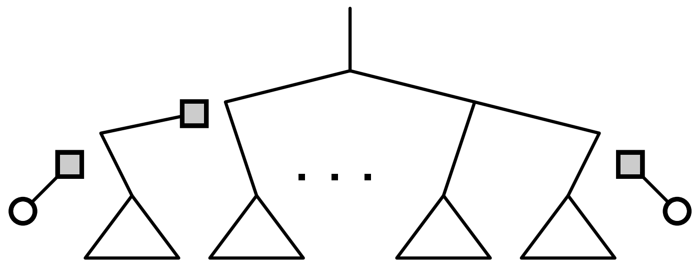
### Kernelization, FPT, Approximation Algorithm

Johannes Zink · WS22









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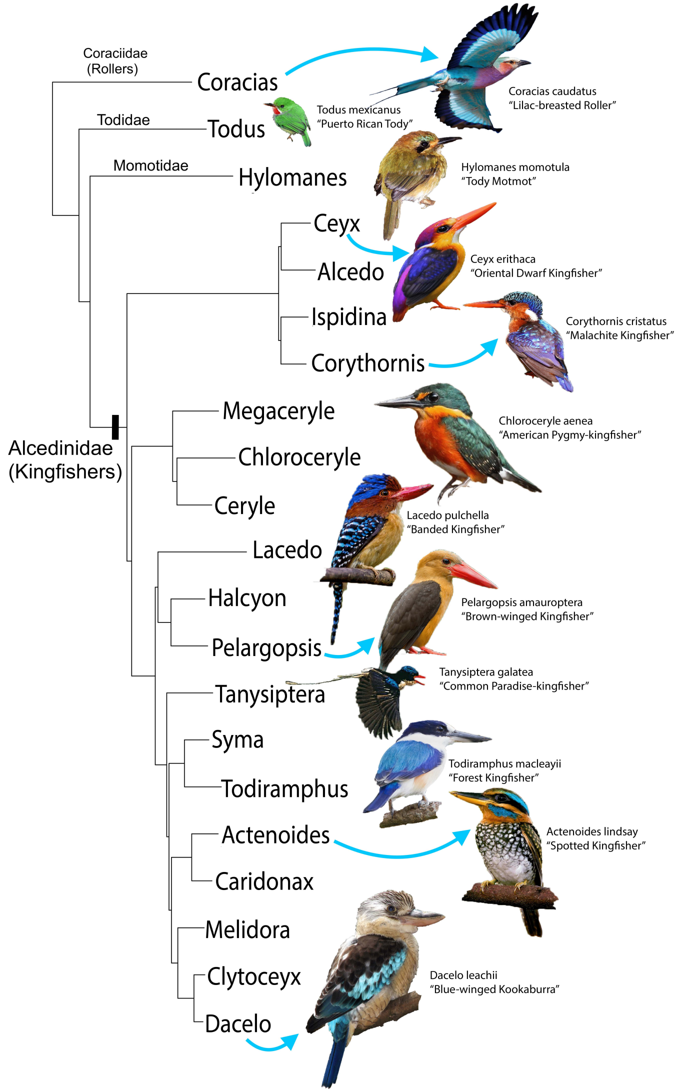


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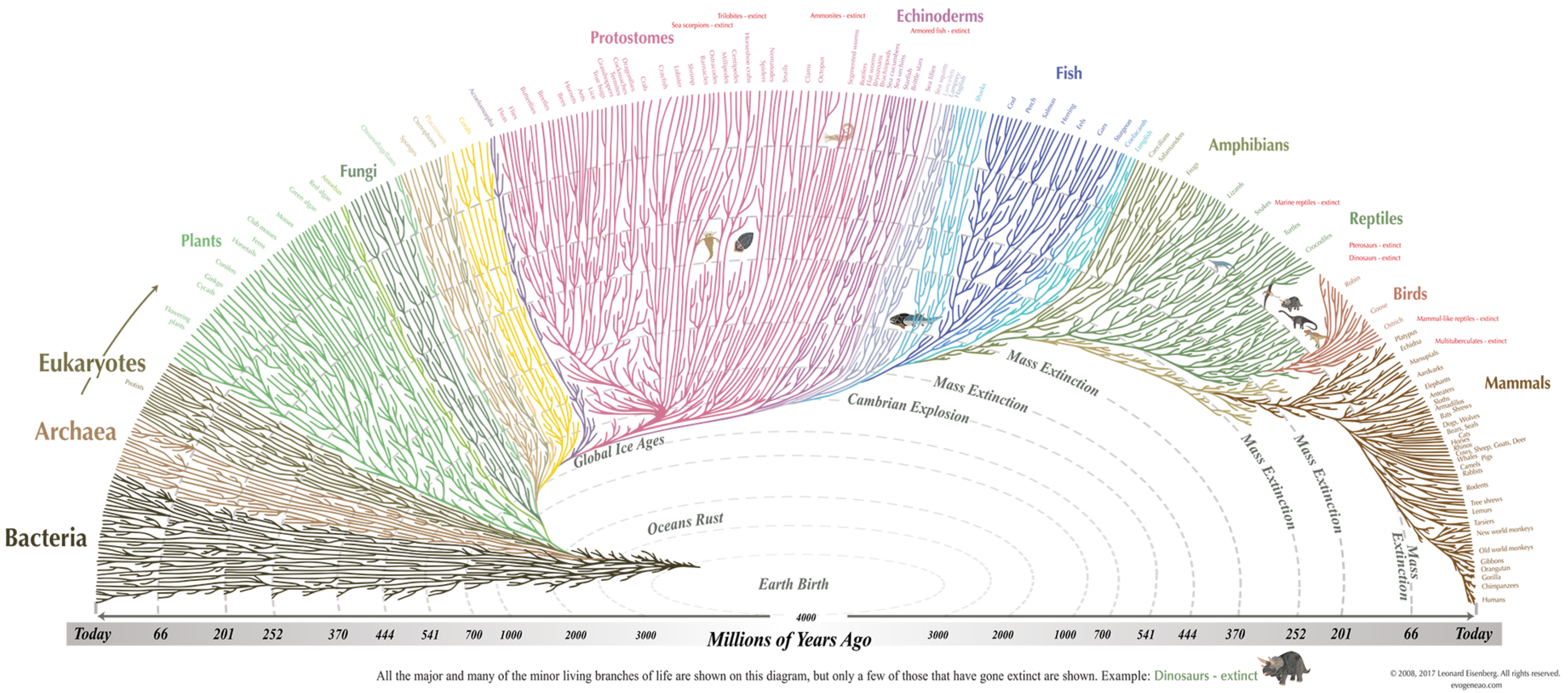


Tree of Life
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(2017)

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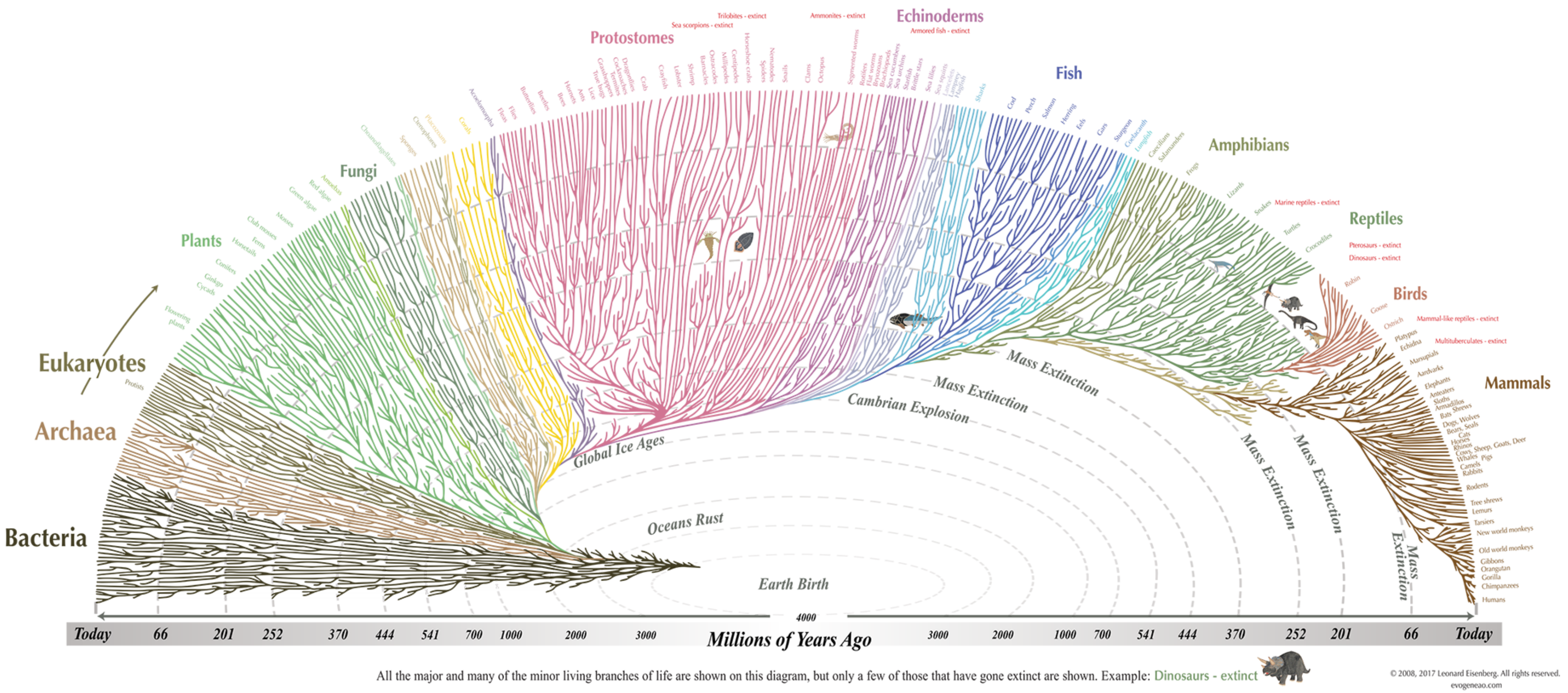


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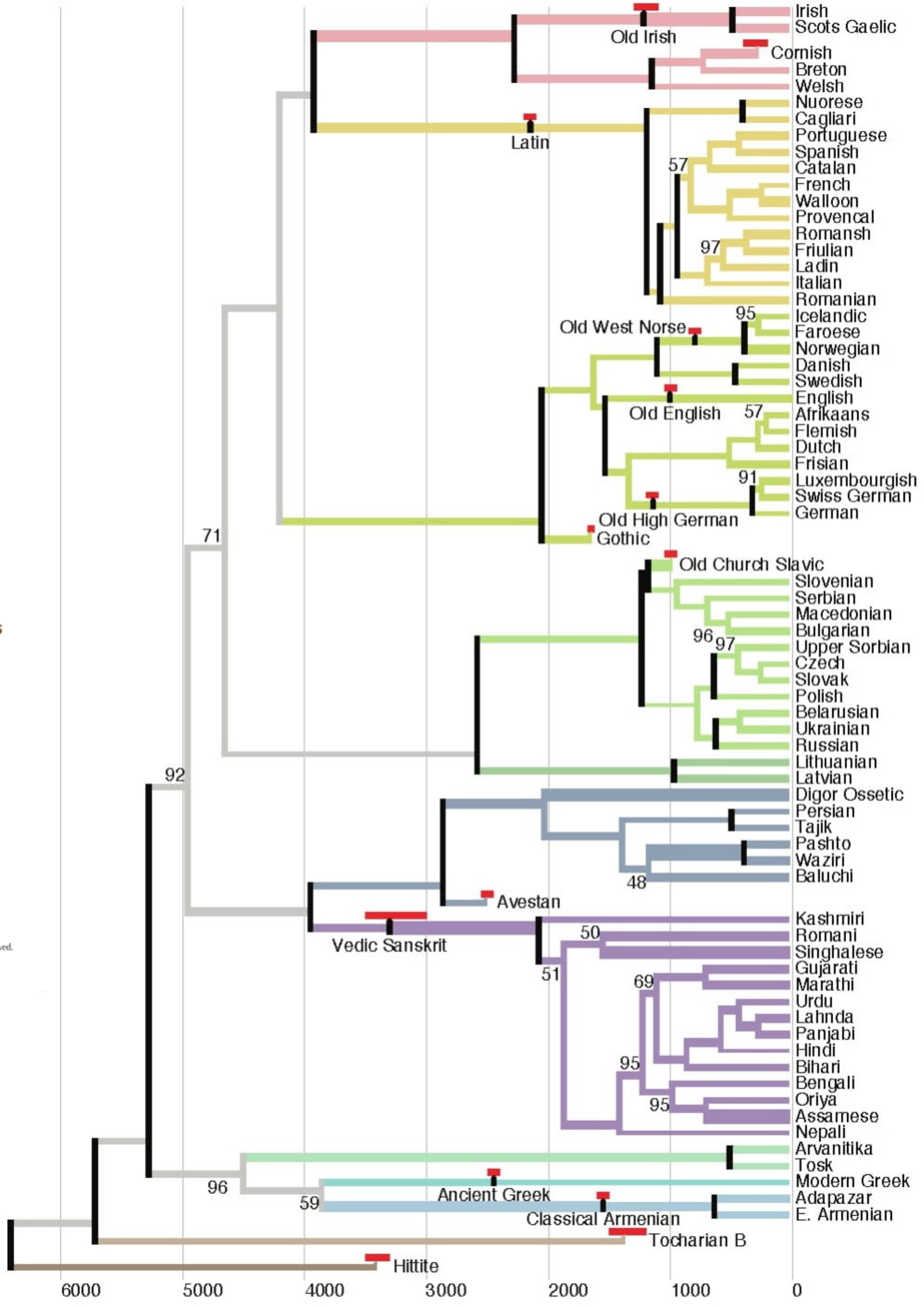


Phylogenetic tree of the Indo-European languages by Chang & Chundra (2015)

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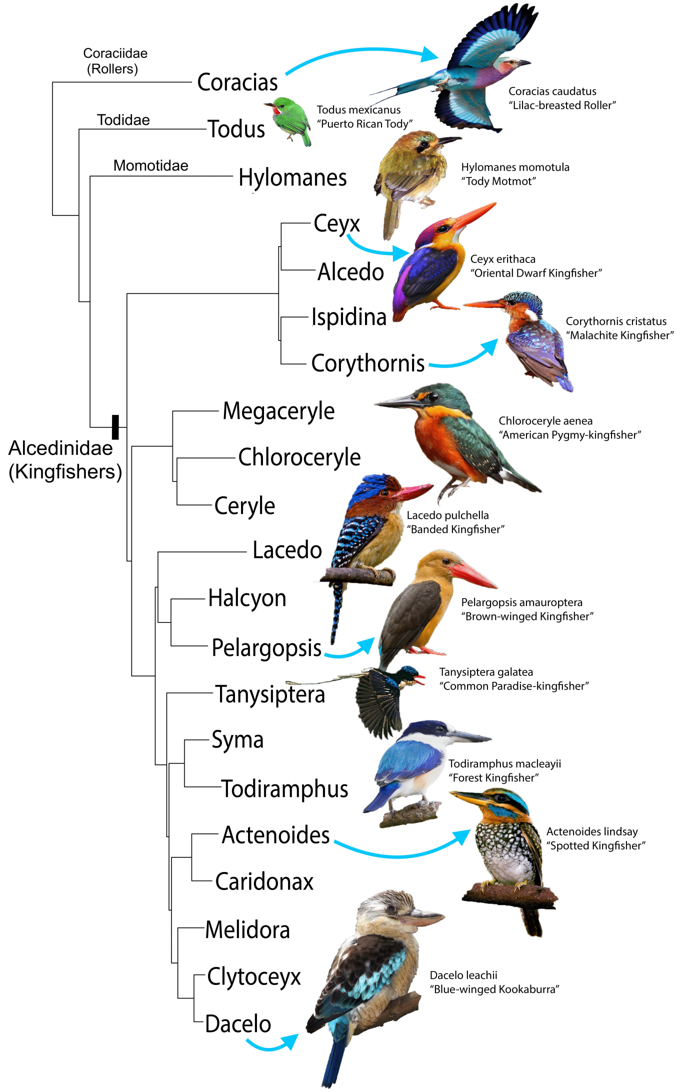


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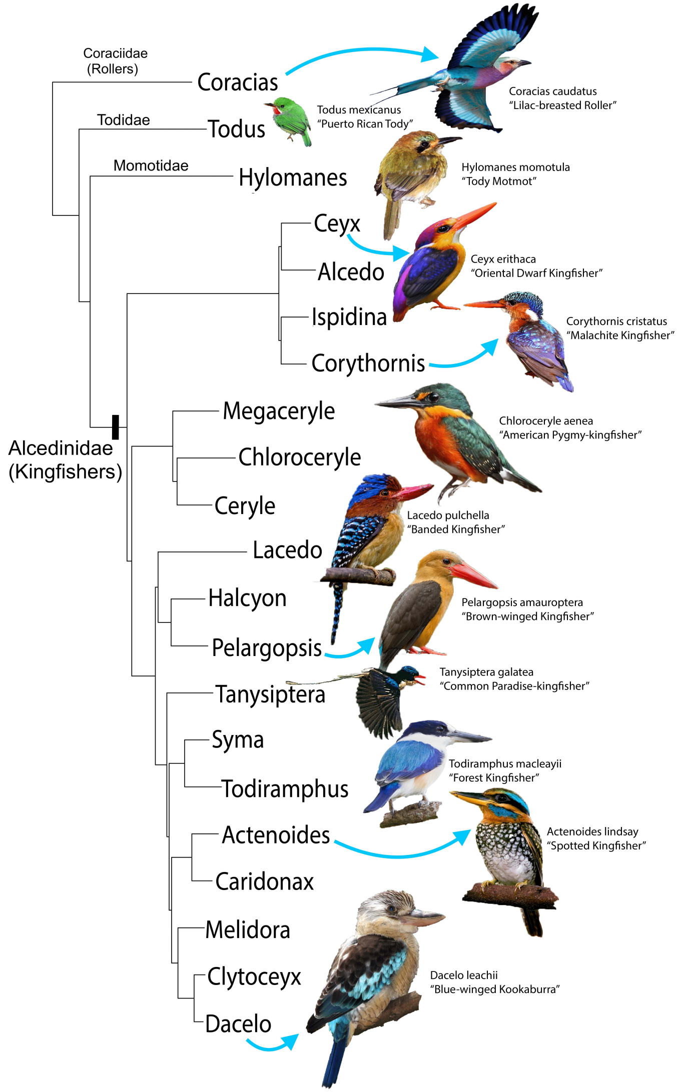


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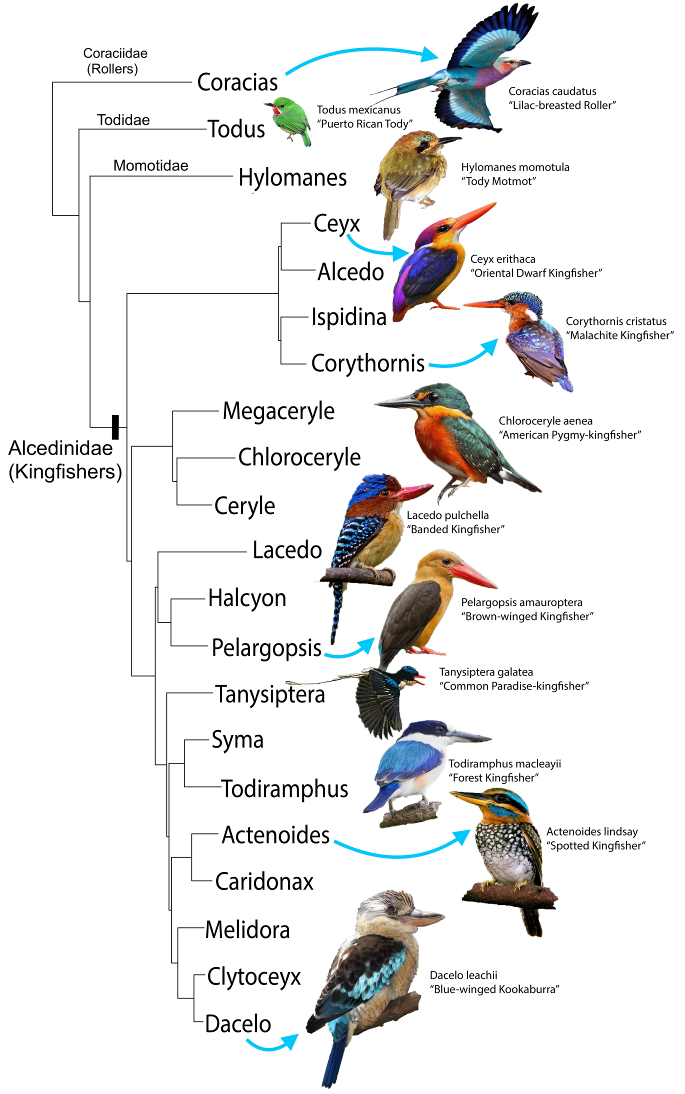


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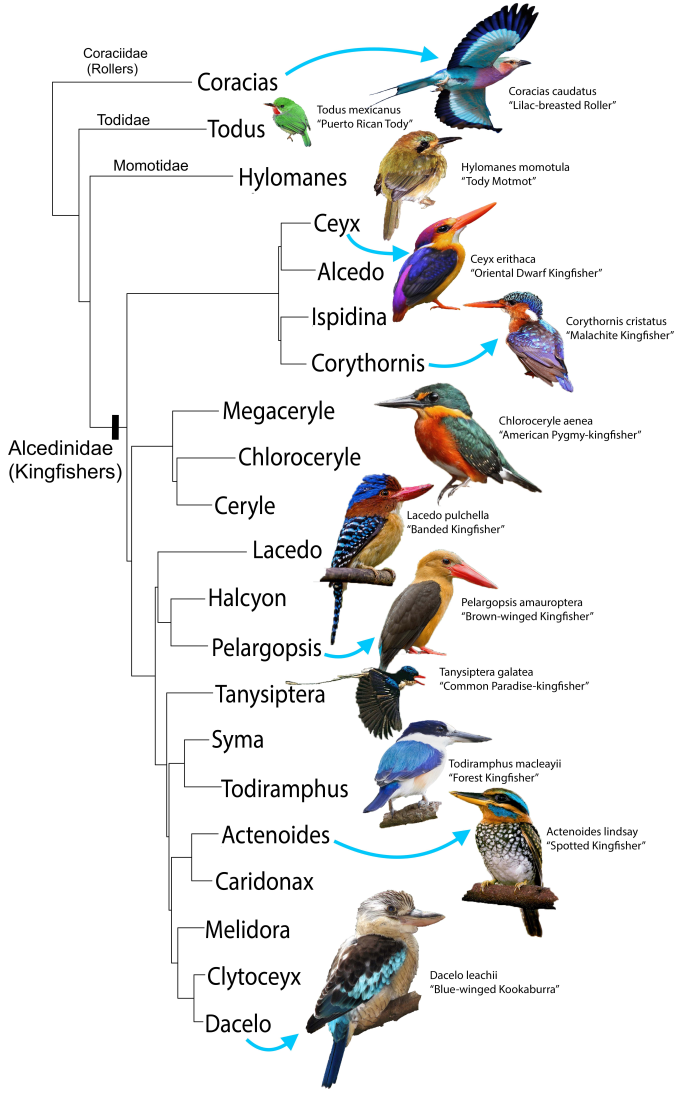


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- Edge length represents an amount of time passed or a genetic distance.
- Inference methods compute a phylogenetic tree based on some model and data.

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A **(rooted, binary) phylogenetic tree** $T$
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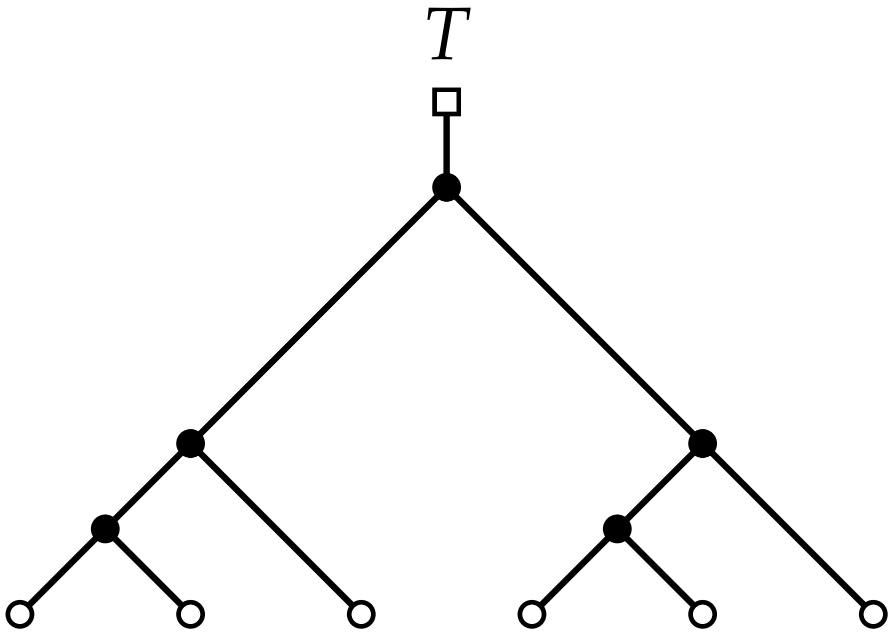

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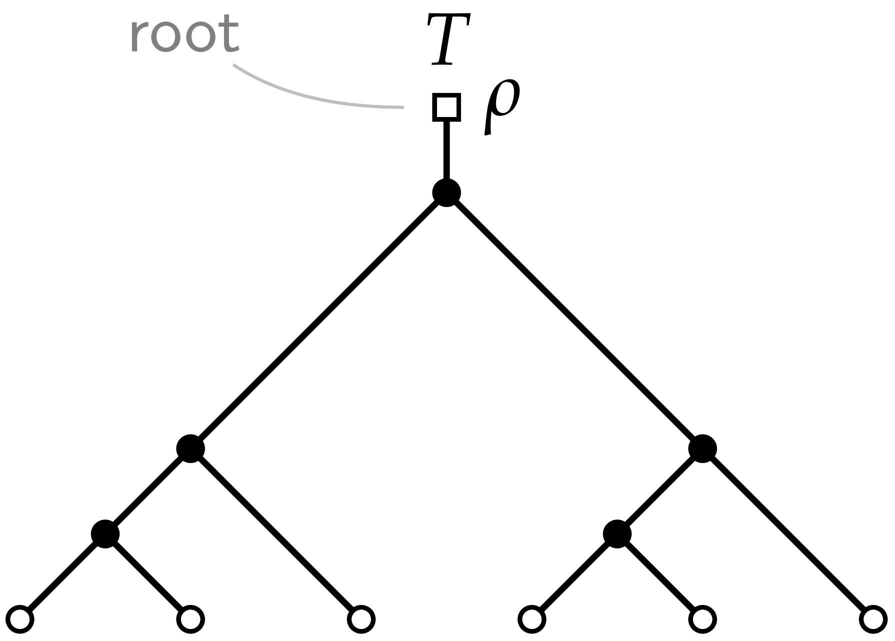

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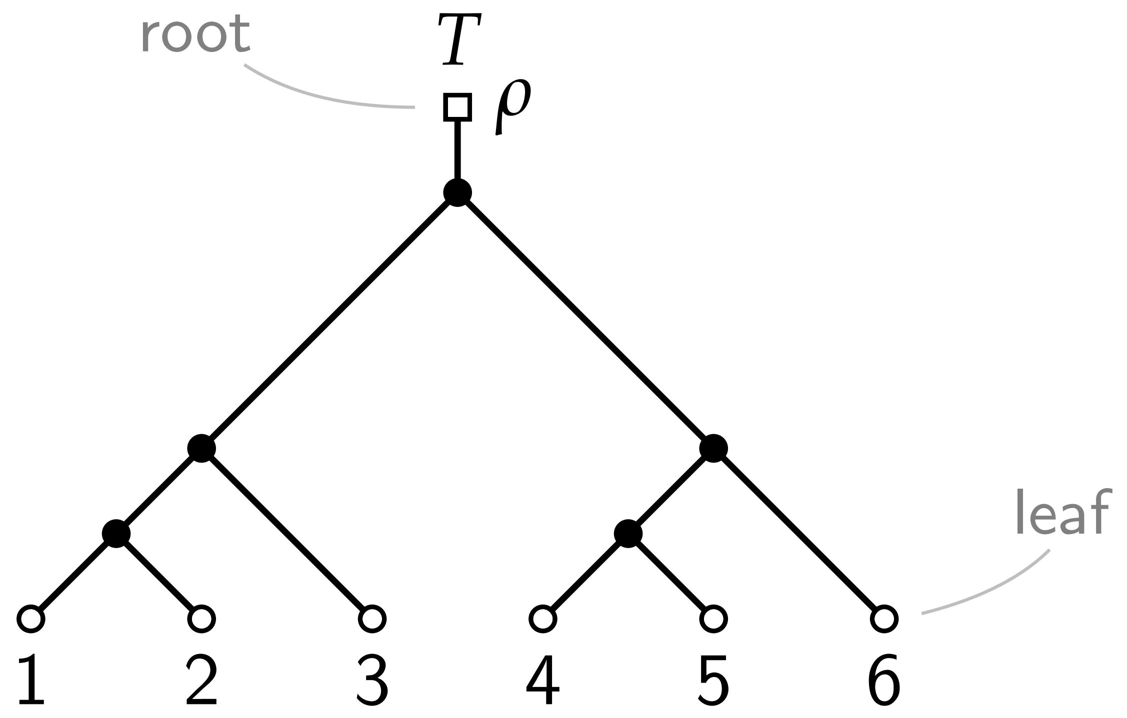

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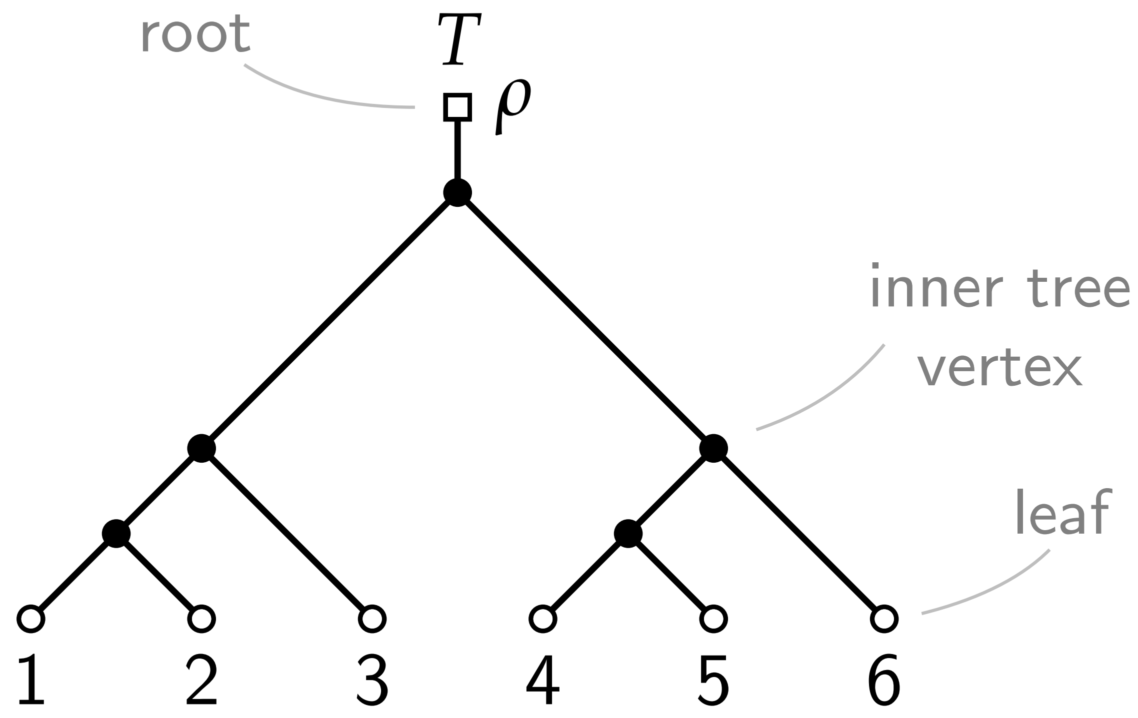

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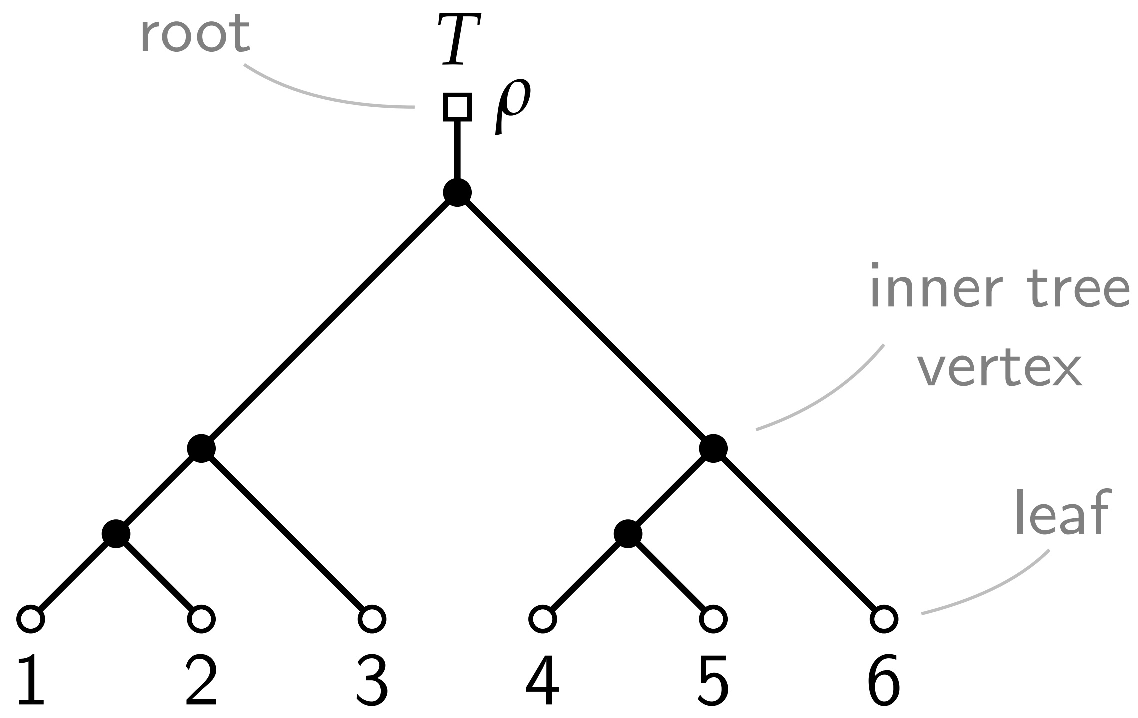
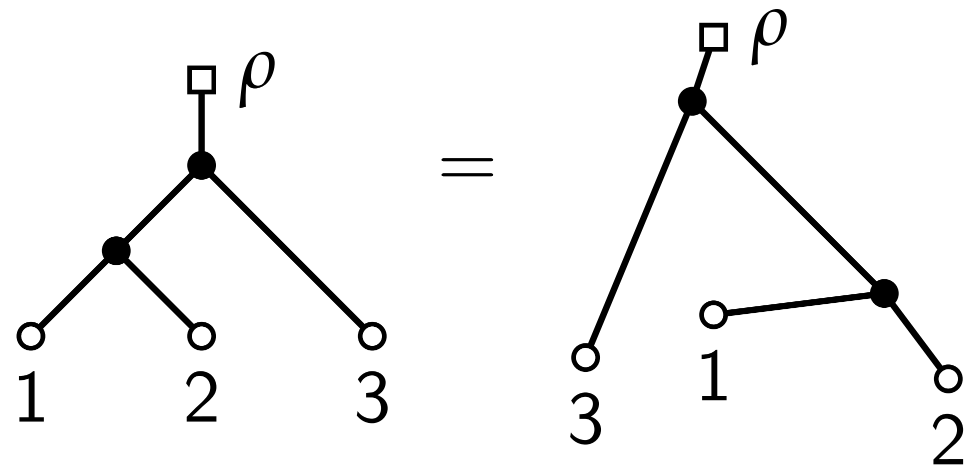
**Remarks.** Here, in our definition

- vertices have **no heights** and
- the order of the children of a vertex does not matter.



# Problem

For the same taxa, we may infer **different** phylogenetic trees because of the use of

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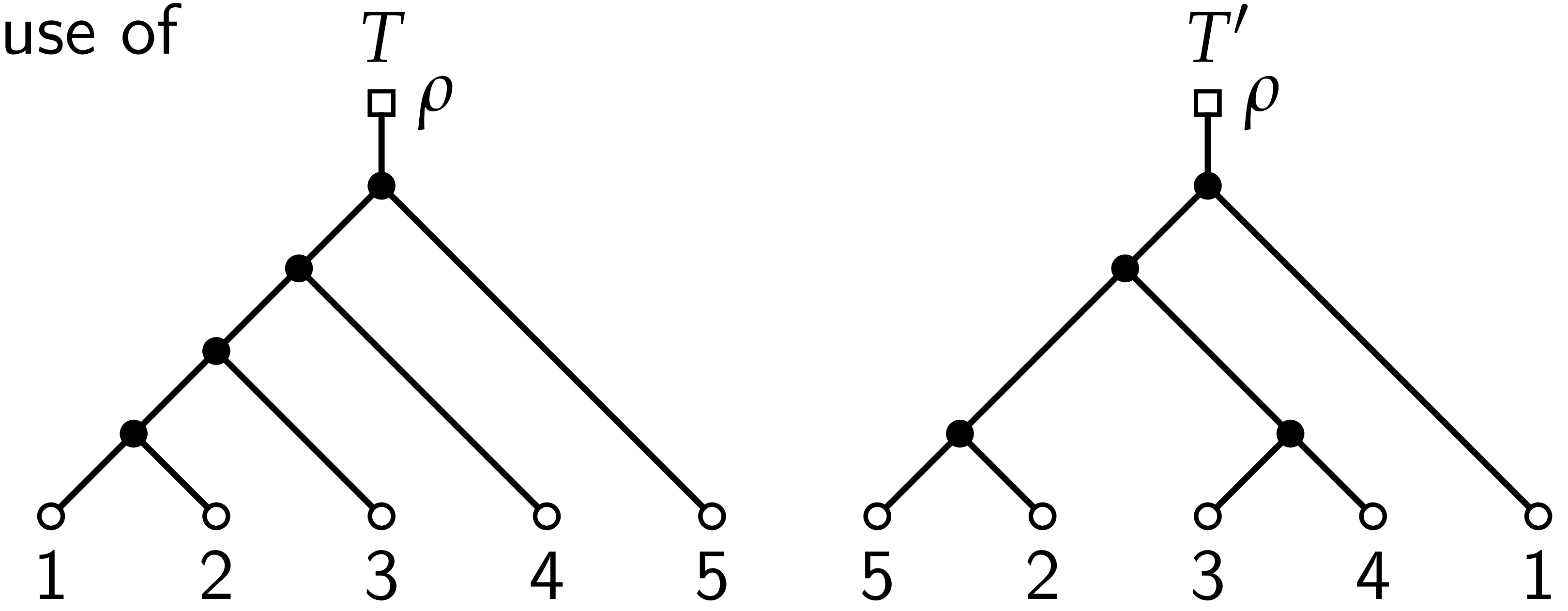

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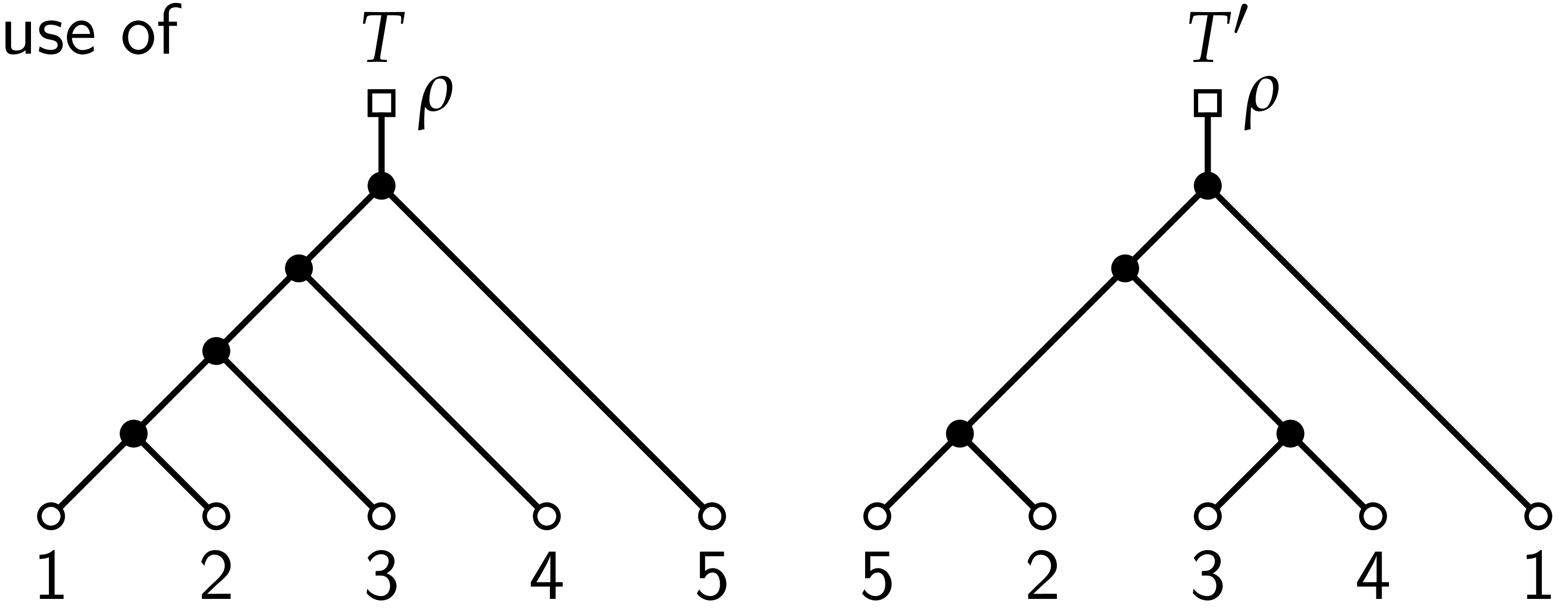

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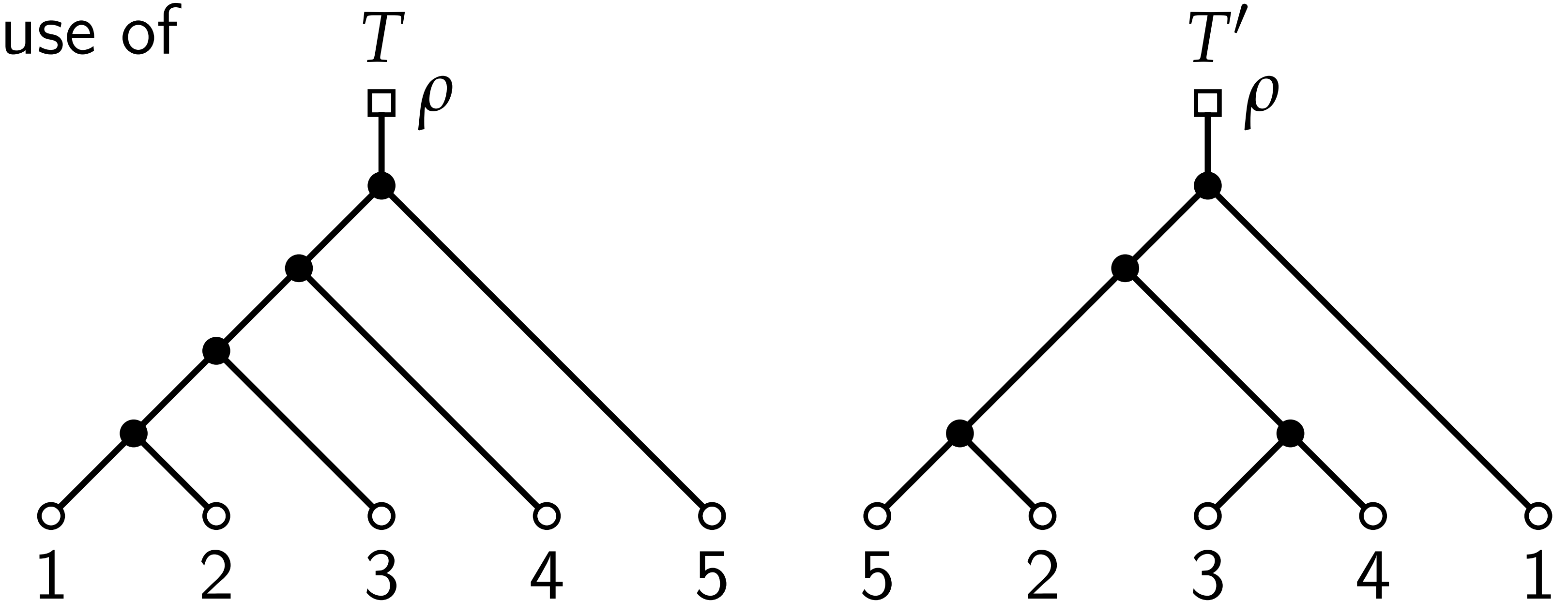


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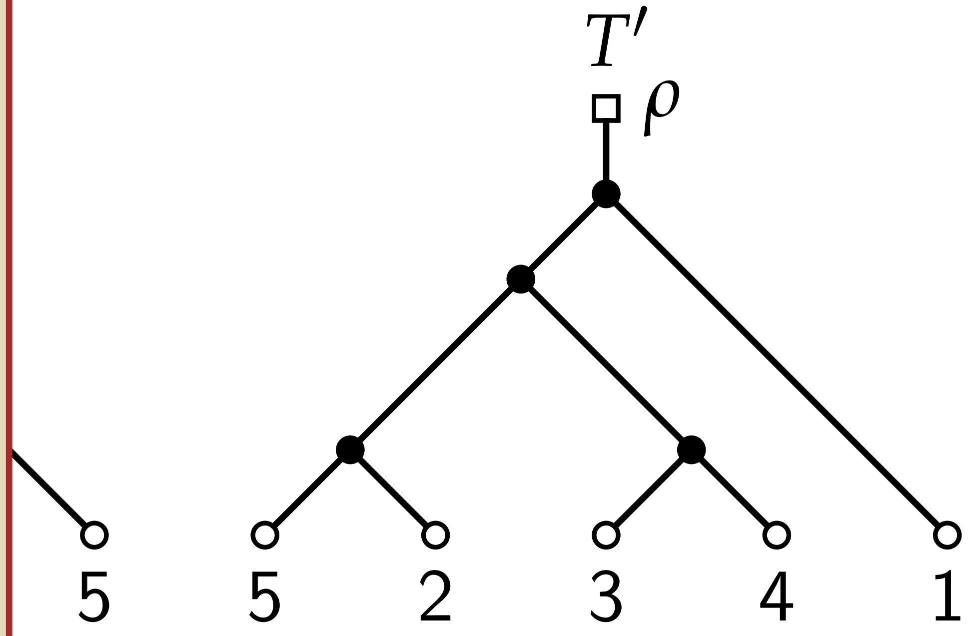


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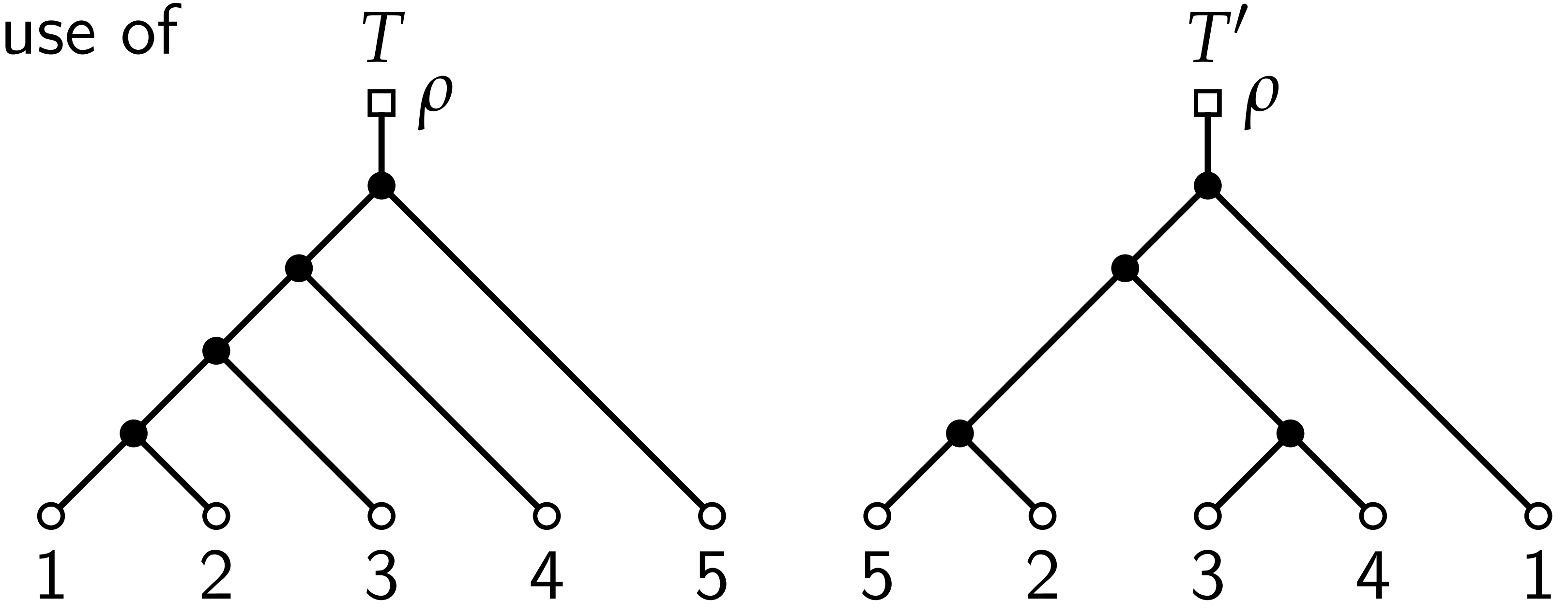


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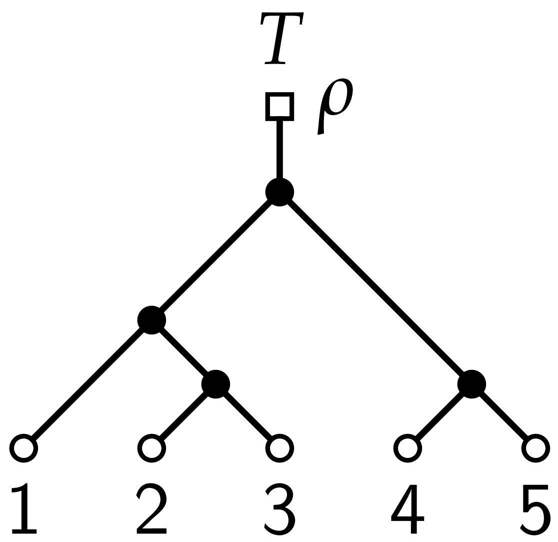
**Idea.**
Count the number of **rearrangement operations** that are necessary to transform $T$ into $T'$.

# Subtree Prune & Regraft (SPR)

An **SPR** operation transforms one phylogenetic tree into another one.



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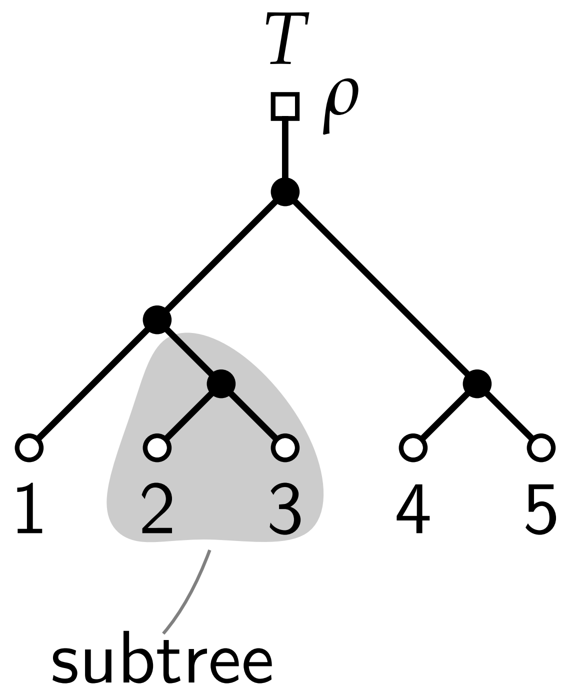

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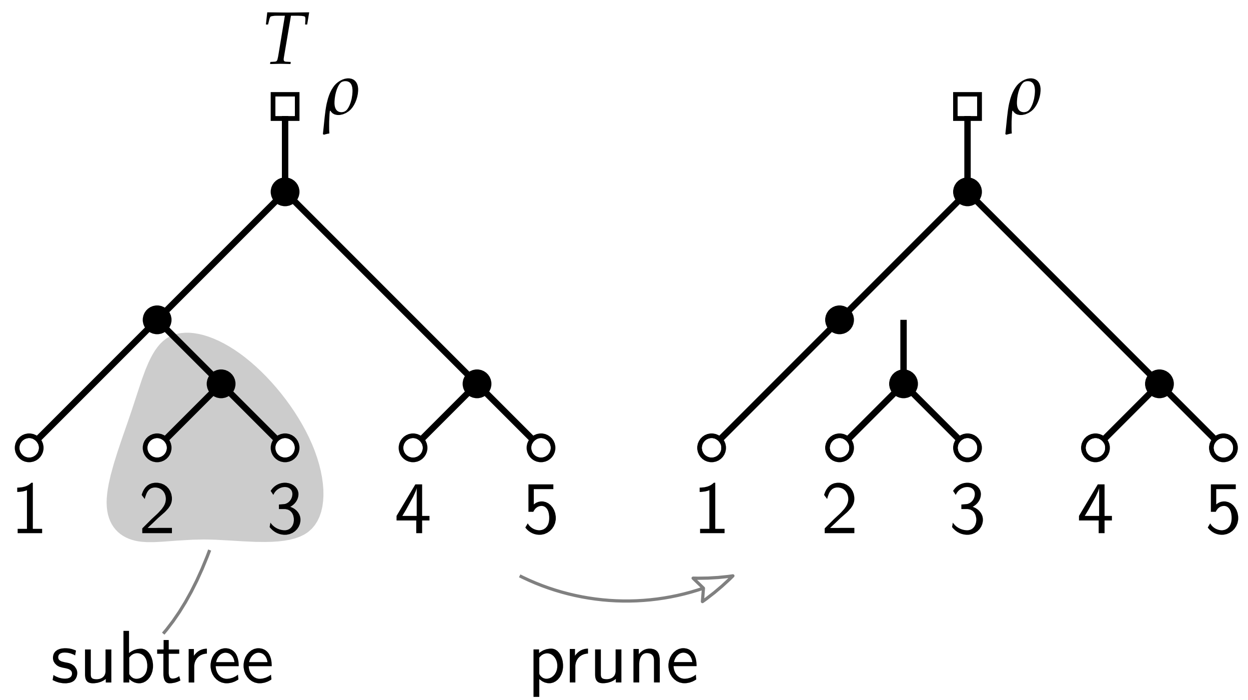

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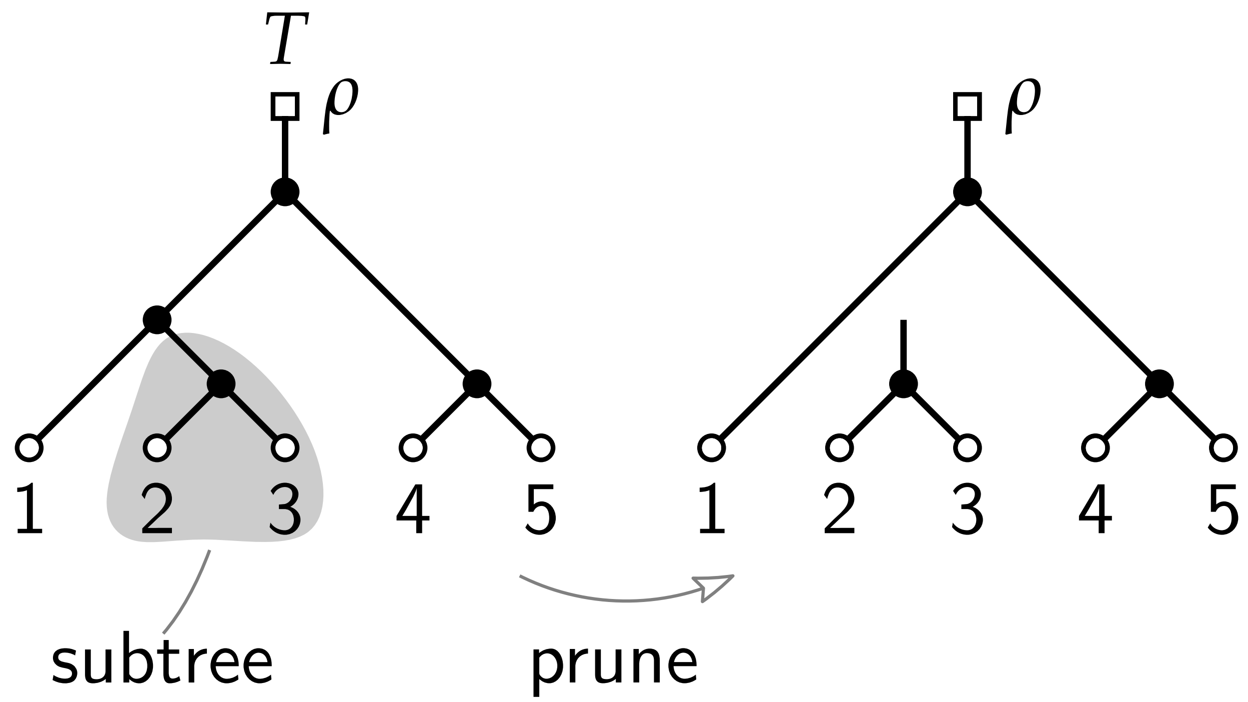

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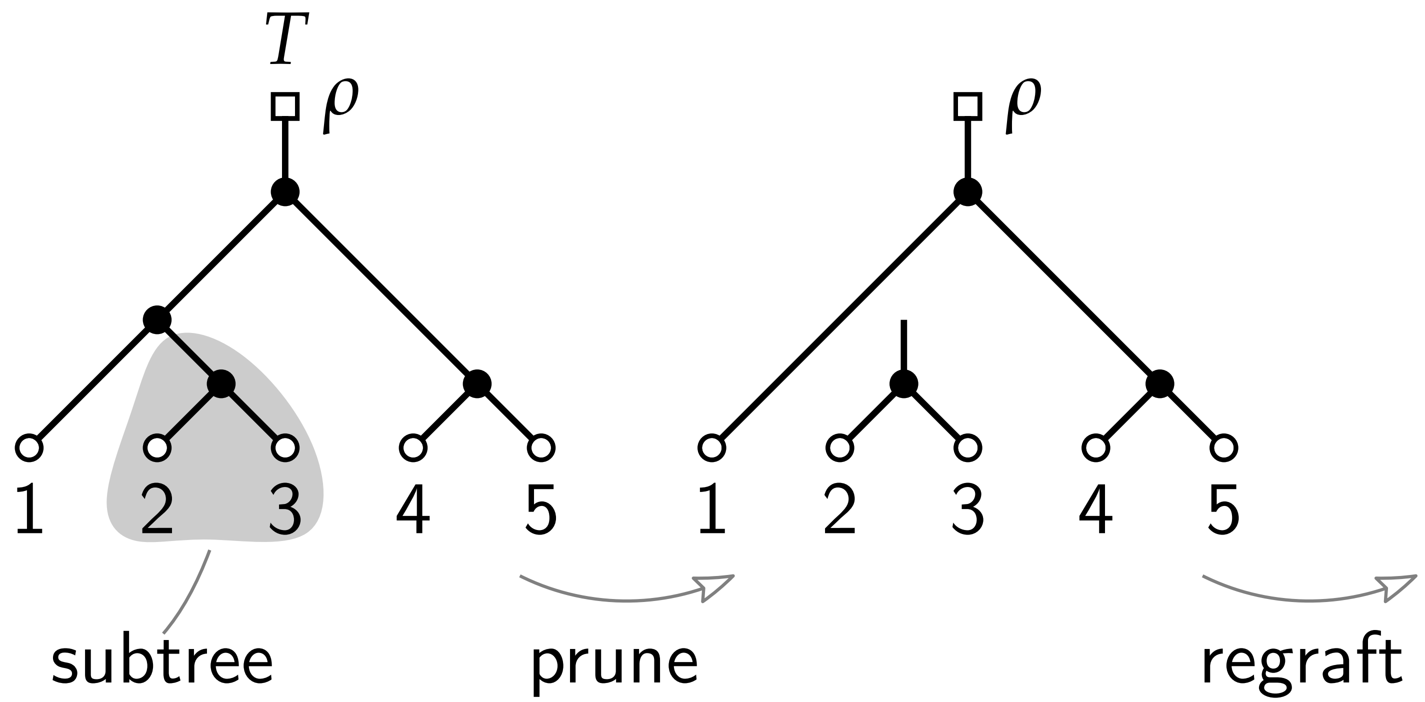

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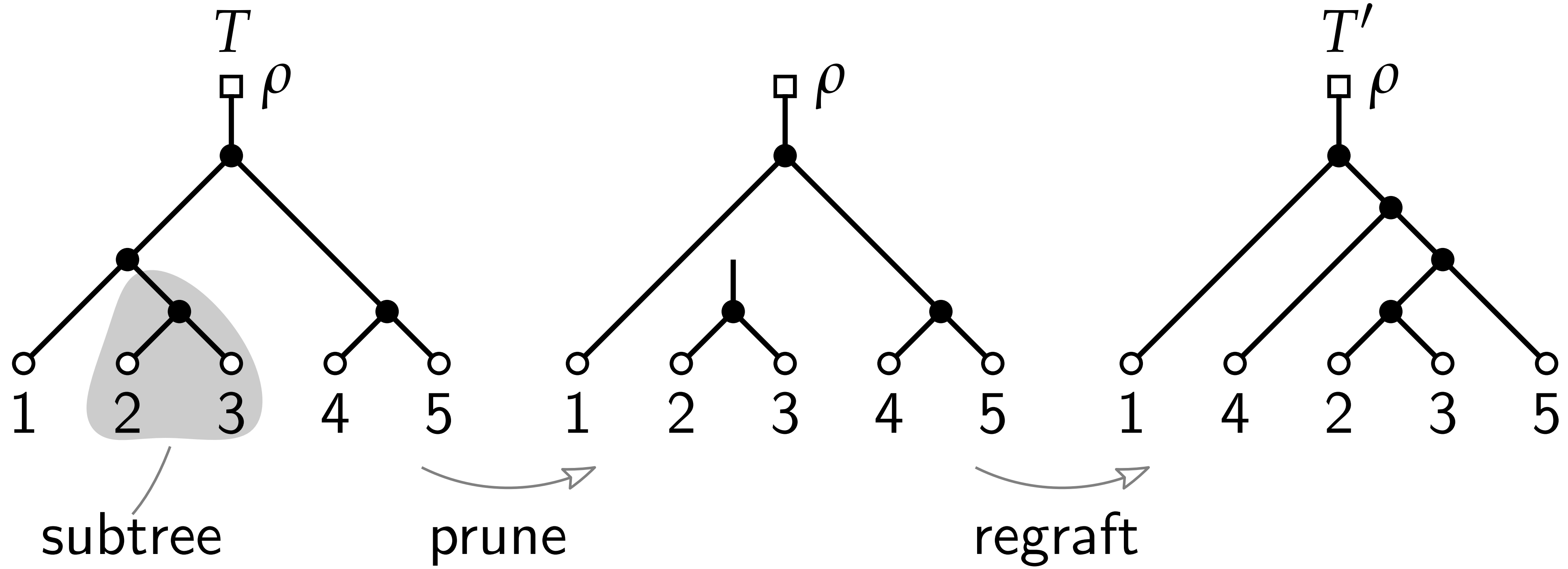

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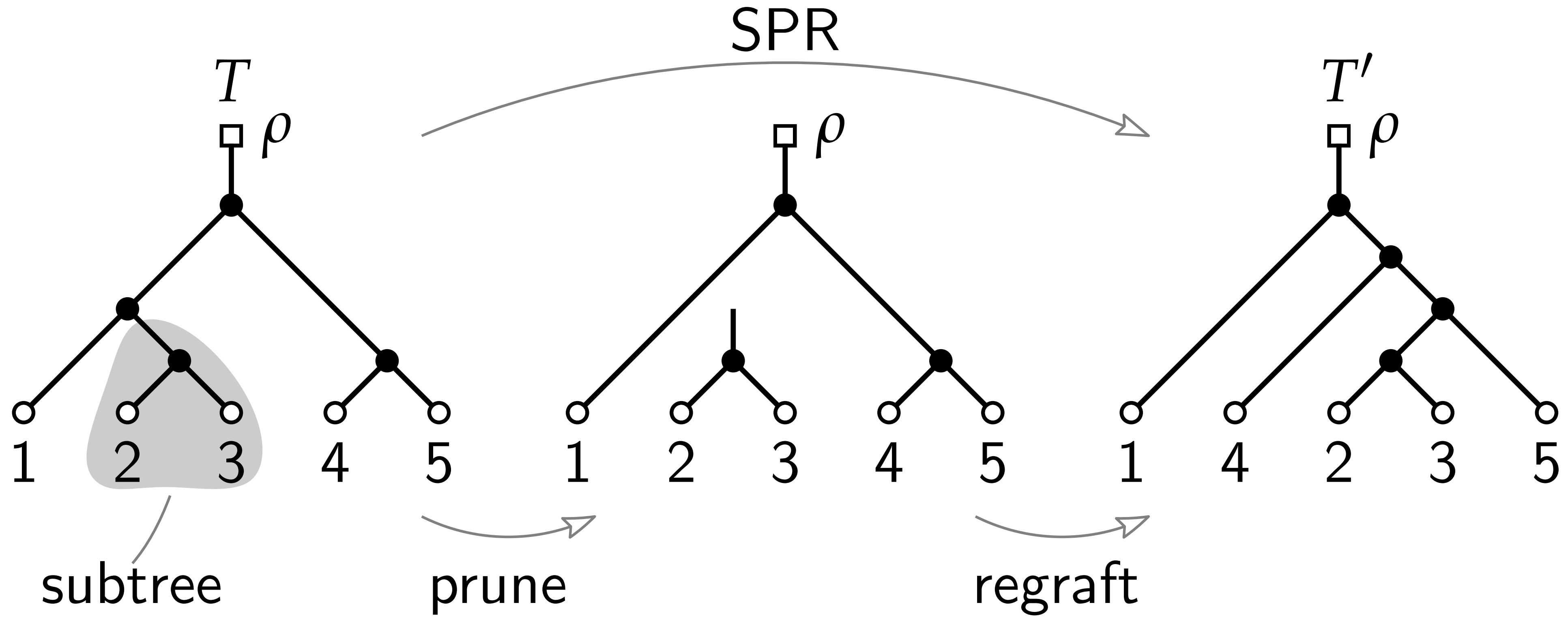

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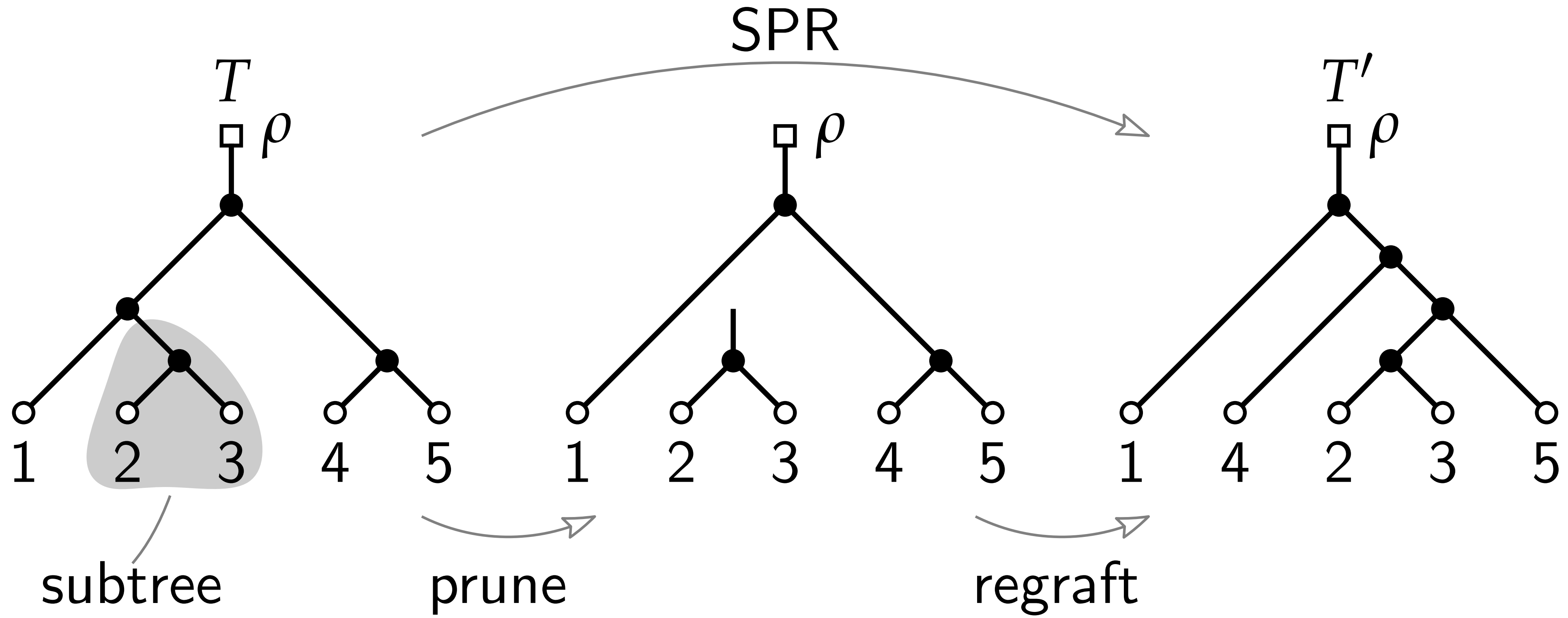


- Note that an SPR operation is reversible.

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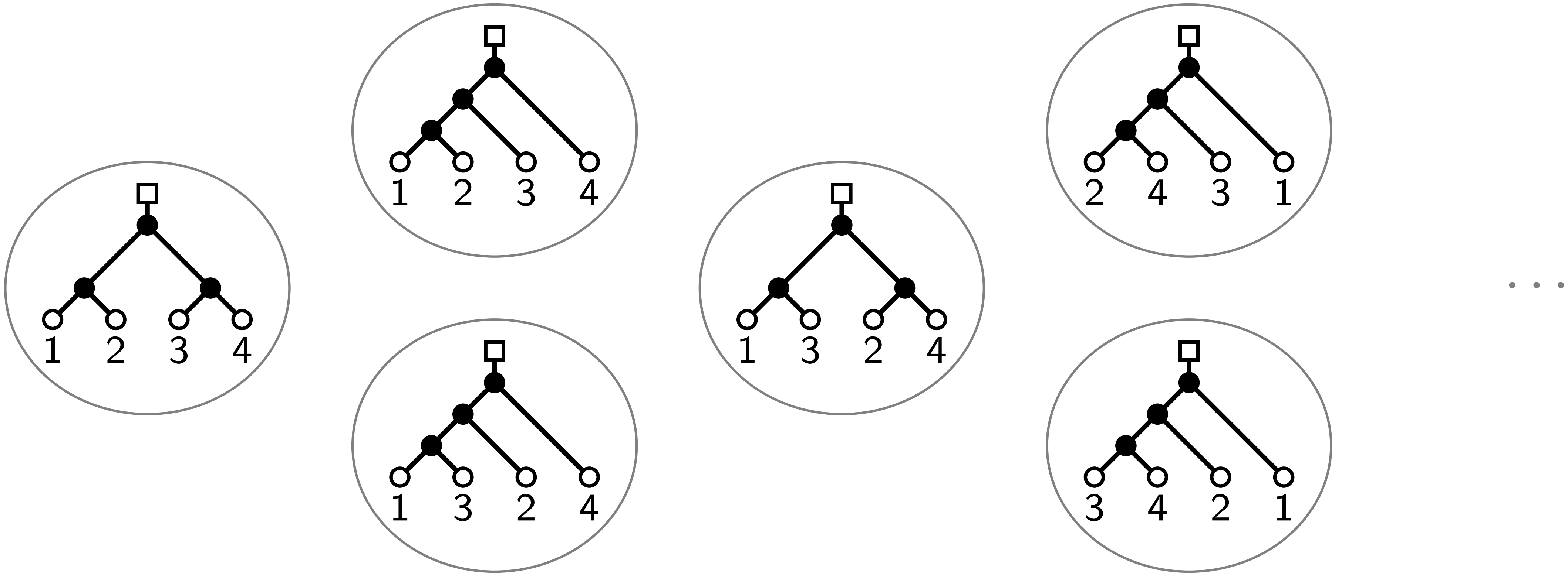

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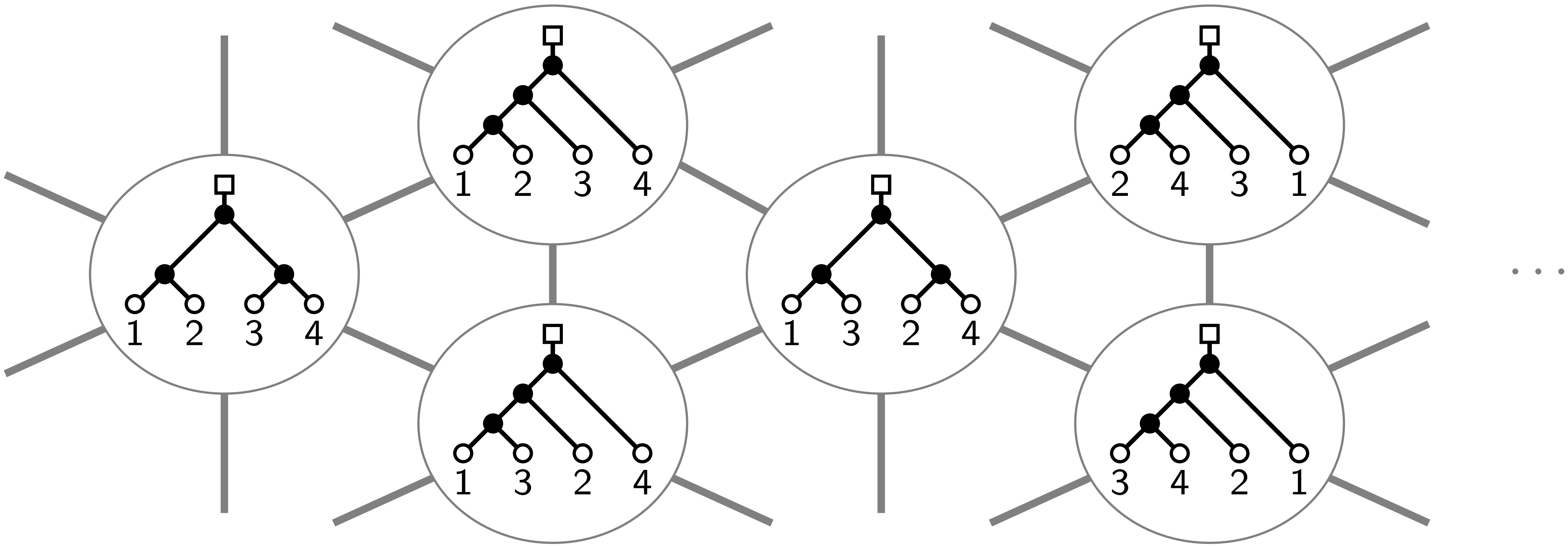
- $V = \{T \mid T$ is a phylogenetic tree on X$\}$
- $E = \{\{T, T'\} \mid T$ can be transformed into $T'$ with a single SPR operation$\}$



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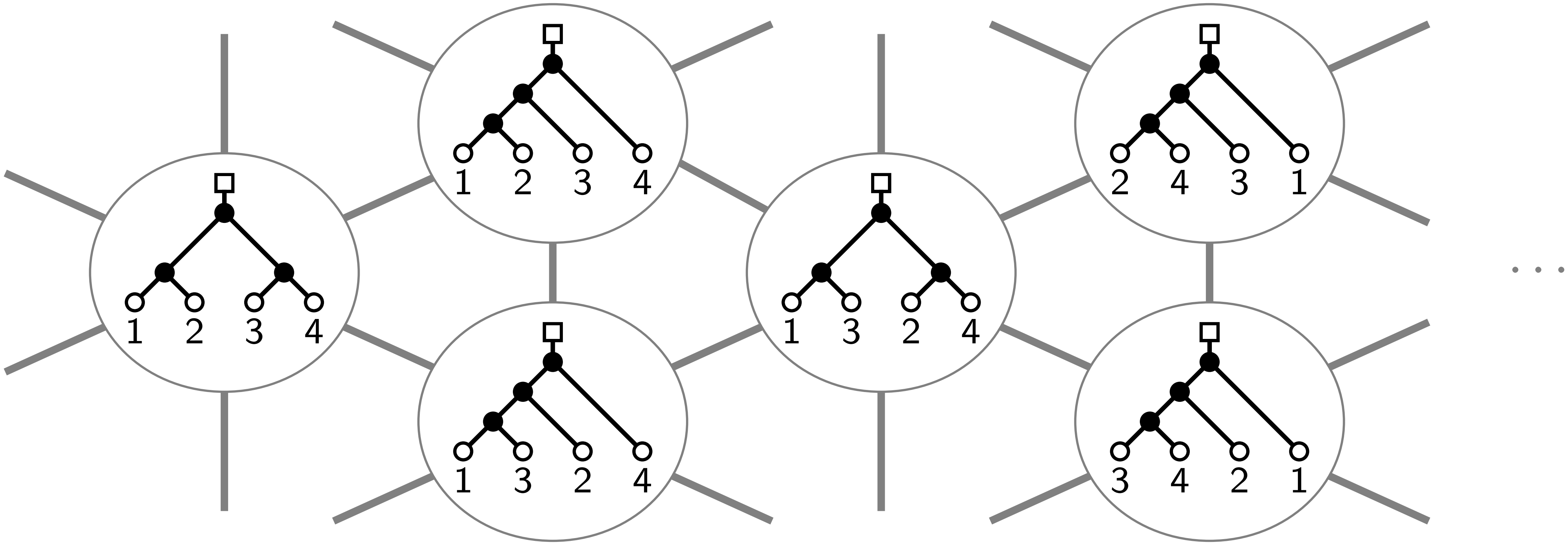

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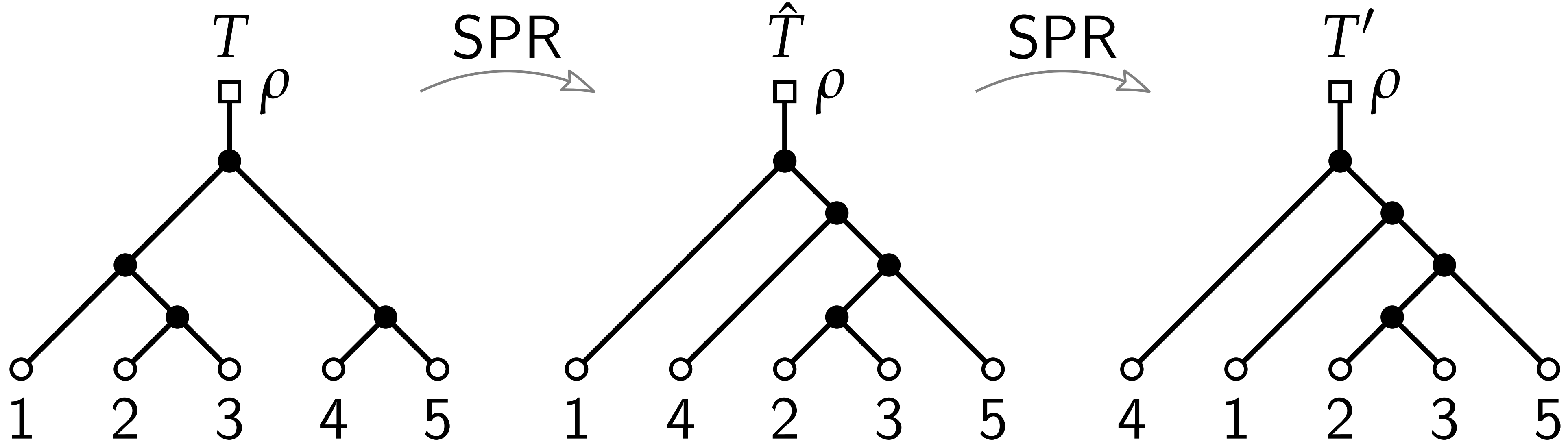
- Can we rephrase the problem?

# Maximum Agreement Forests



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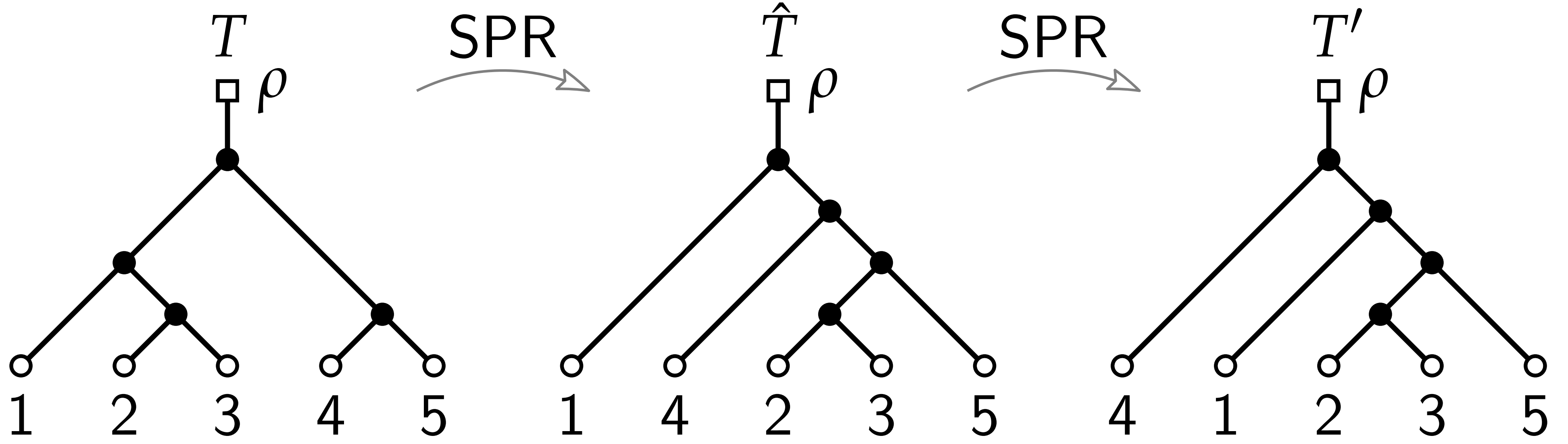


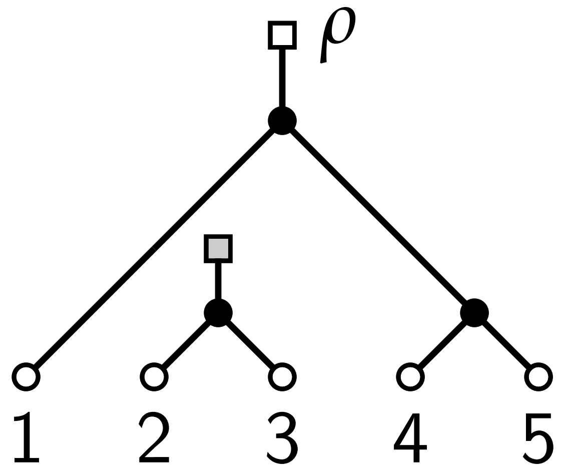

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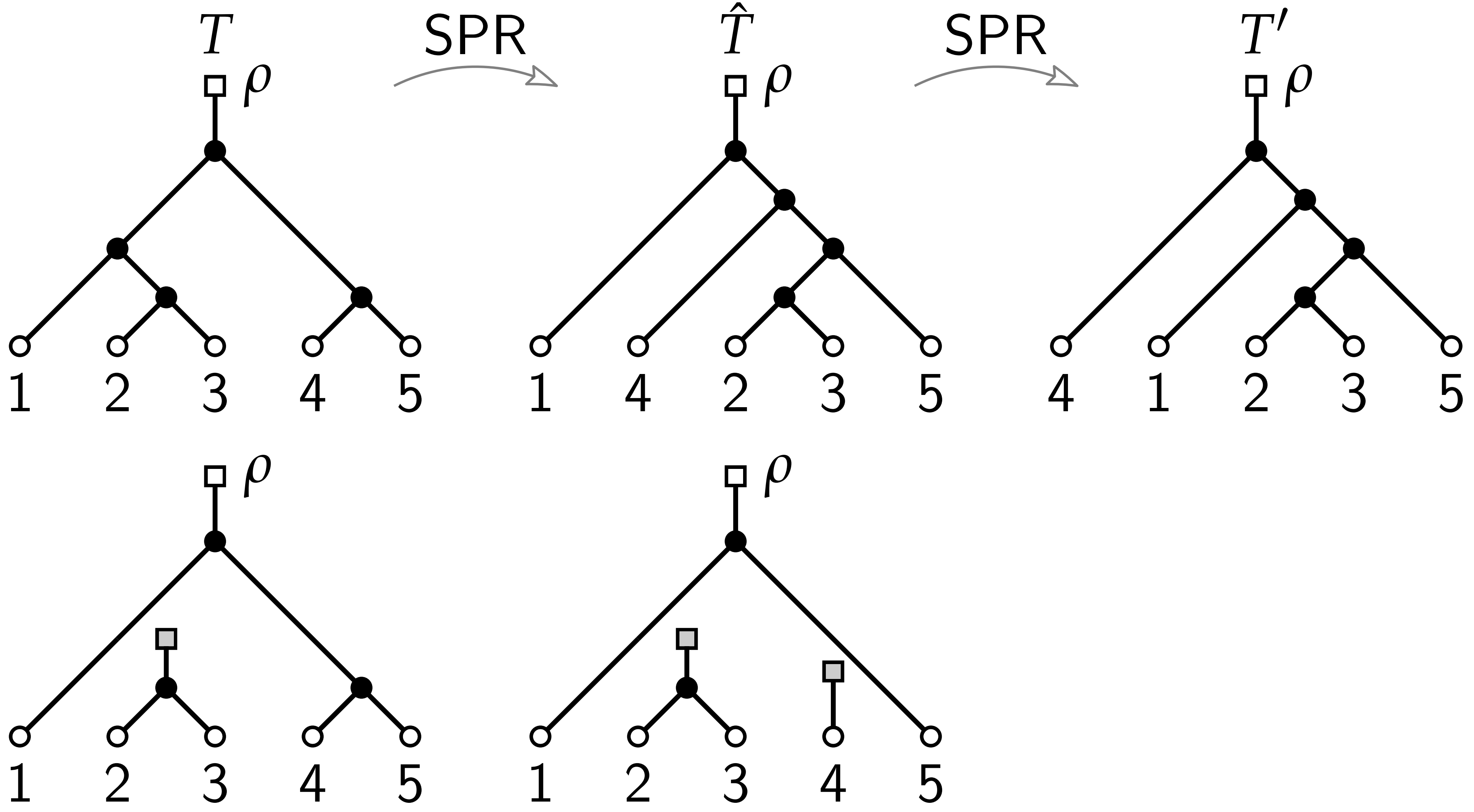

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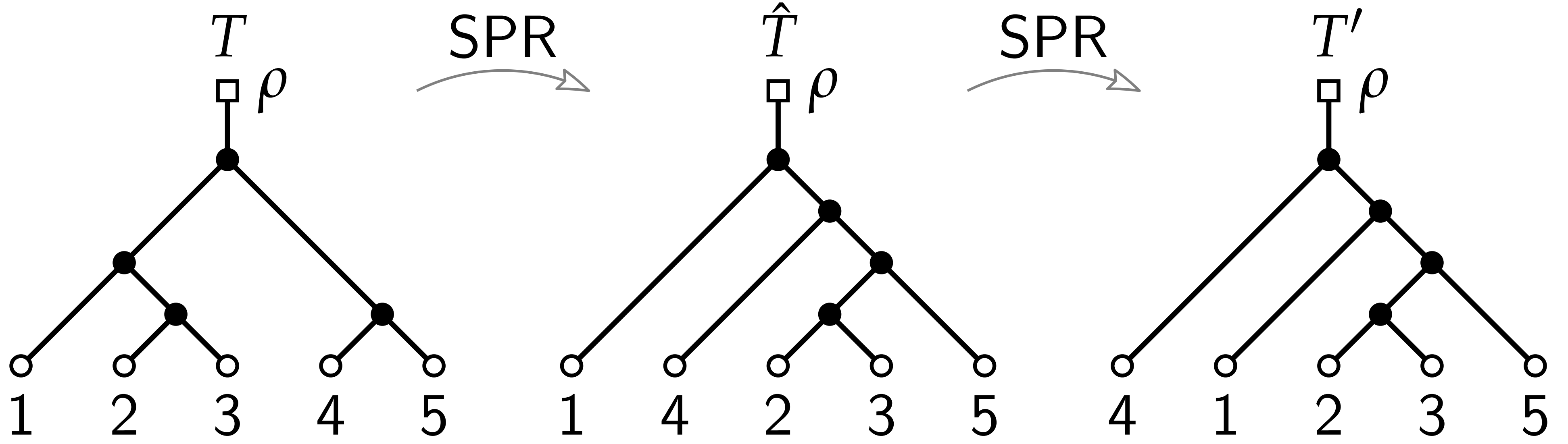


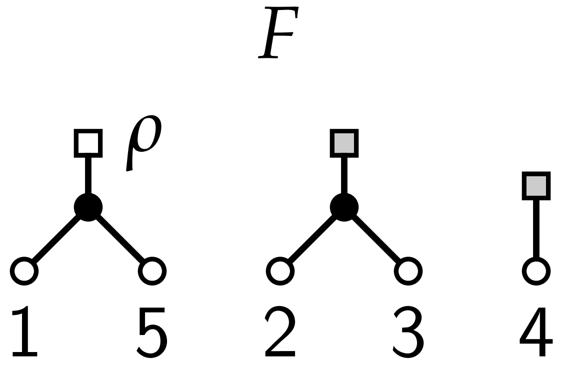

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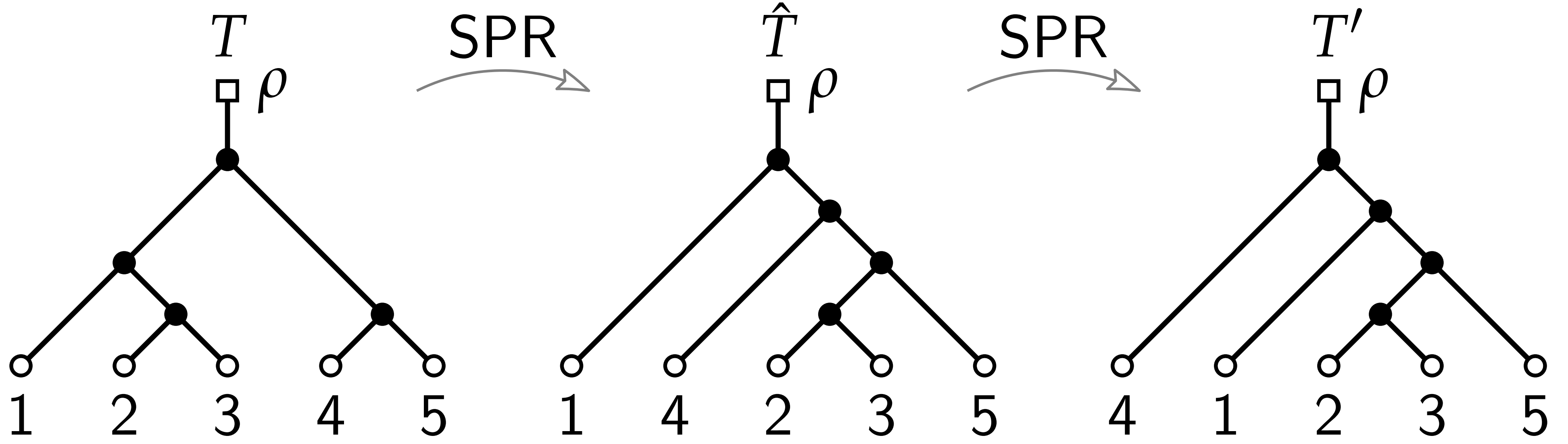


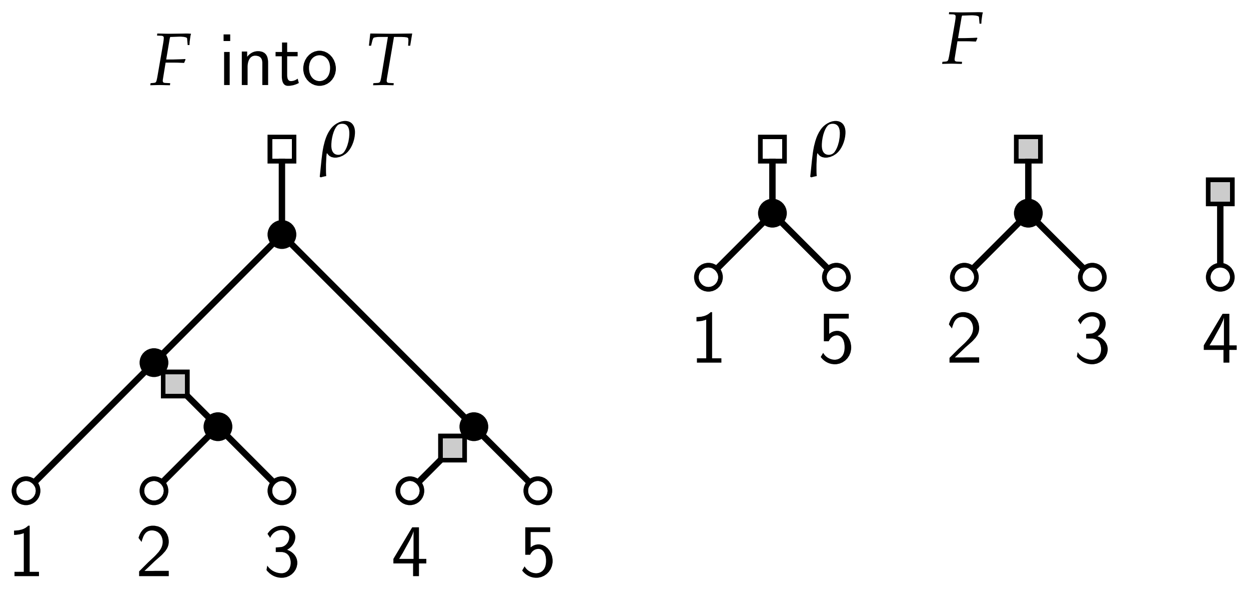

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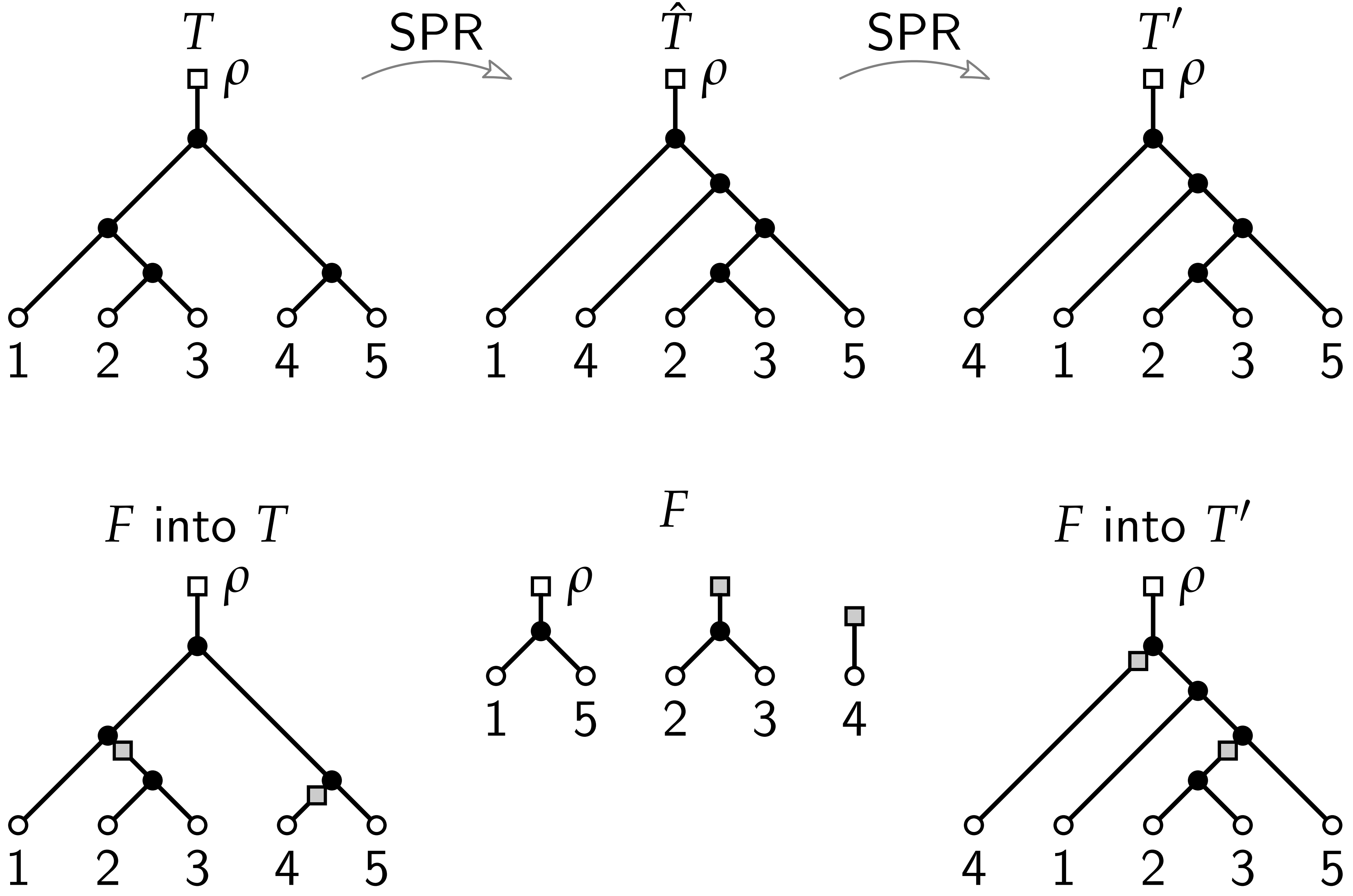

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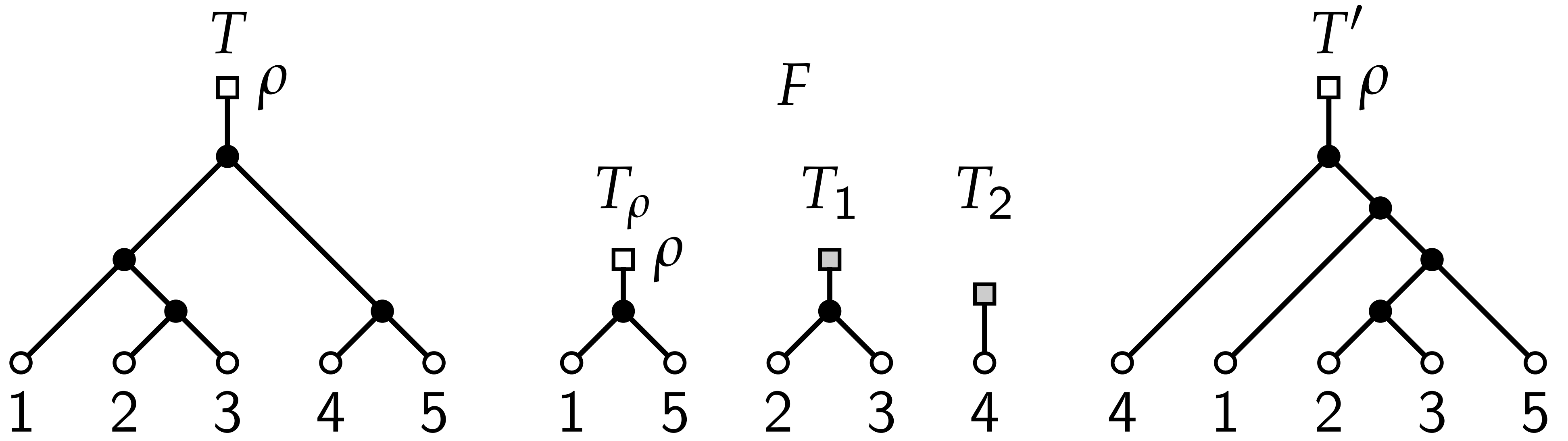


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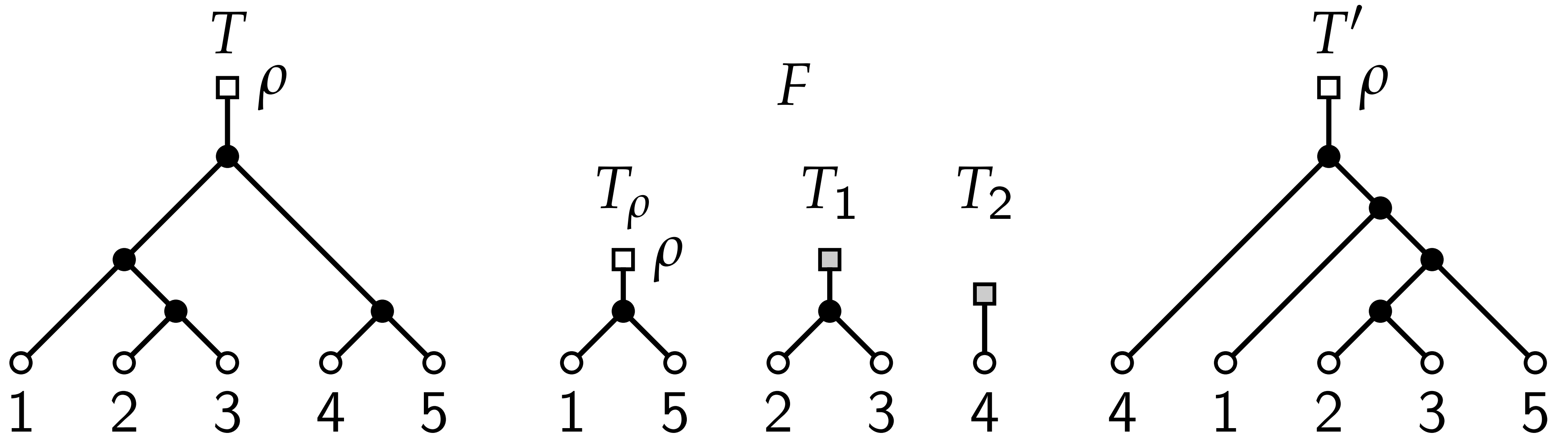


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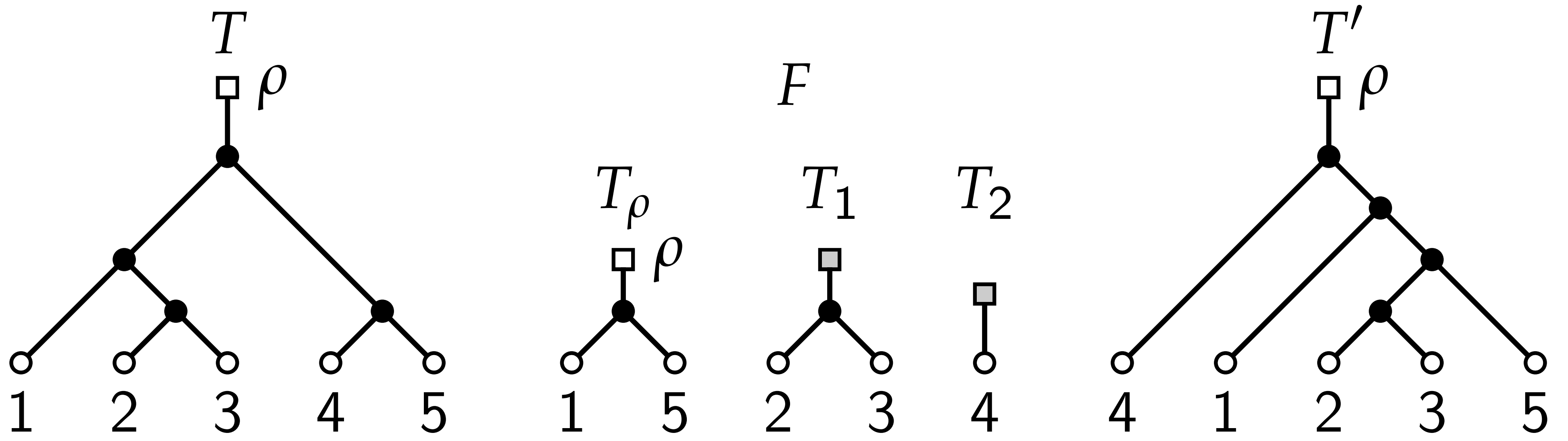


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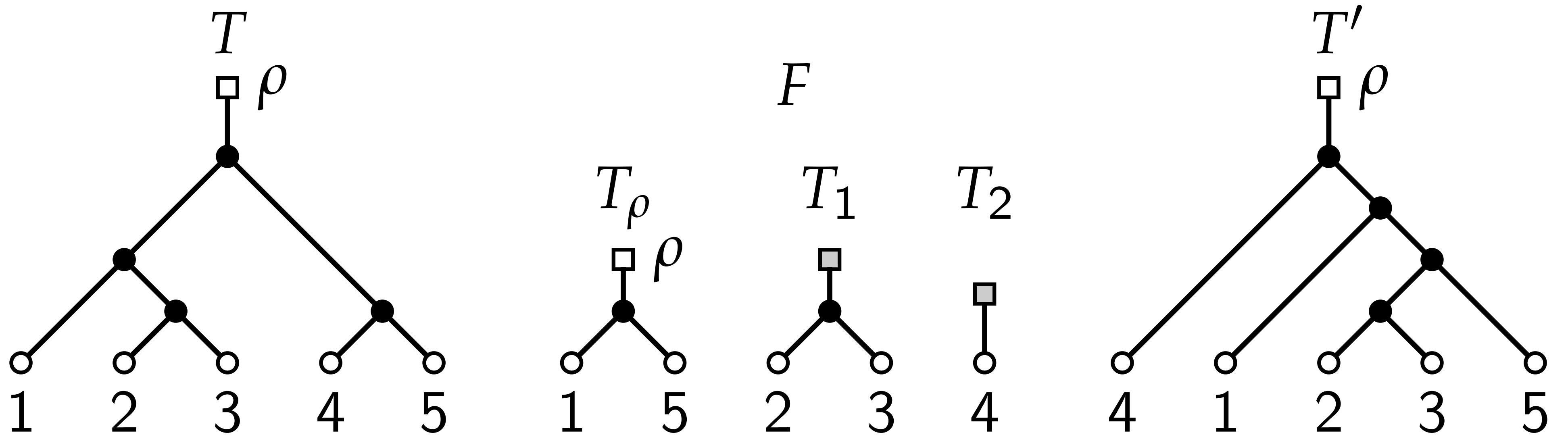


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If $k$ is minimum, $F$ is a **maximum agreement forest (MAF)**.

# Characterization

Let $T$ and $T'$ be two phylogenetic trees on $X$ and let $F = \{T_\rho, T_1, T_2, \ldots, T_k\}$ be a MAF of $T$ and $T'$.
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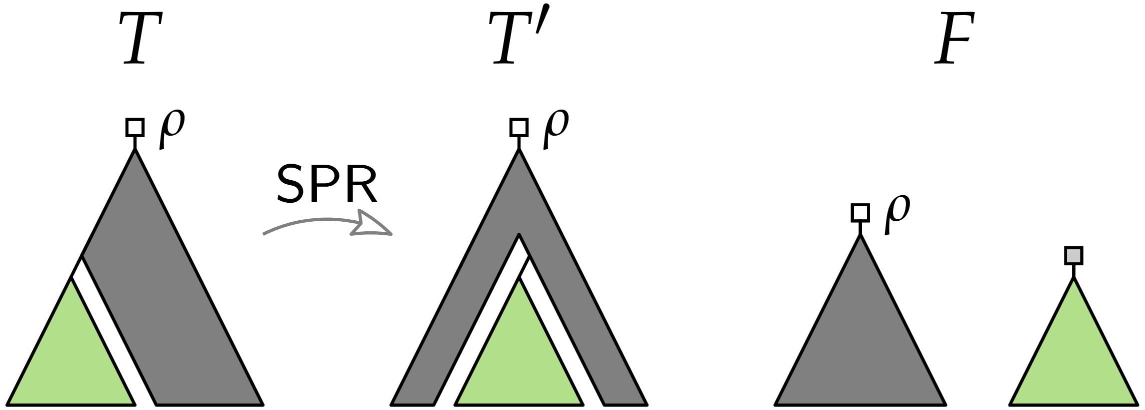

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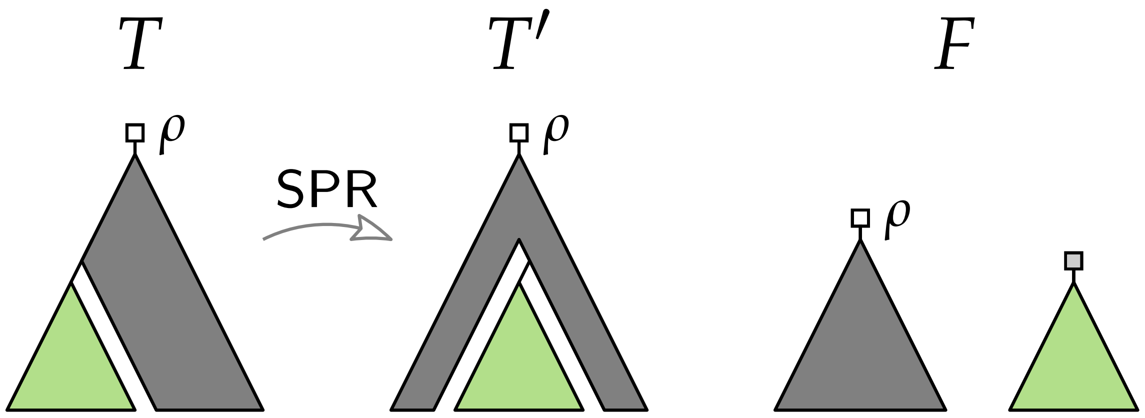

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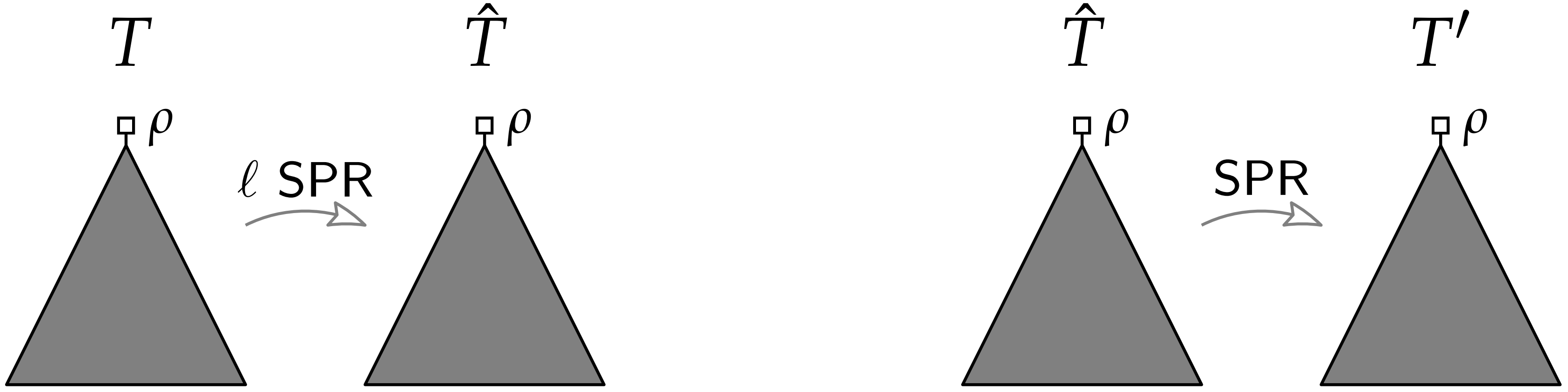

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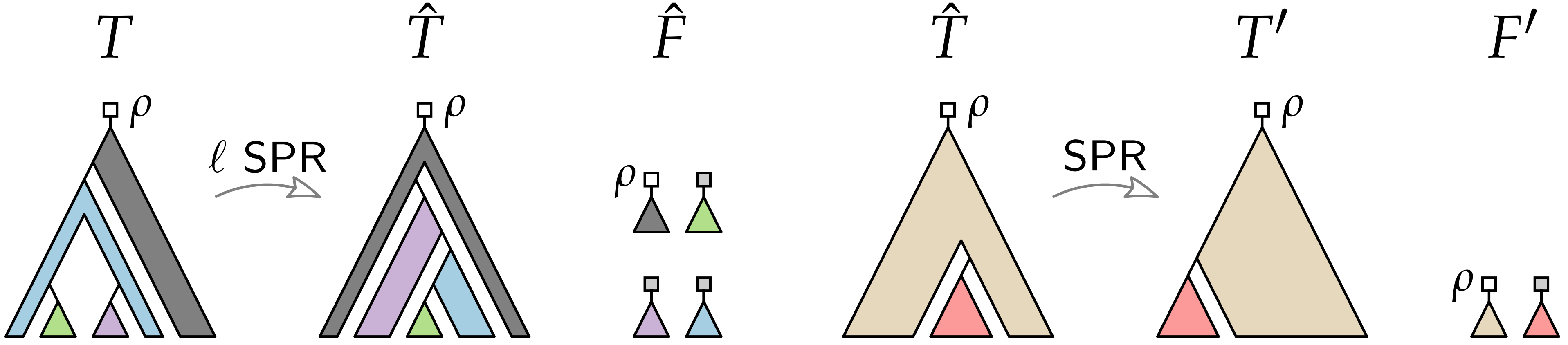

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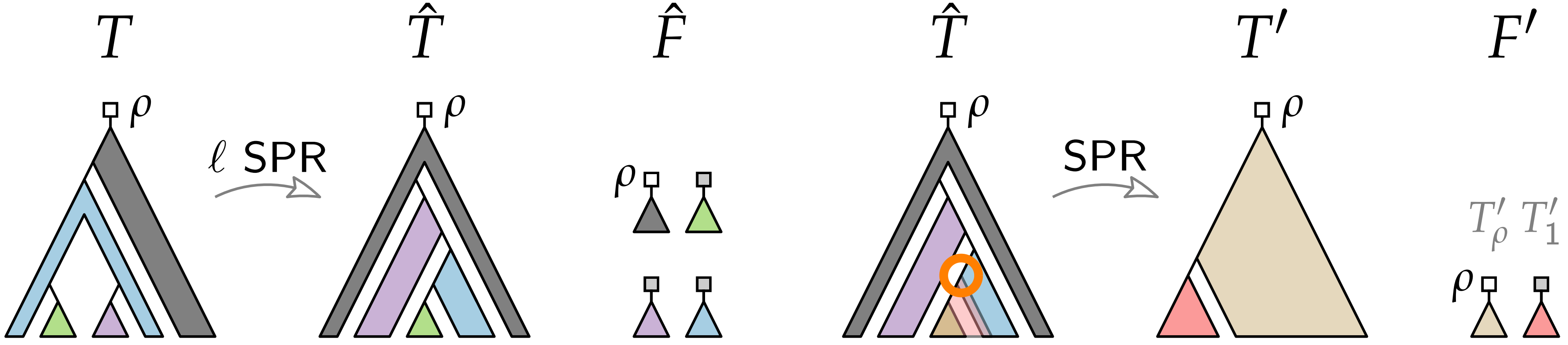

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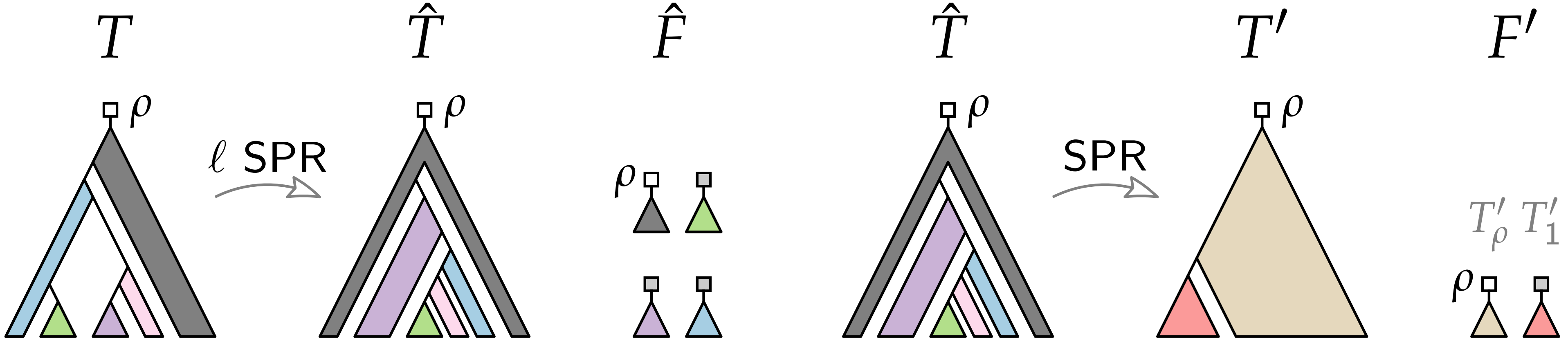

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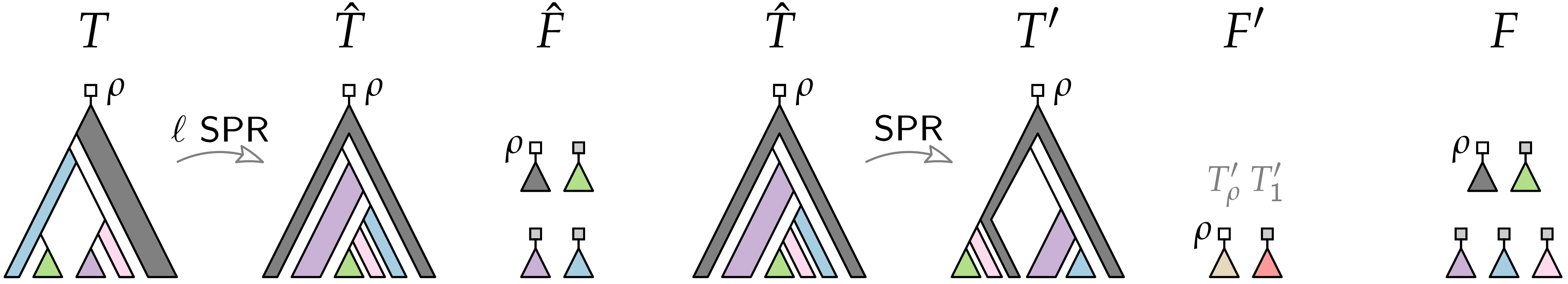
- Subdivide the corresponding tree to obtain $F$ from $\hat{F}$, which is an AF for $T$ and $T'$.



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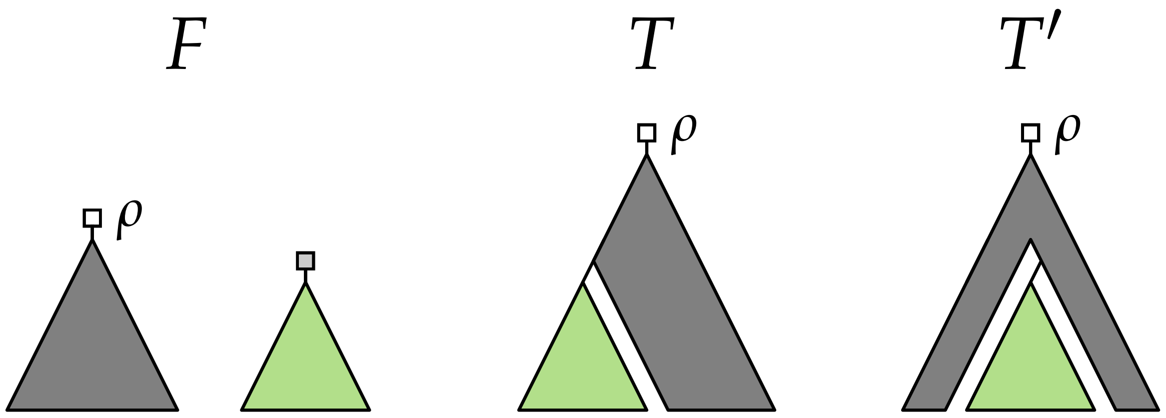

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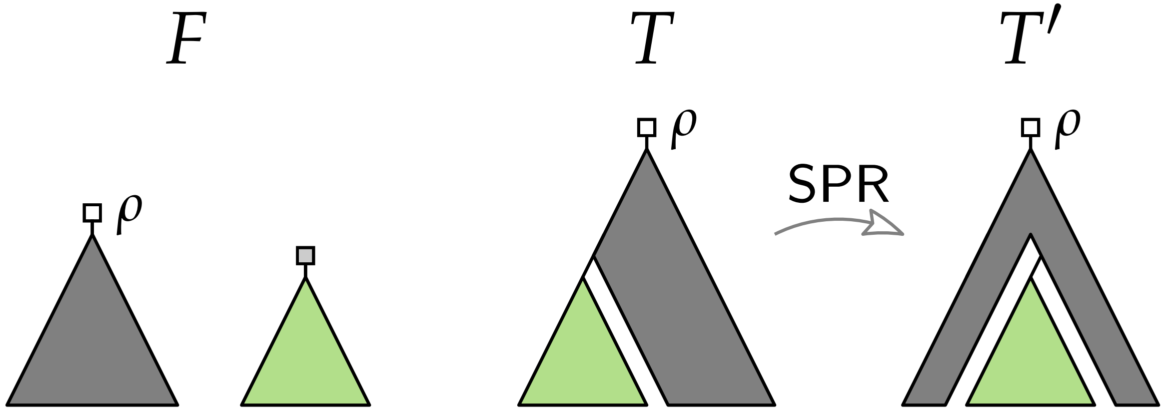

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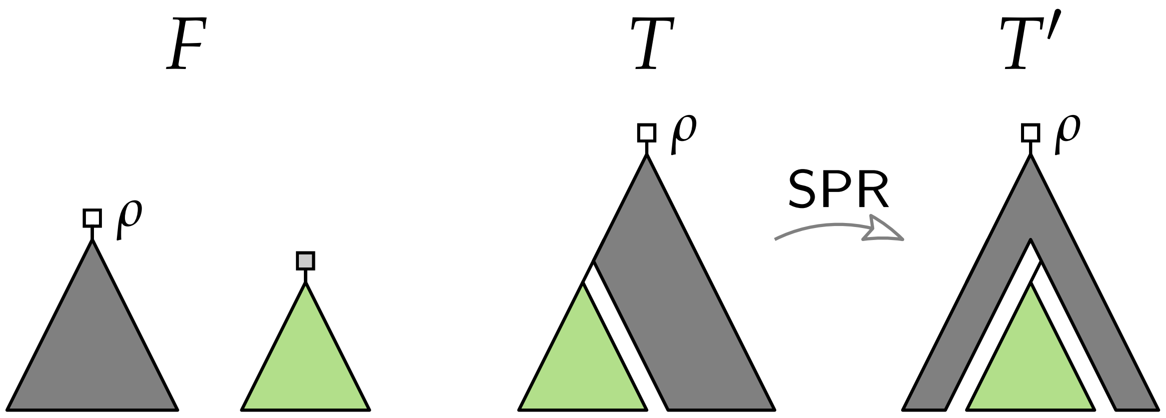

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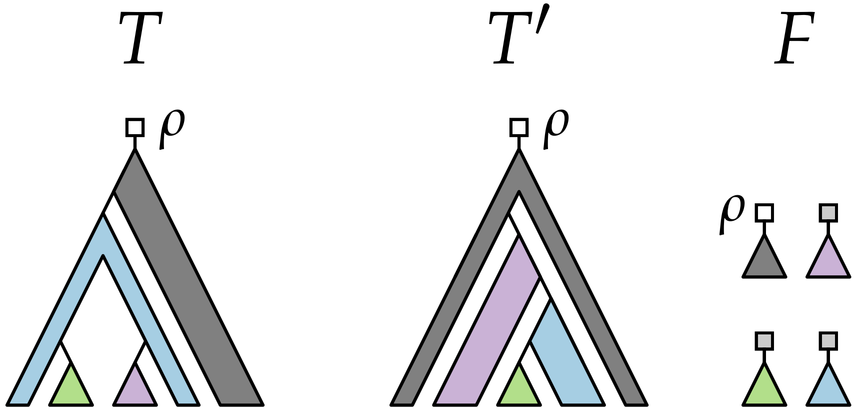

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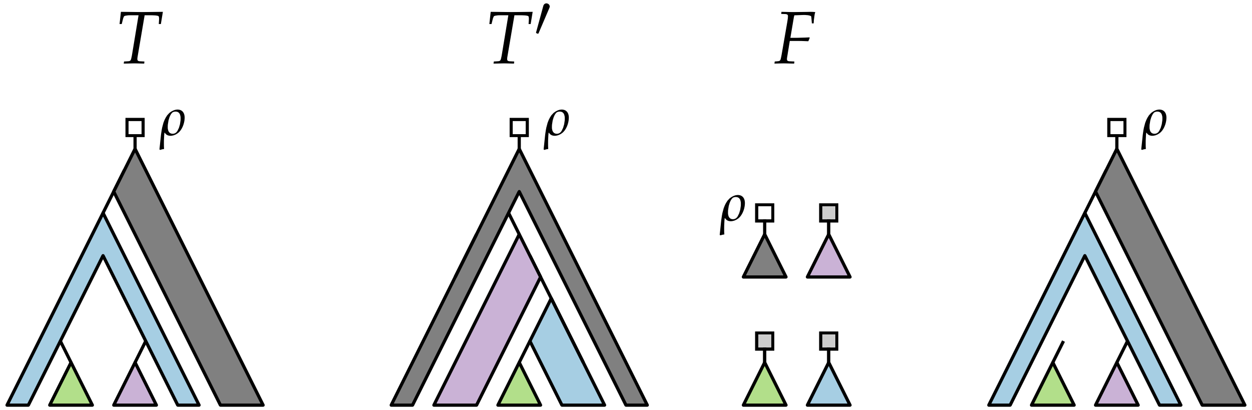

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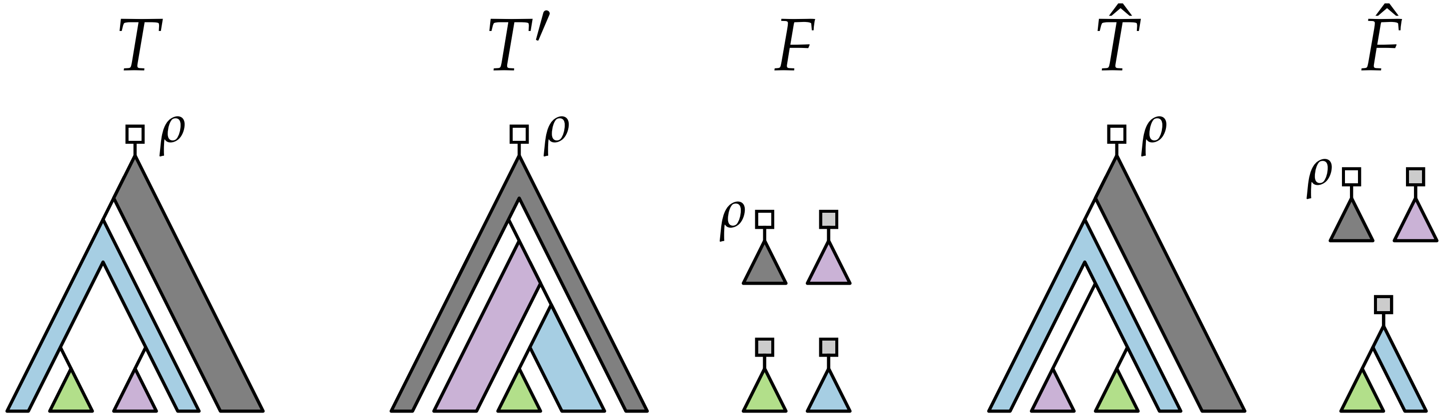

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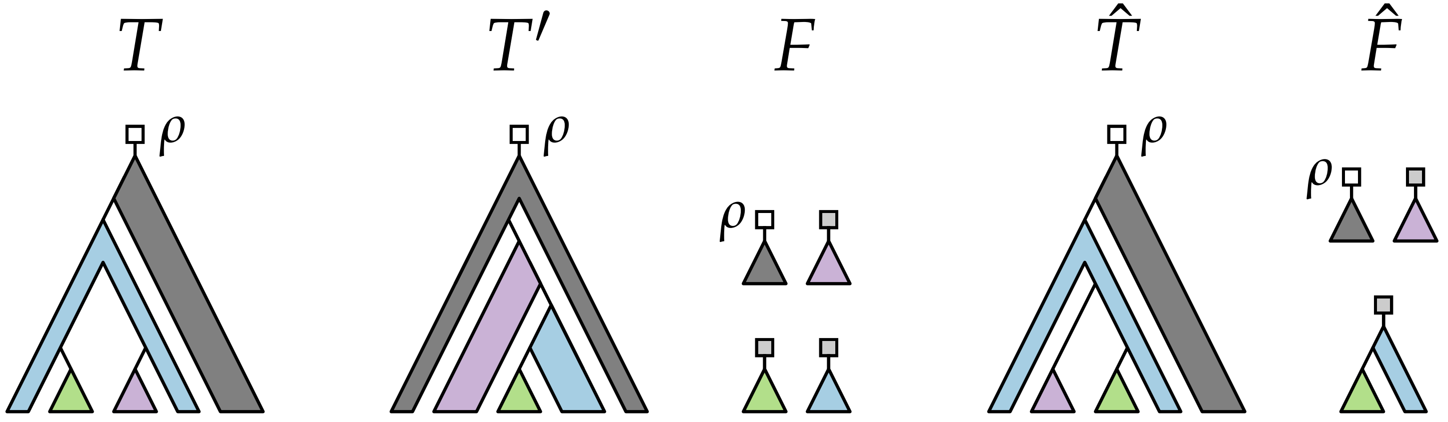


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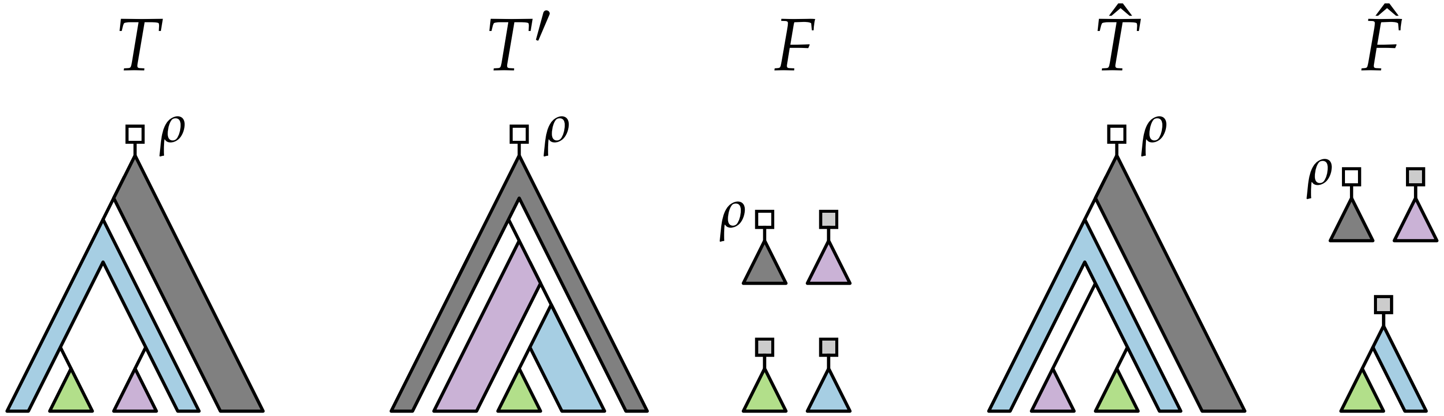


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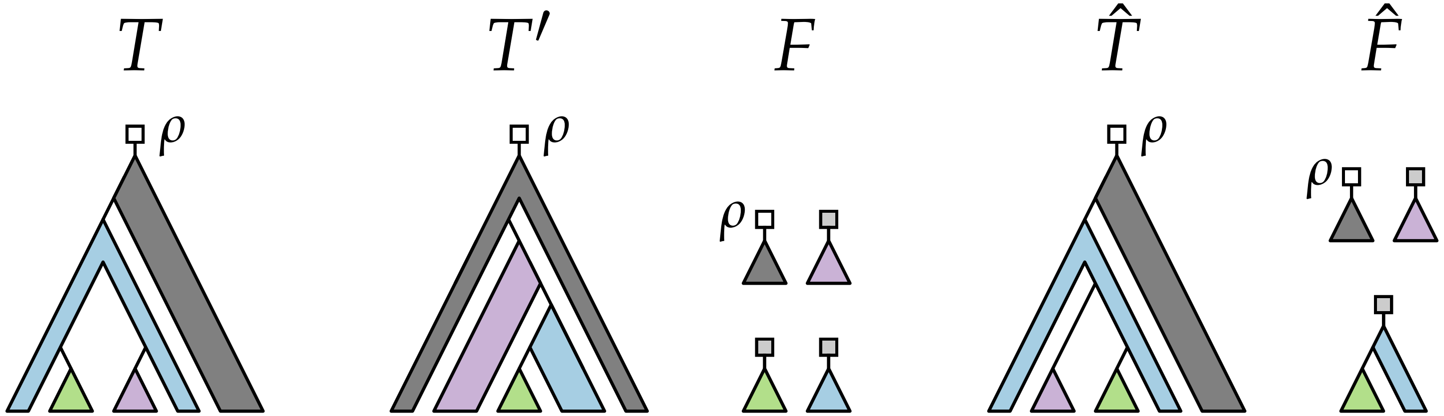


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□

# Problem & Plan

**Theorem 4.** [HJWZ '96, BS '05]
Computing $\mathsf{d}_{\mathsf{SPR}}(T, T')$ is NP-hard.

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**Plan.**

- Construct **kernel** of the problem.
  - Replace $T$ and $T'$ with smaller $S$ and $S'$.
  - Derive $\mathrm{d_{SPR}}(T, T')$ from $\mathrm{d_{SPR}}(S, S')$.

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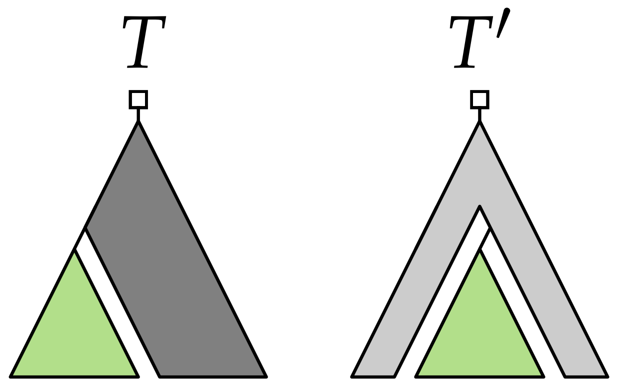

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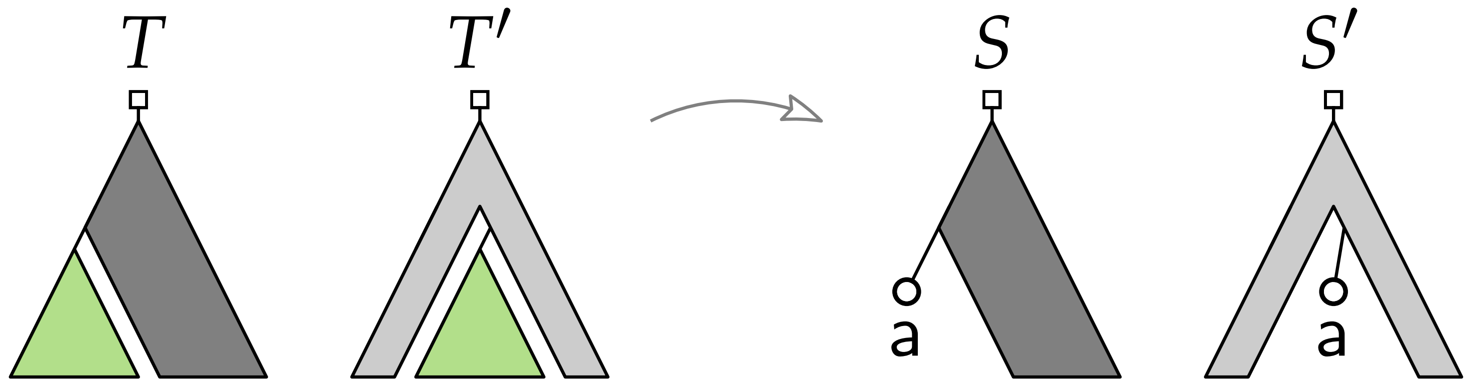

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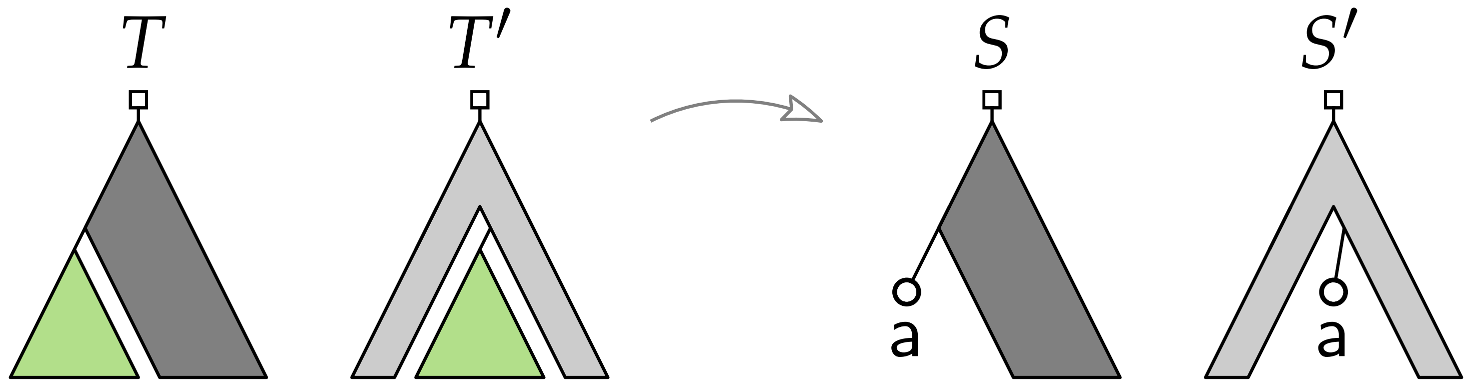


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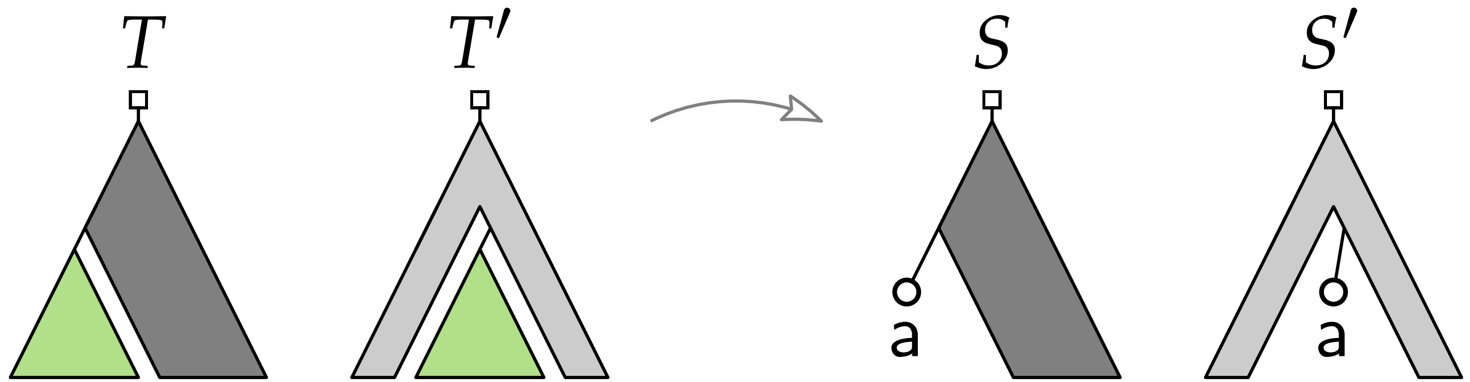


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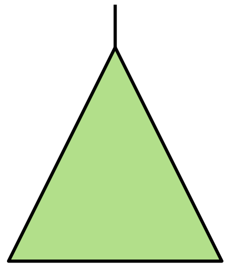
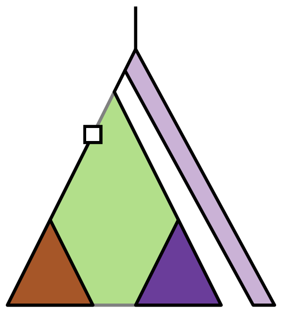
Suppose  is covered by two trees of MAF 

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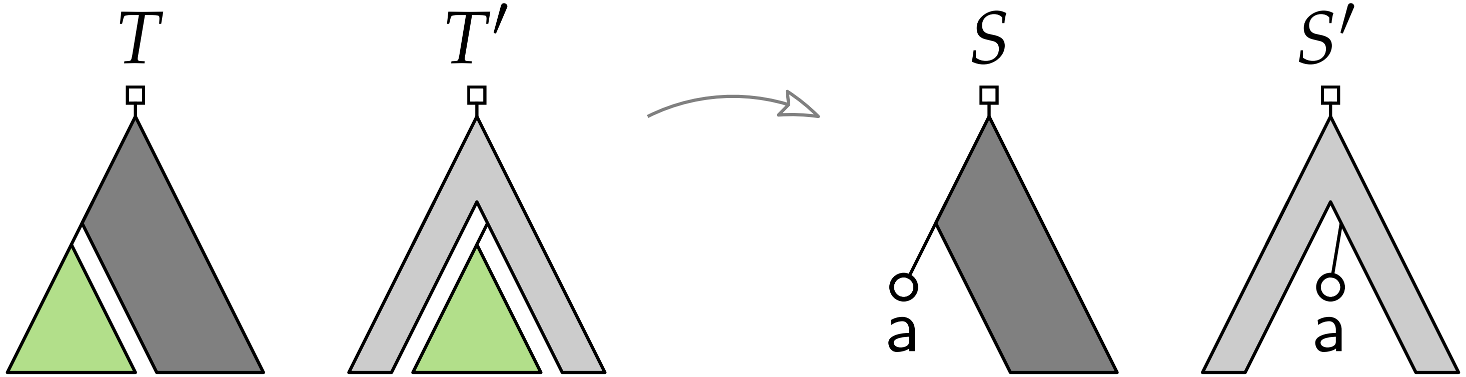


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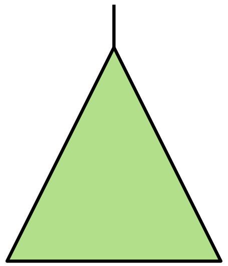
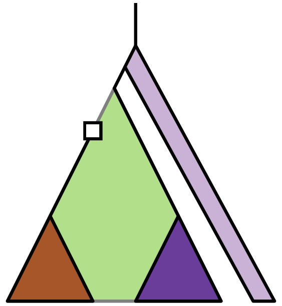
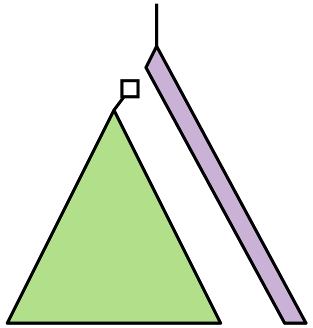
Suppose  is covered by two trees of MAF  then there is an alternative MAF of the same size 

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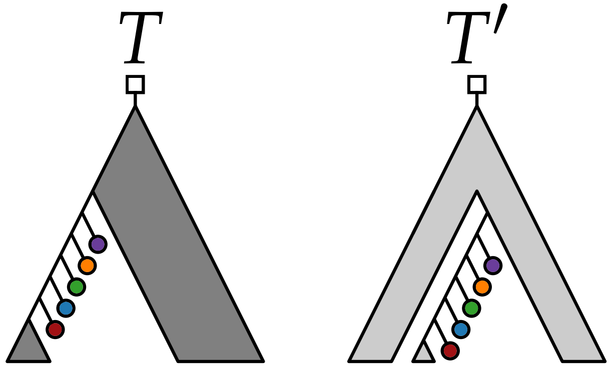

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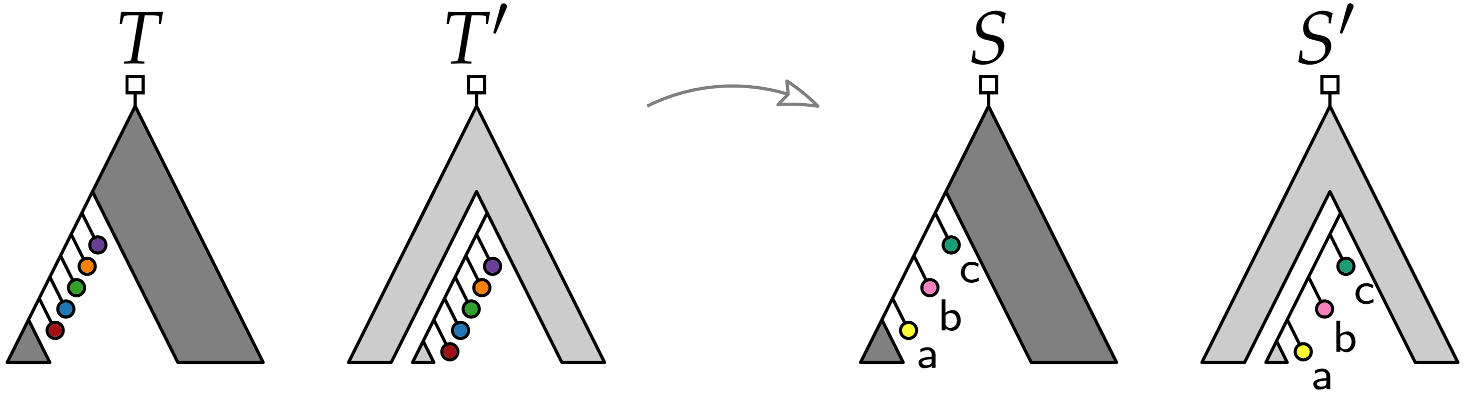

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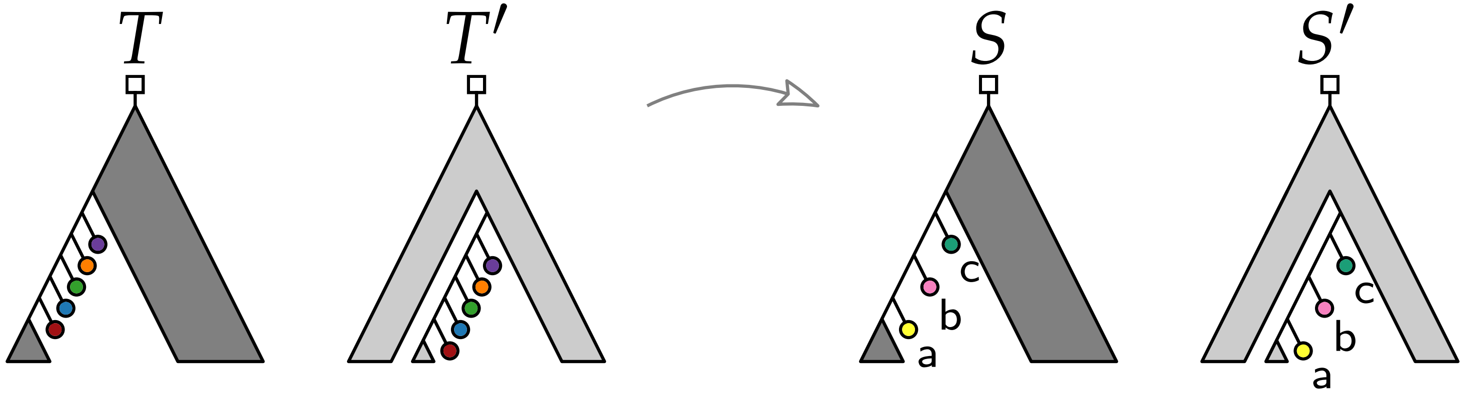


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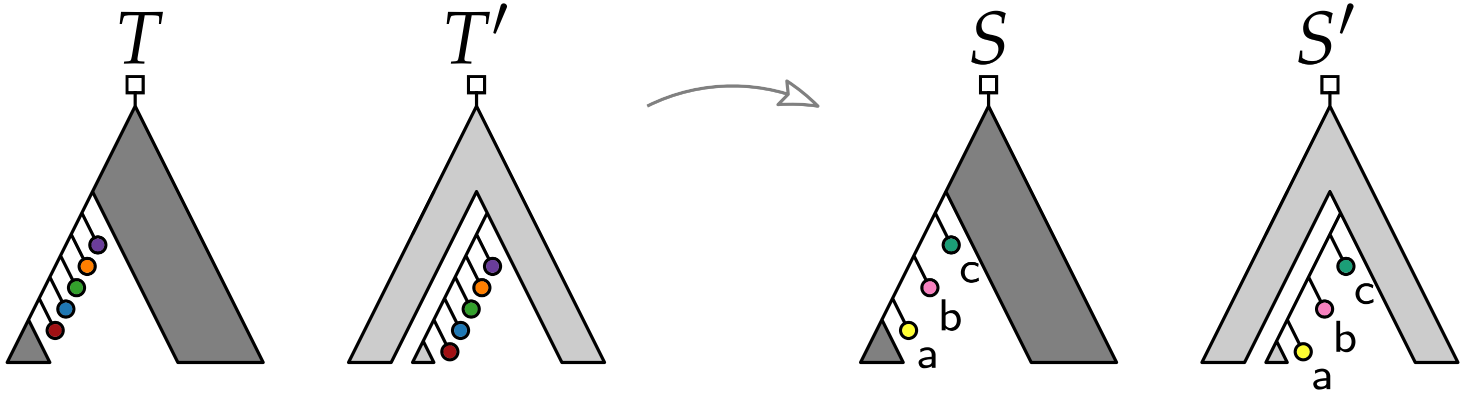


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- Show there is a tree with abc-chain in a MAF of $S$ and $S'$.
- Swap abc-chain with original chain for MAF of $T$ and $T'$.

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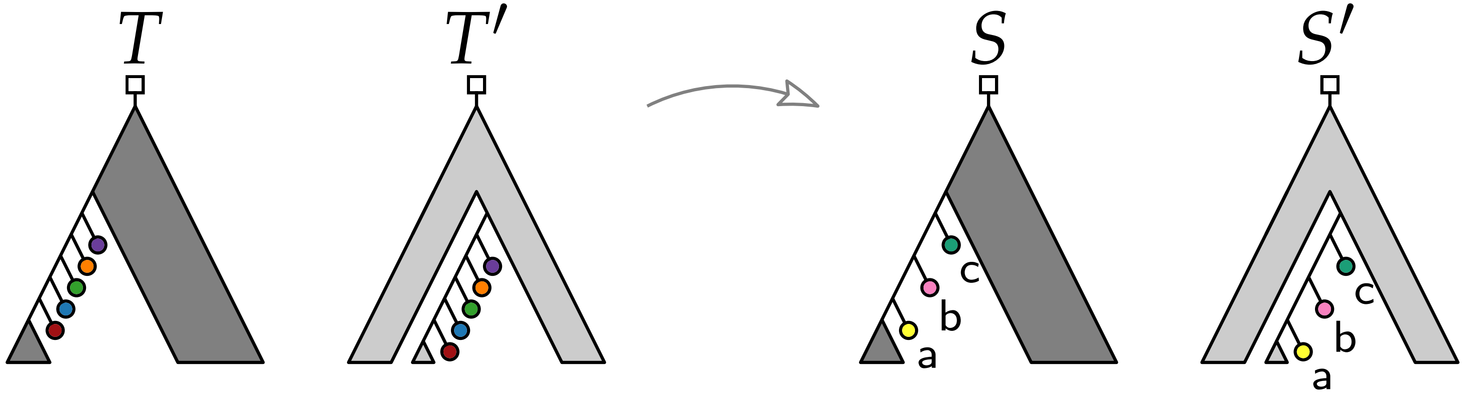


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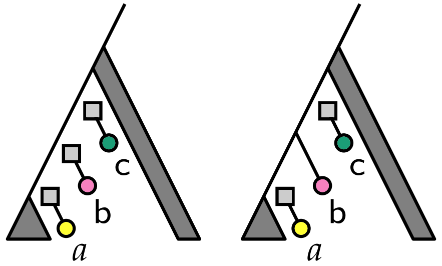

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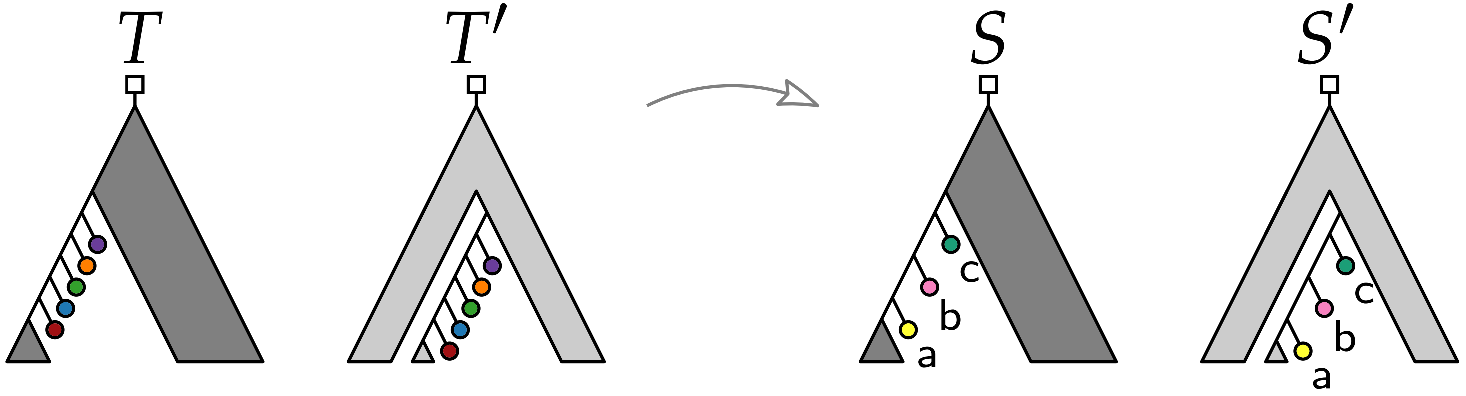


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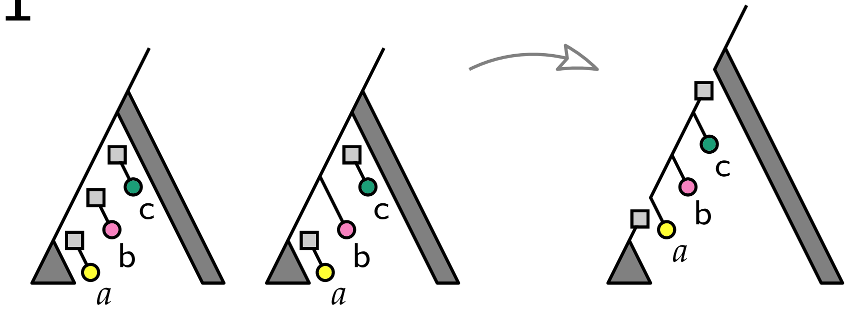

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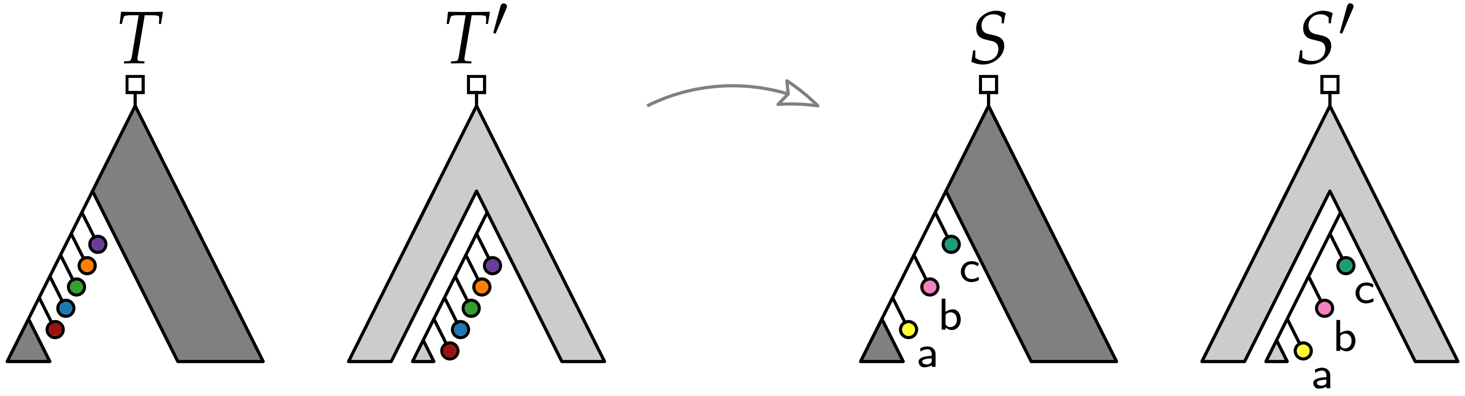


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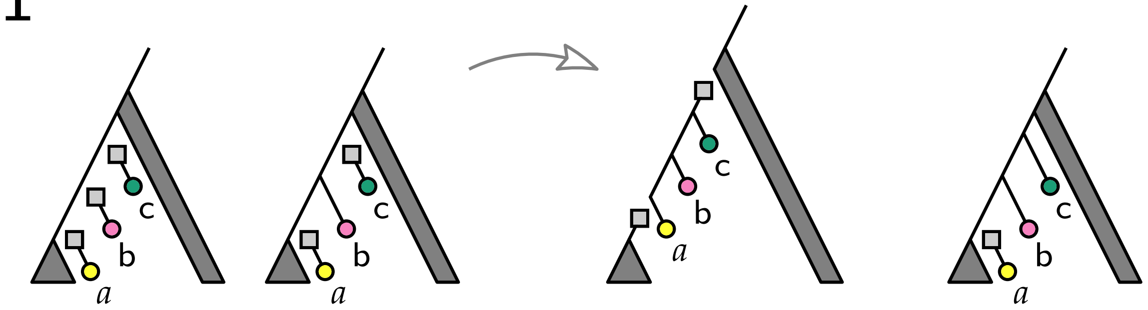

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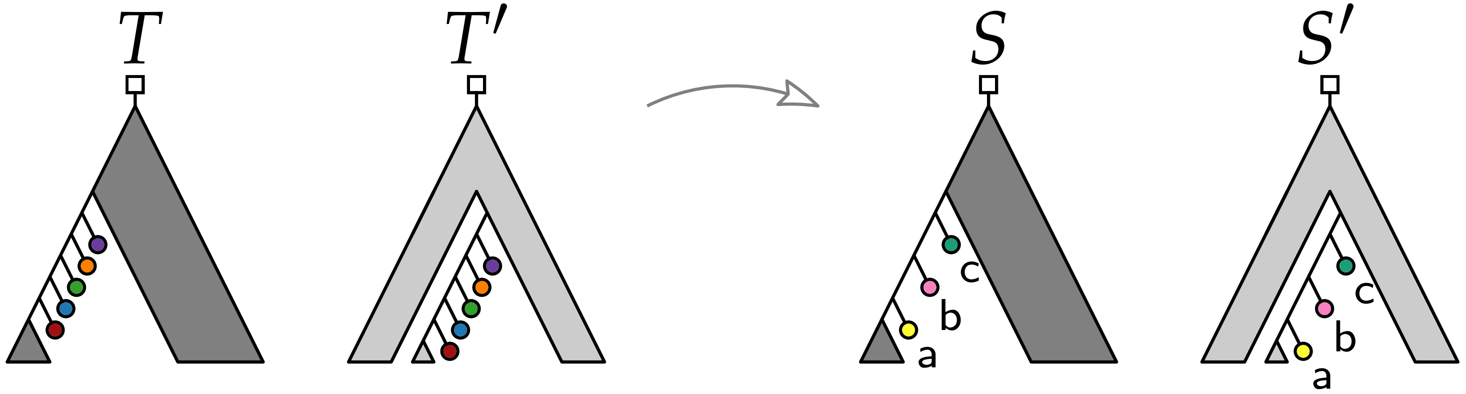


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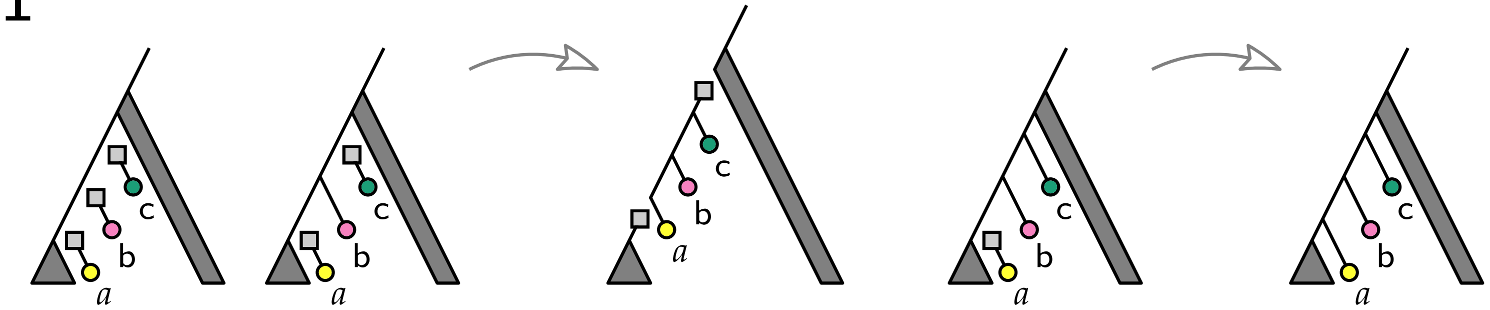

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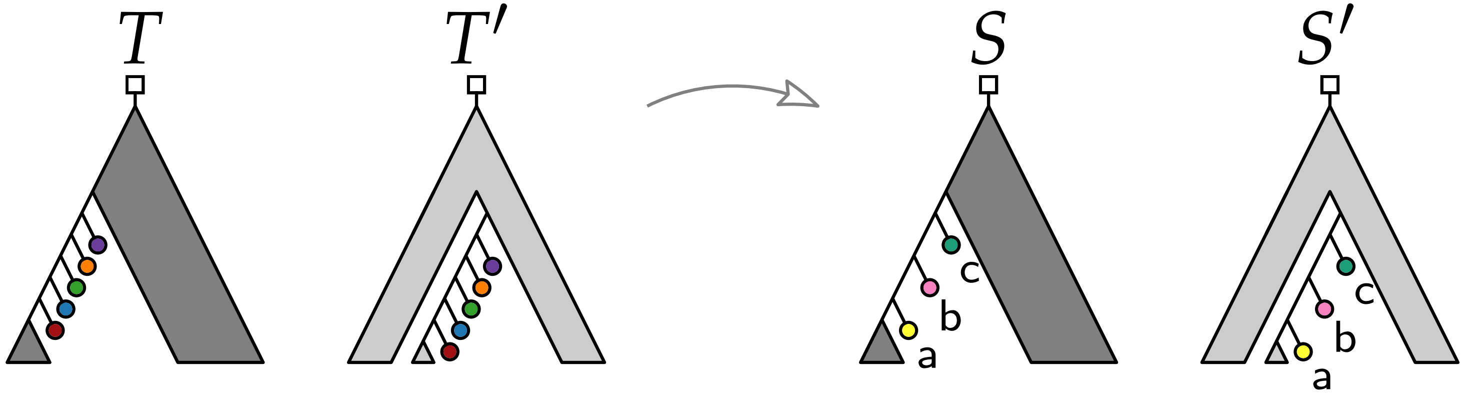


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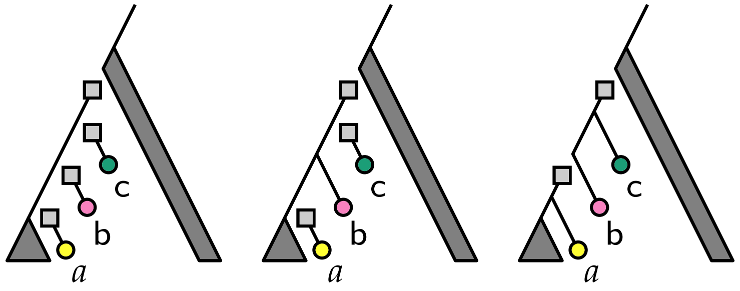

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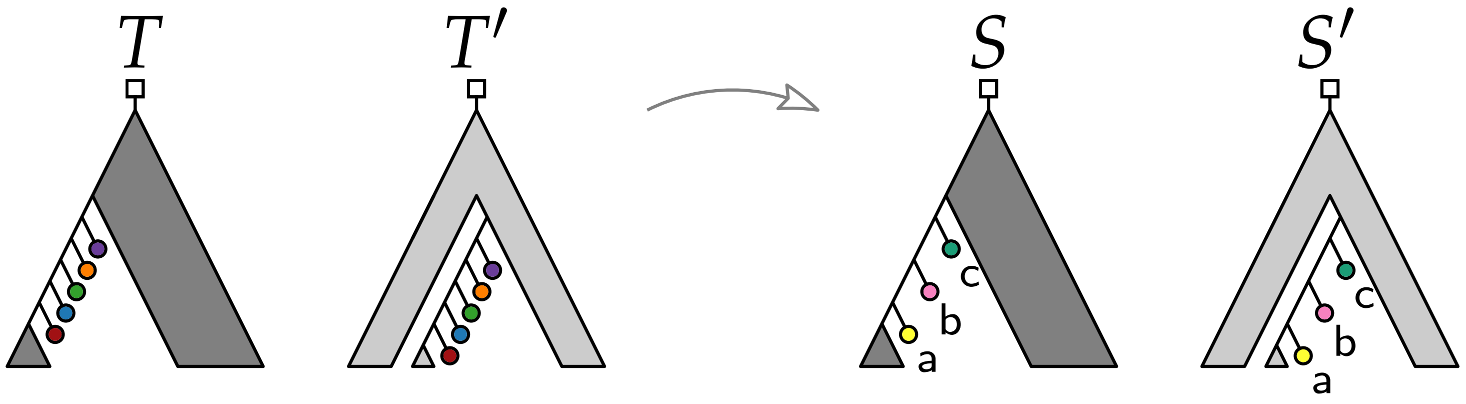


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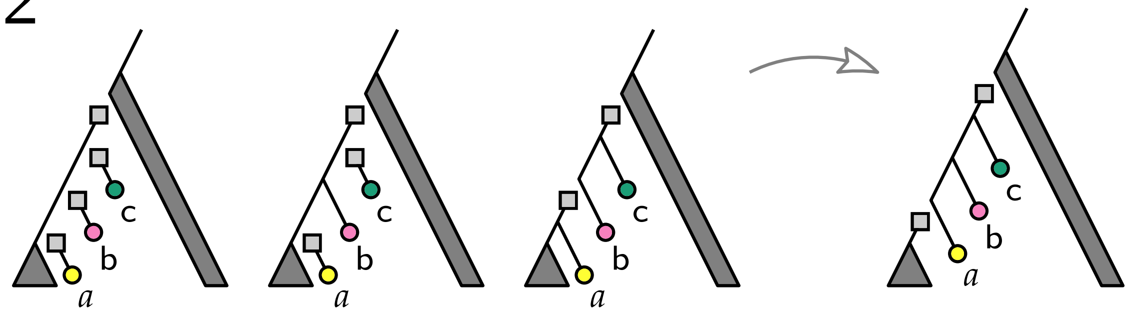

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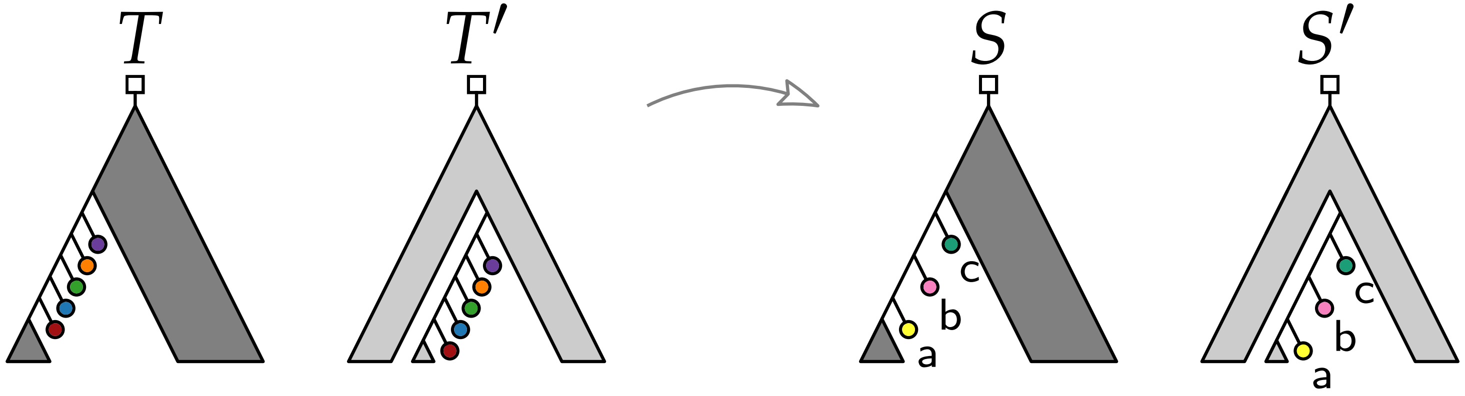


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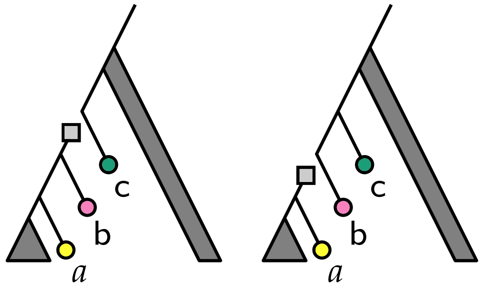

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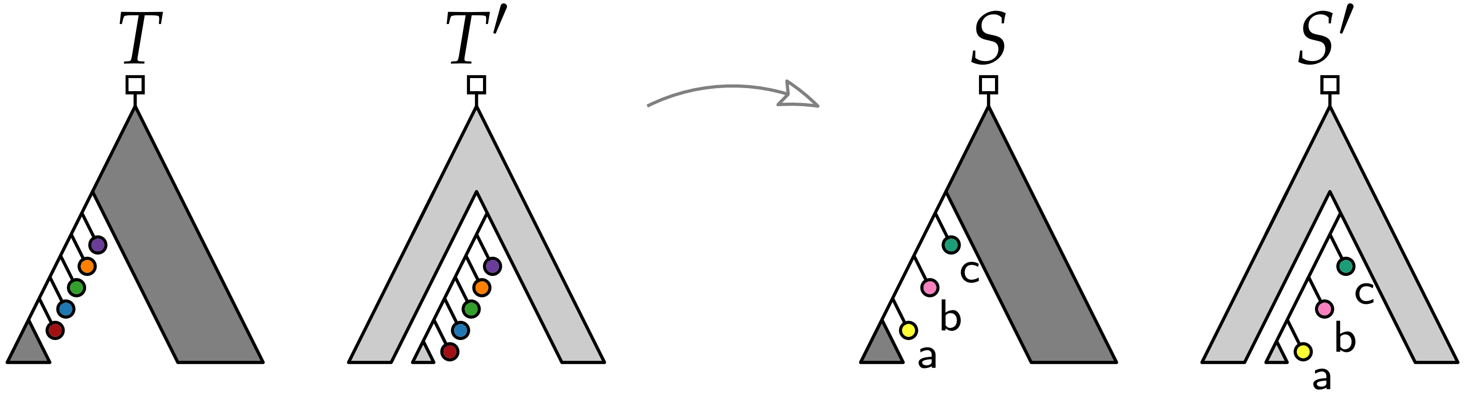


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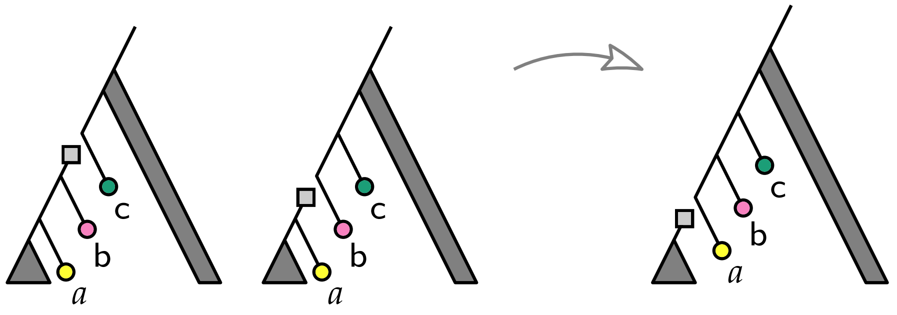

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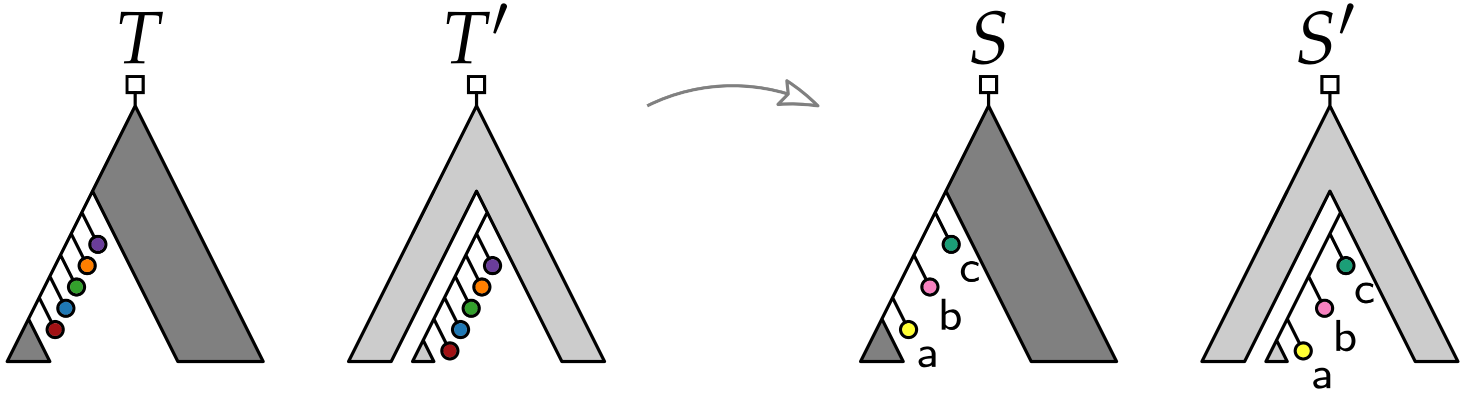


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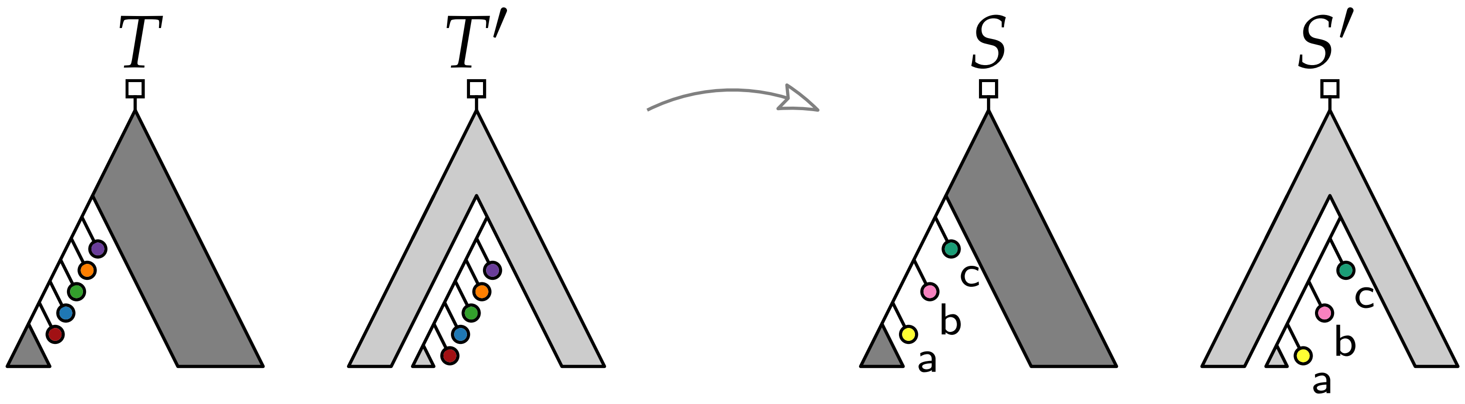


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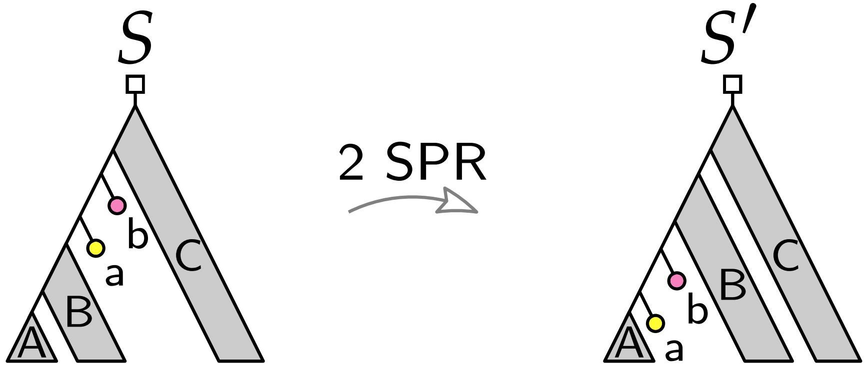


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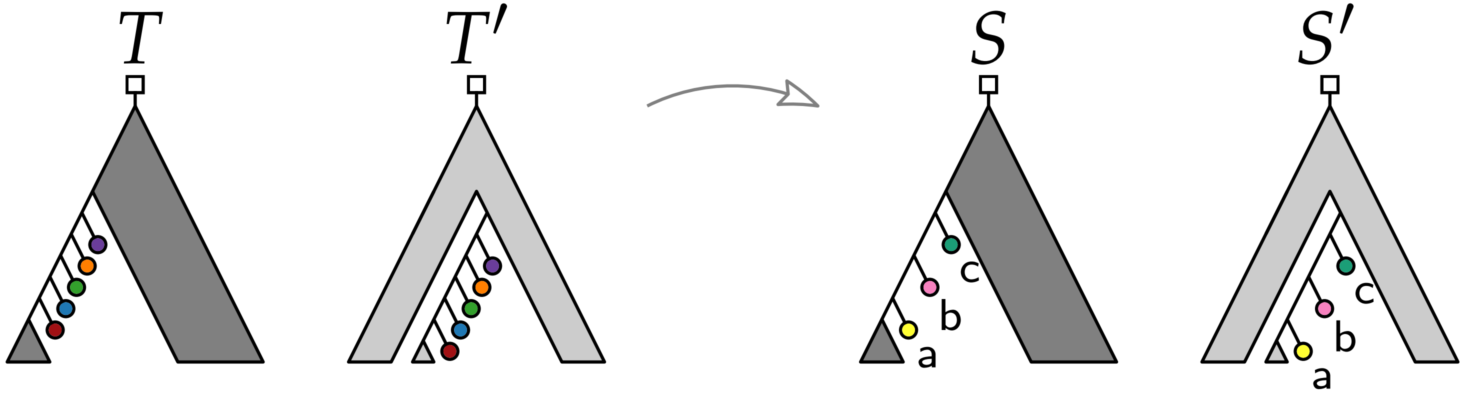


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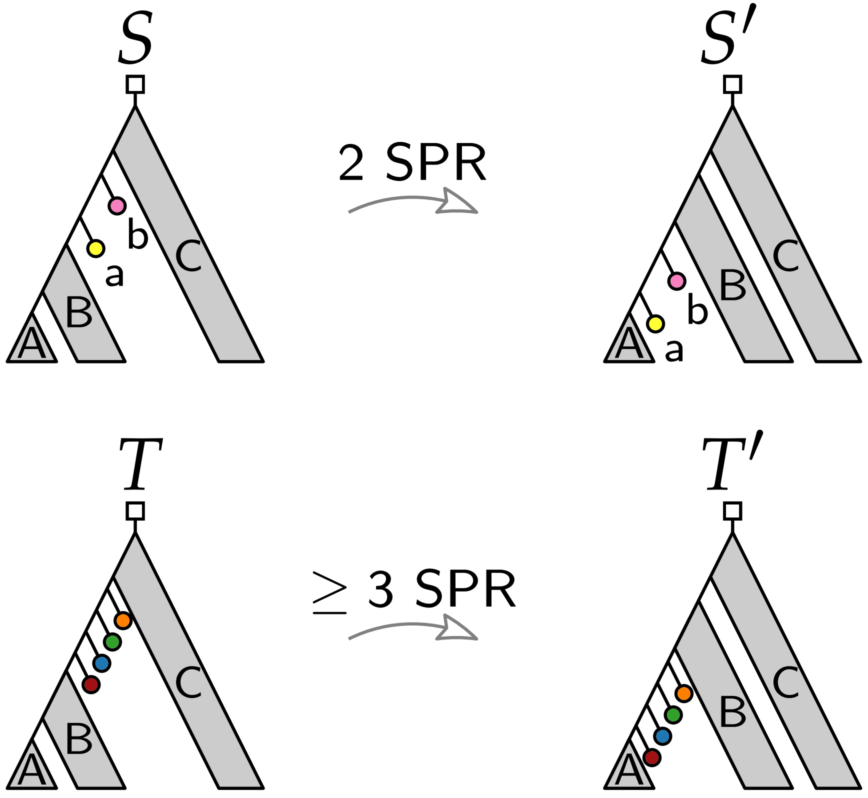

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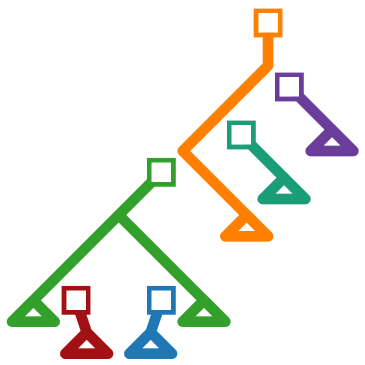

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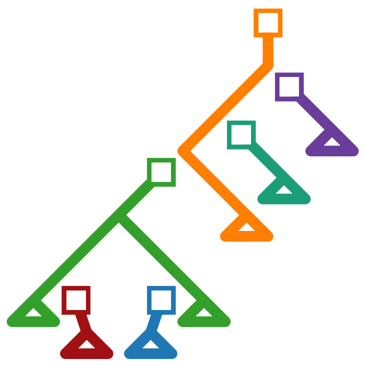

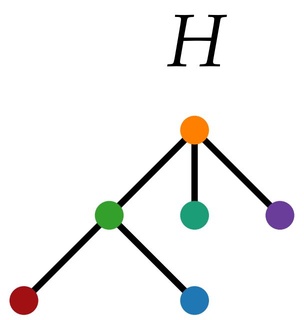

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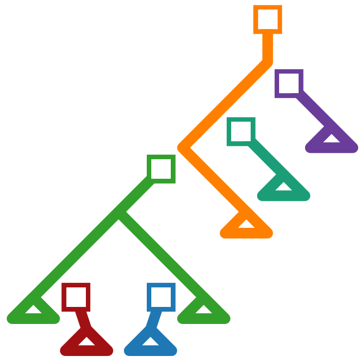
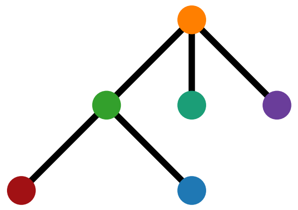


$H$



$|V(H)| = k + 1$

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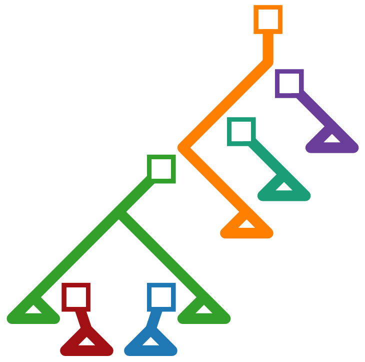

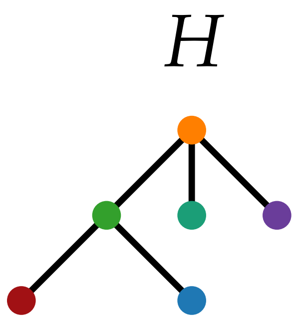


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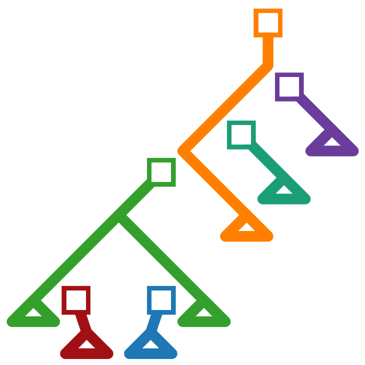

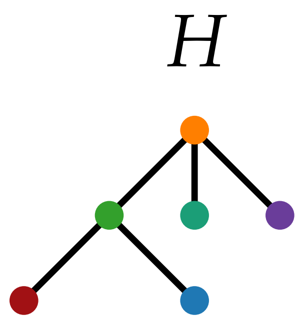


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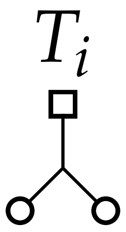

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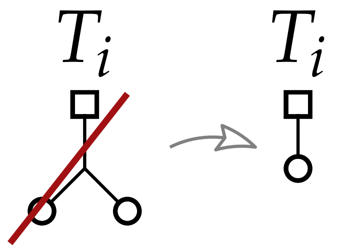

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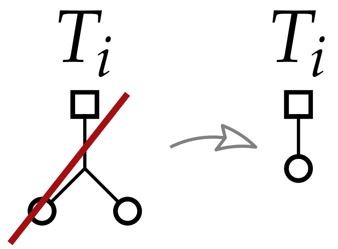


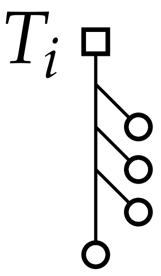

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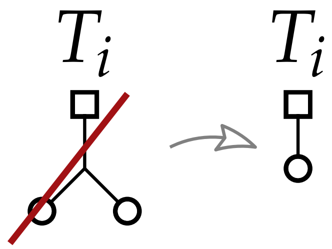


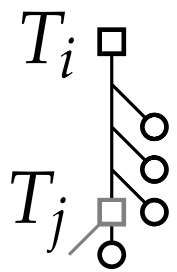

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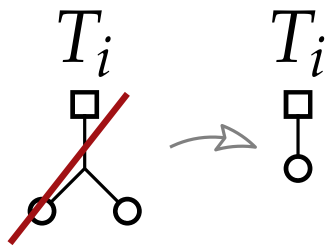


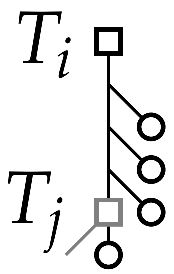


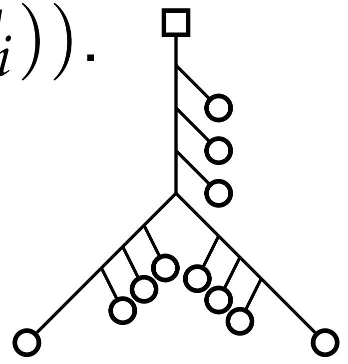

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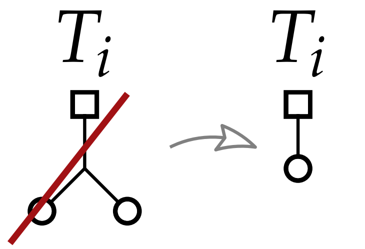


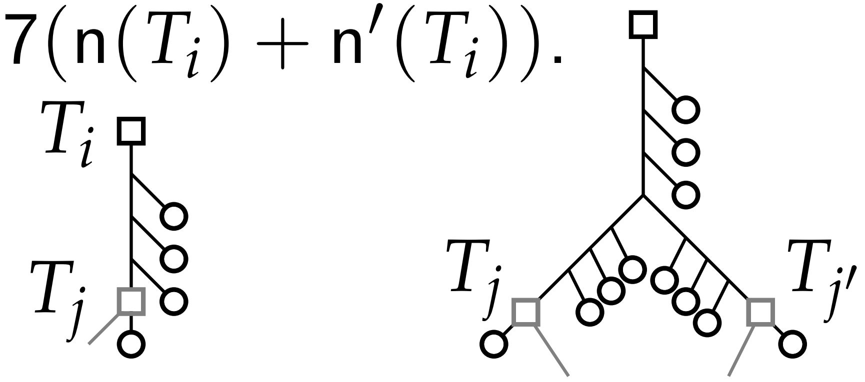

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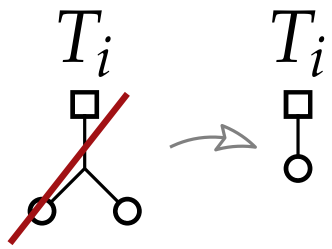


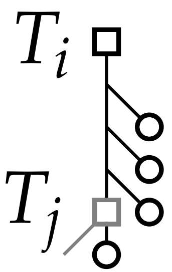


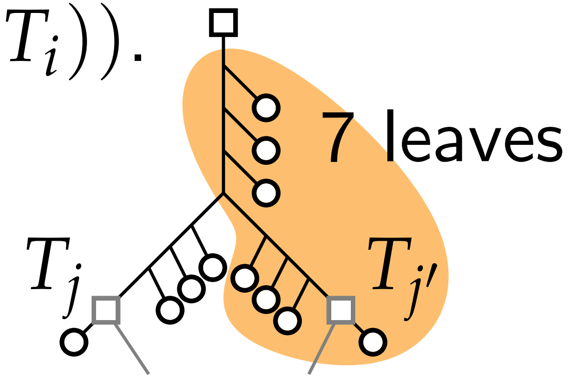

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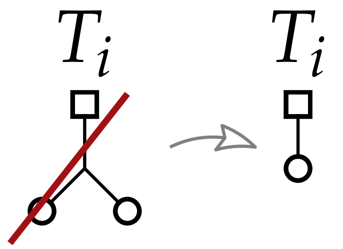


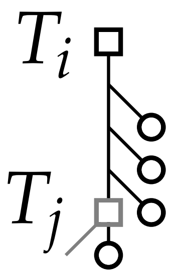


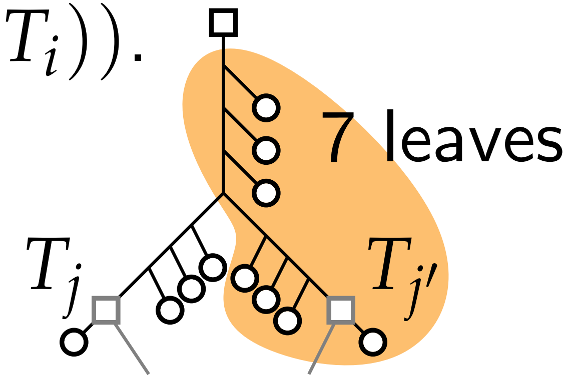

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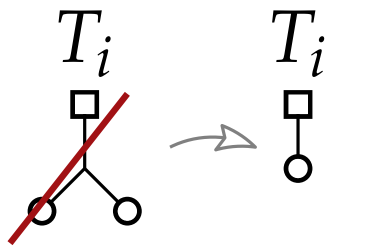


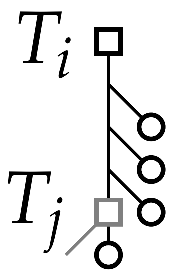


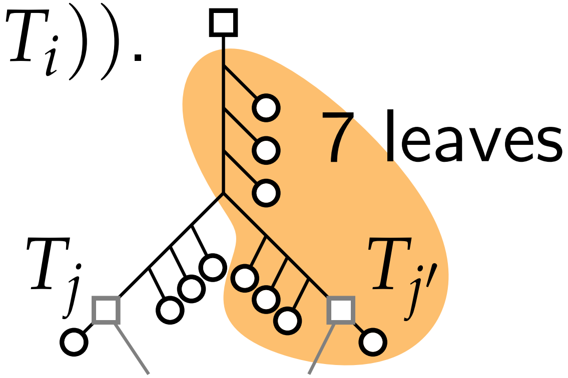

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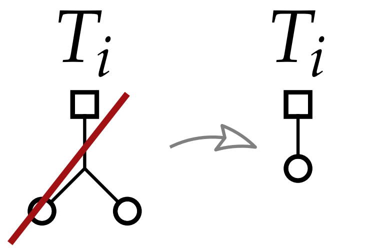


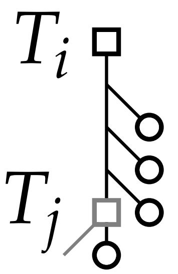


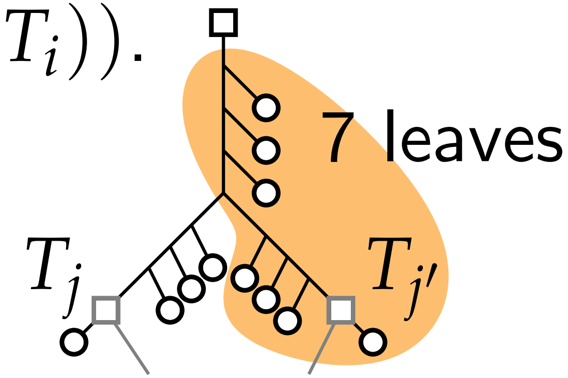

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- Length-$k$ BFS from $S$ visits at most $O\left(\left(4|X'|^2\right)^k\right) = O\left((56k)^{2k}\right)$ trees.

# FPT Algorithm

**Theorem 8.**
Computing $\mathrm{d_{SPR}}(T, T')$ is fixed-parameter tractable when parameterized by $\mathrm{d_{SPR}}(T, T')$.

**Proof.**

- Reduce $T$ and $T'$ to $S$ and $S'$ by exhaustively applying the reduction rules.
- Let $S$ and $S'$ be on $X'$ and let $k = \mathrm{d_{SPR}}(S, S')$.
- $S$ has at most $4|X'|^2$ neighbors in the SPR-graph $G$.
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- Length-$k$ BFS from $S$ visits at most $O\left(\left(4|X'|^2\right)^k\right) = O\left((56k)^{2k}\right)$ trees.

by Lemma 7

# FPT Algorithm

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- Length-$k$ BFS from $S$ visits at most $O\left(\left(4|X'|^2\right)^k\right) = O\left((56k)^{2k}\right)$ trees. (by Lemma 7)
- Since $k = \mathsf{d}_{\mathsf{SPR}}(S, S') = \mathsf{d}_{\mathsf{SPR}}(T, T')$, this yields an FPT algorithm.

# Approximation Algorithm

**Idea.**

- Given trees $T$ and $T'$, which are reduced by the previous rules, we compute an agreement forest $F$ by
- successively making “cuts” and “eliminations”.
- These steps let $T$ and $T'$ shrink further and further.
- Show that $|F|$ is at most $3|F^*|$, where $F^*$ is a MAF of $T$ and $T'$.

# Approximation Algorithm

$\textsc{approx}\mathrm{DSPR}(T, T')$

$i \leftarrow 1$
$G_i \leftarrow T$
$H_i \leftarrow T'$
**while** $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ **do**

**return** $|H_i| - 1$

# Approximation Algorithm

$\textsc{approxDSPR}(T, T')$

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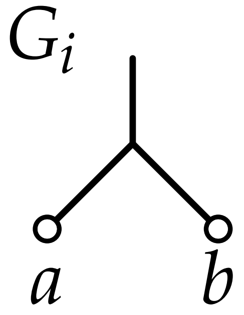

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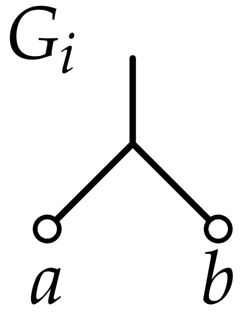

# Approximation Algorithm

APPROXDSPR$(T, T')$

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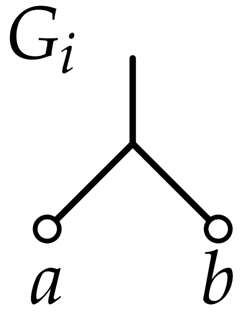
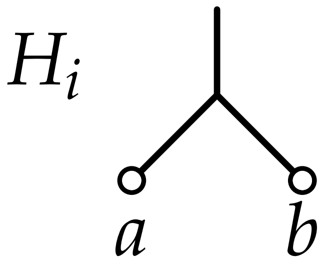



Case 1



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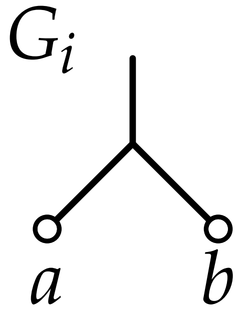
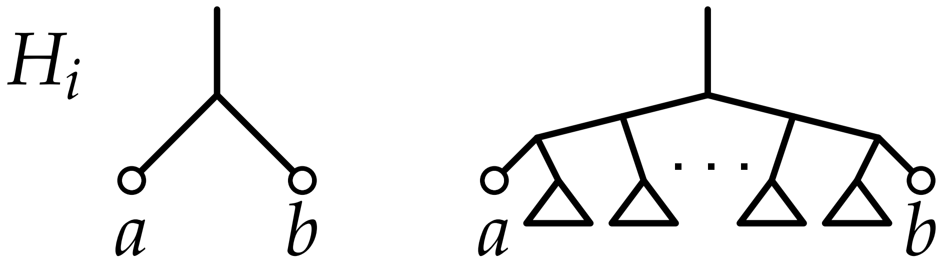



Case 1 Case 2



# Approximation Algorithm

APPROXDSPR$(T, T')$

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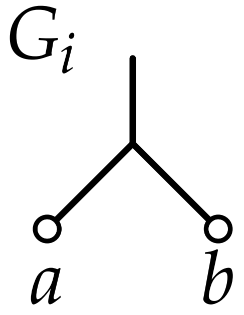
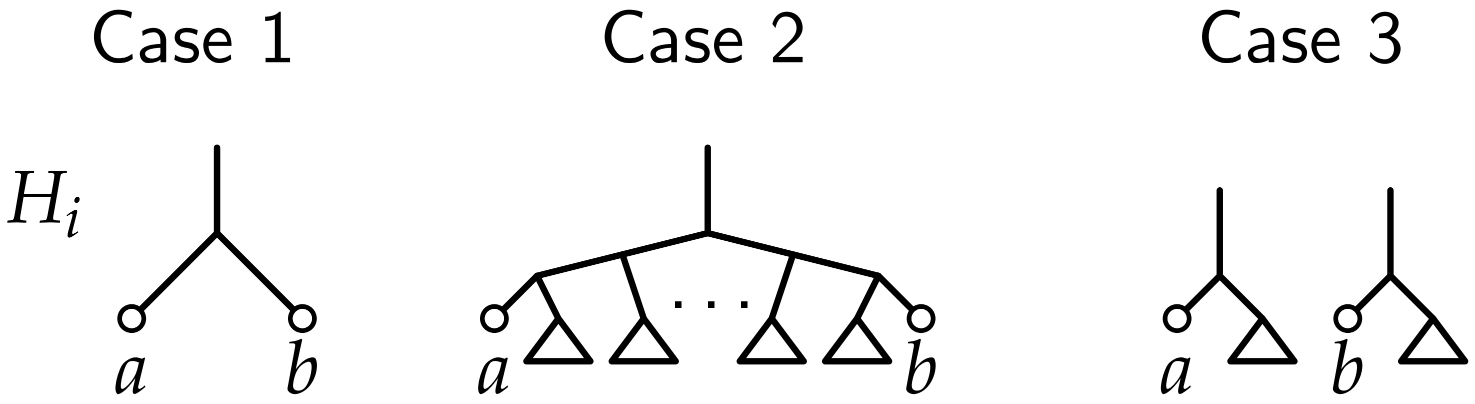
**return** $|H_i| - 1$



# Approximation Algorithm

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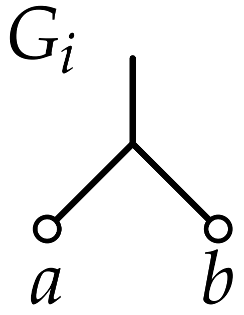
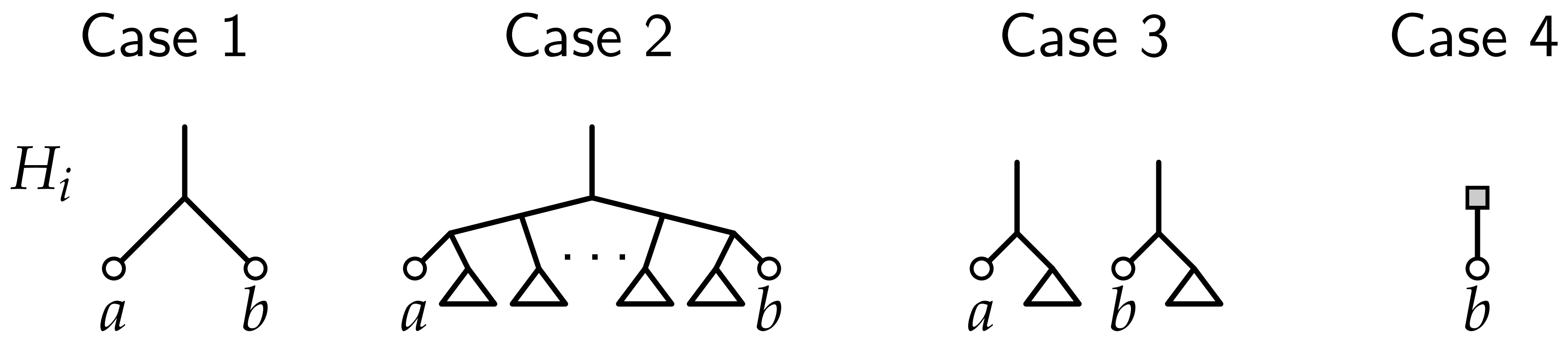
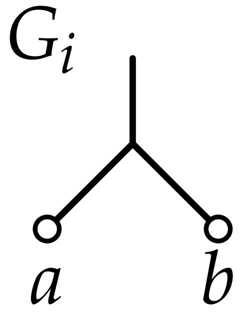


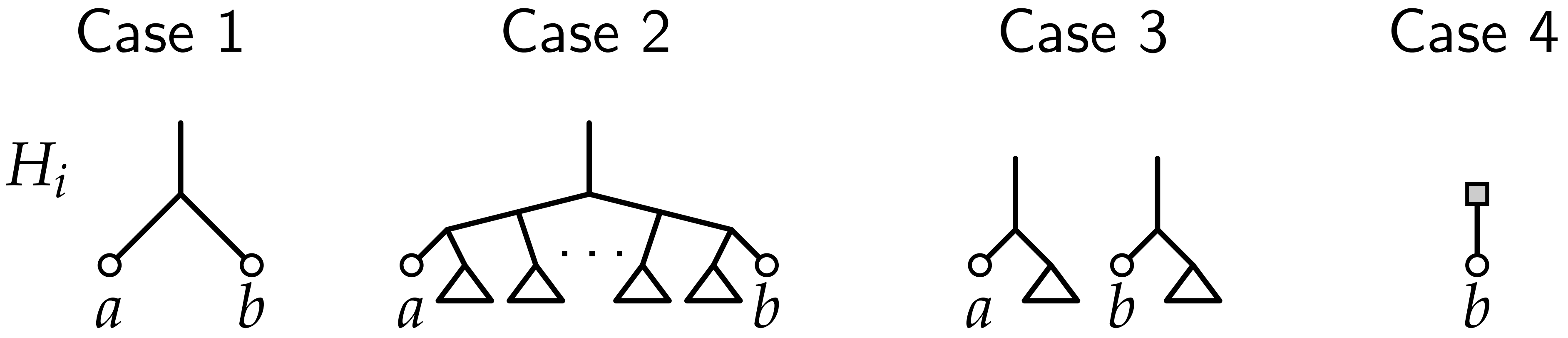



# Approximation Algorithm

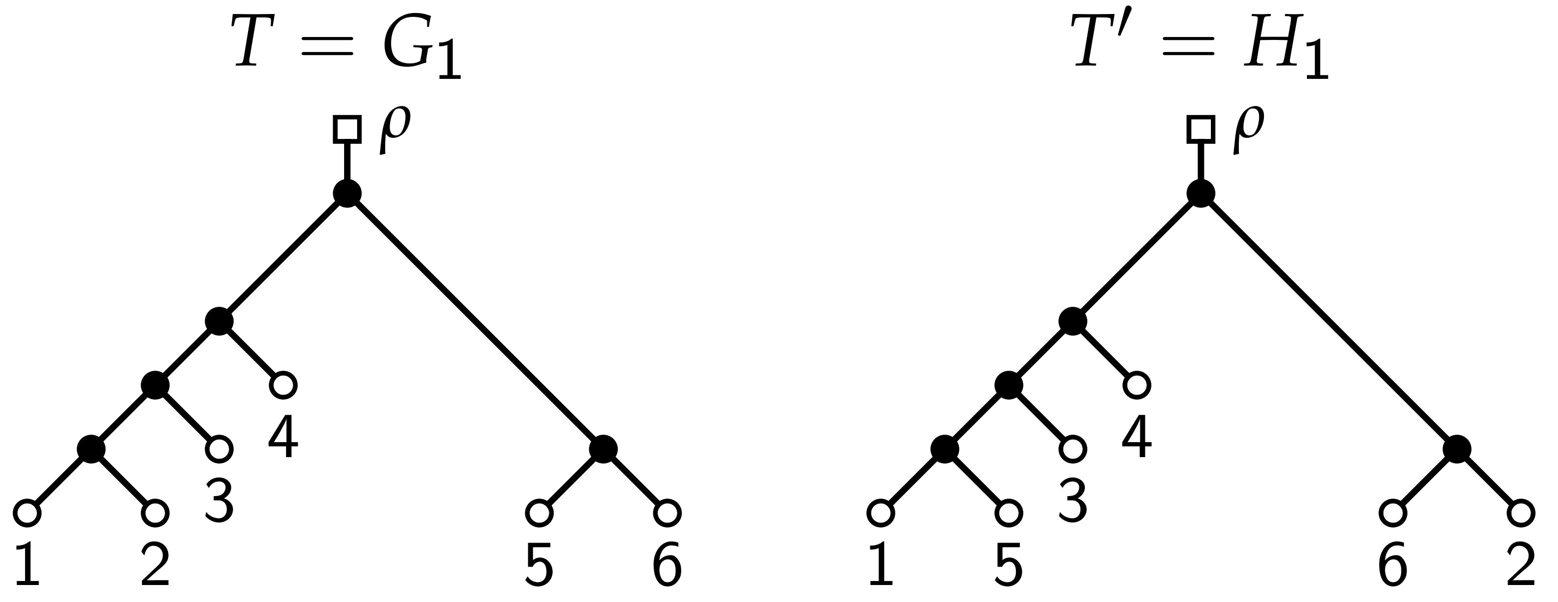
$\textsc{approx}\mathrm{DSPR}(T, T')$

$i \leftarrow 1$
$G_i \leftarrow T$
$H_i \leftarrow T'$
**while** $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ **do**
  find the case that applies to $a$ and $b$ in $H_i$
  apply the corresponding modification
  to obtain $G_{i+1}$ from $G_i$ and $H_{i+1}$ from $H_i$
  $i++$
**return** $|H_i| - 1$



# Approximation Algorithm – Example



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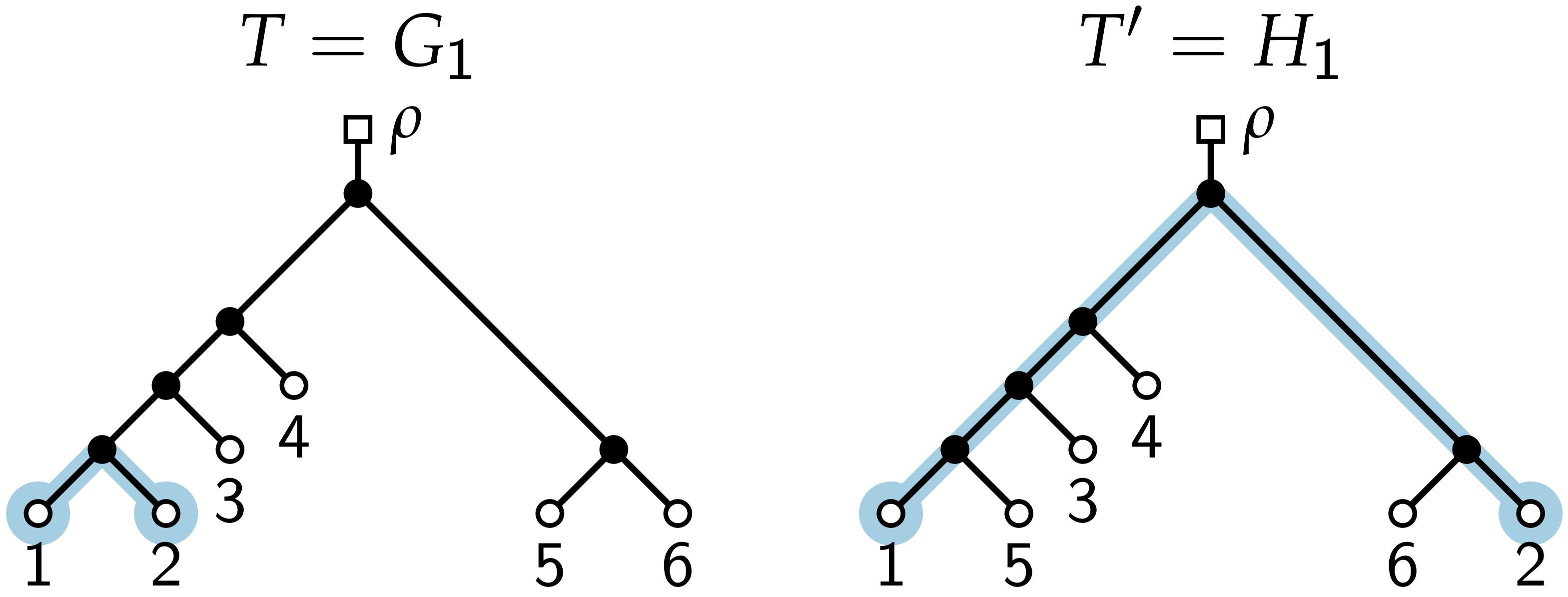

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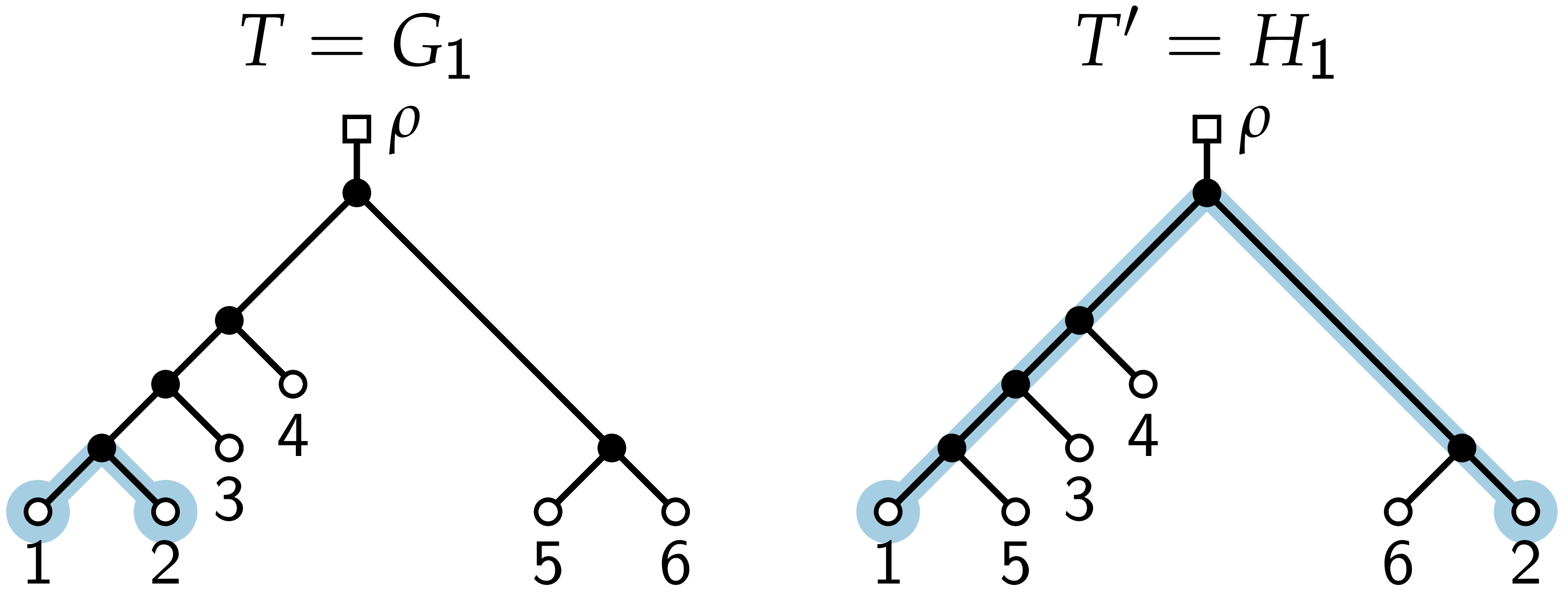
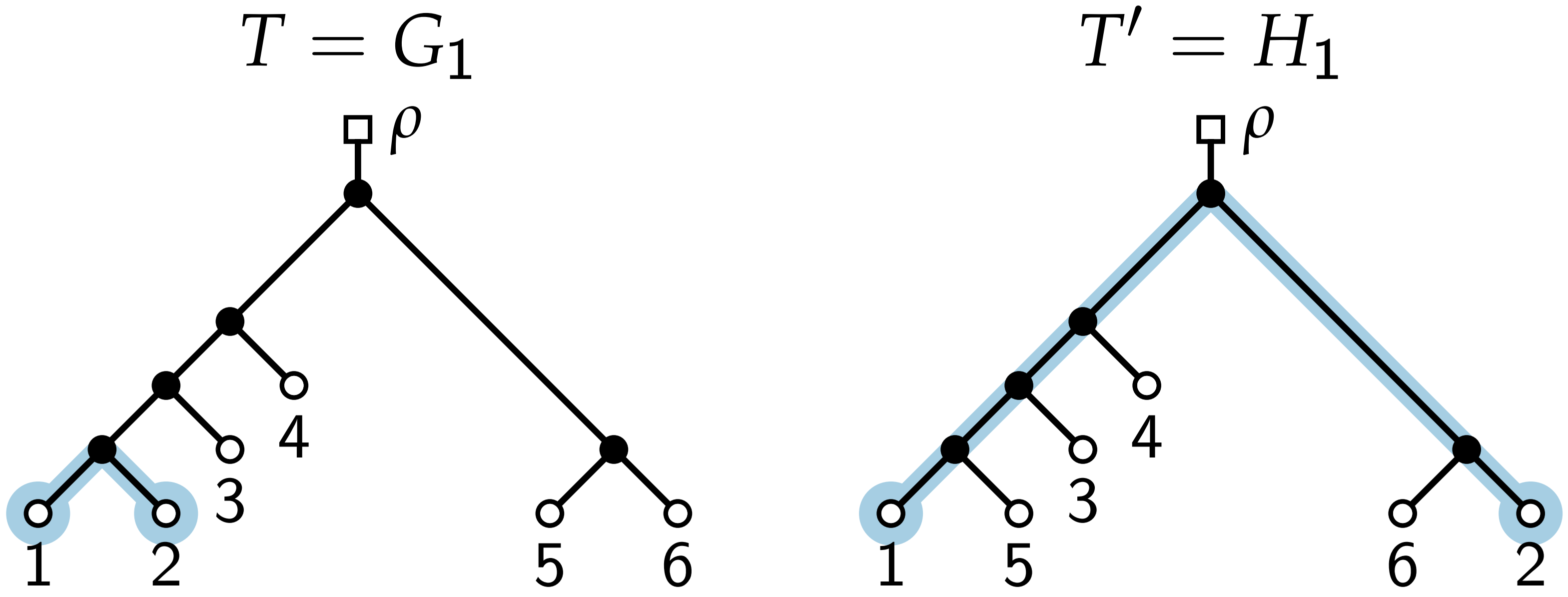



- Should we cut off leaf 1 or leaf 2 or everything between them in $H_1$?

# Approximation Algorithm – Example

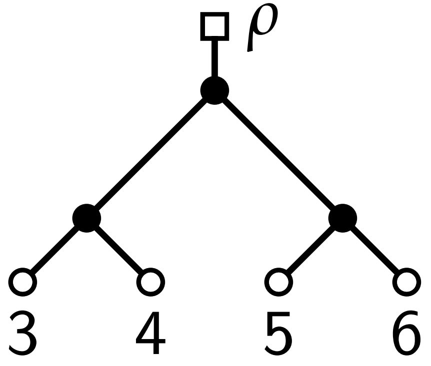



**Case 2**

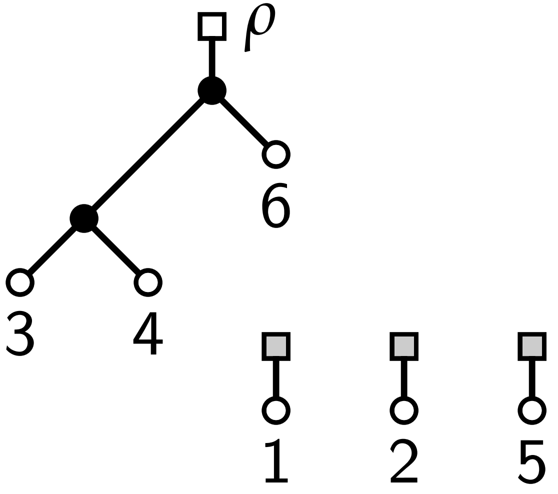
- Should we cut off leaf 1 or leaf 2 or everything between them in $H_1$?
- Do parts of each!

# Approximation Algorithm – Example

$G_2$



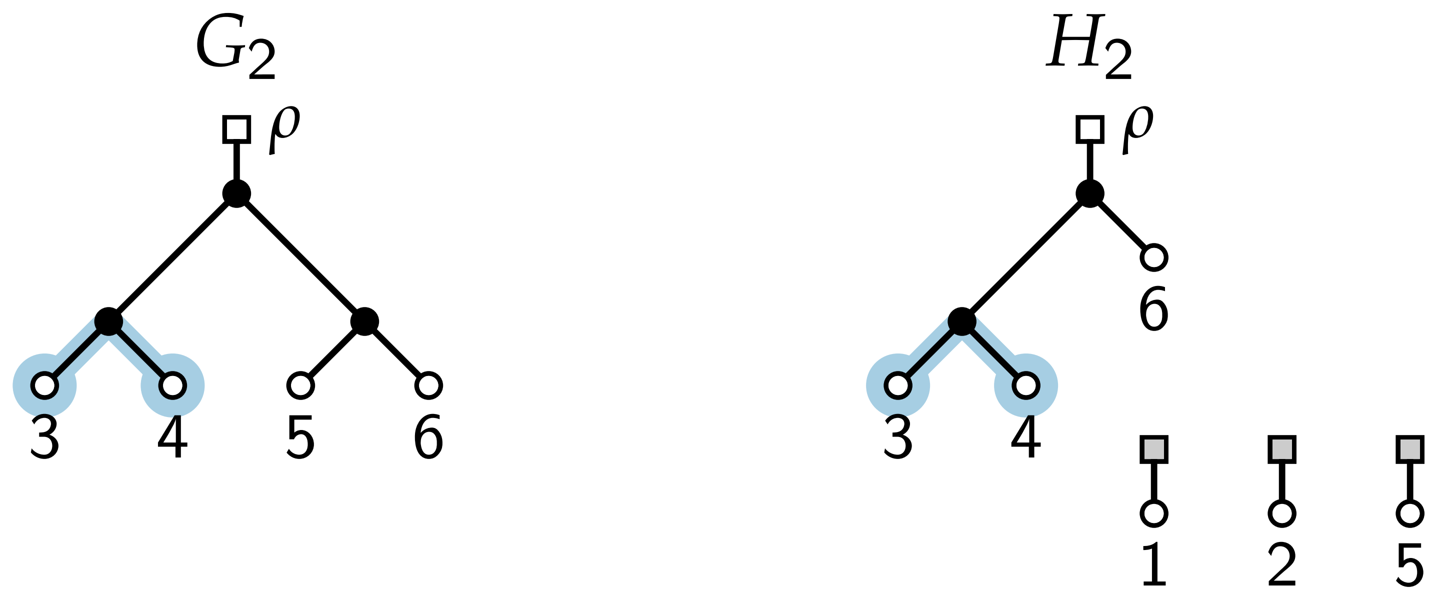

$H_2$



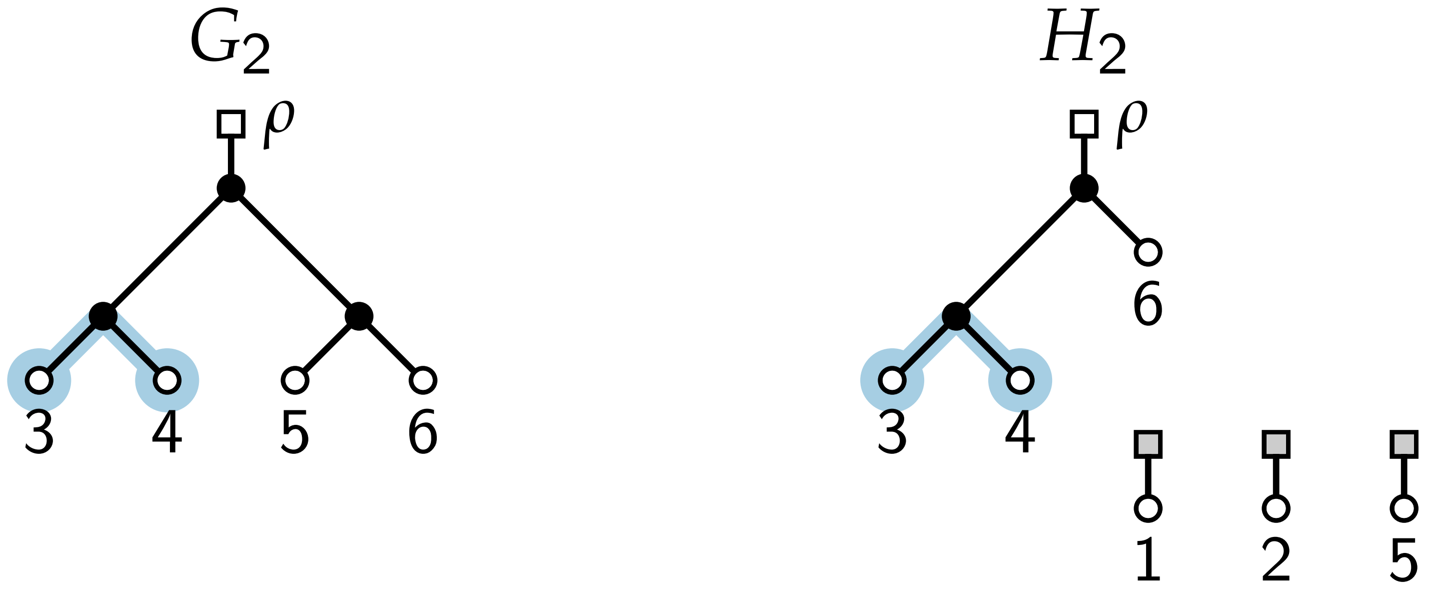

**Case 2**

- Should we cut off leaf 1 or leaf 2 or everything between them in $H_1$?
- Do parts of each!

# Approximation Algorithm – Example



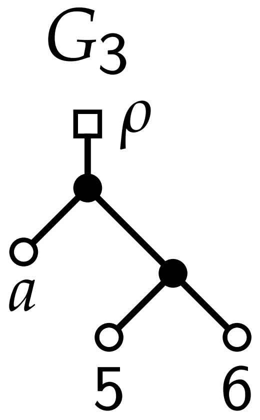
# Approximation Algorithm – Example

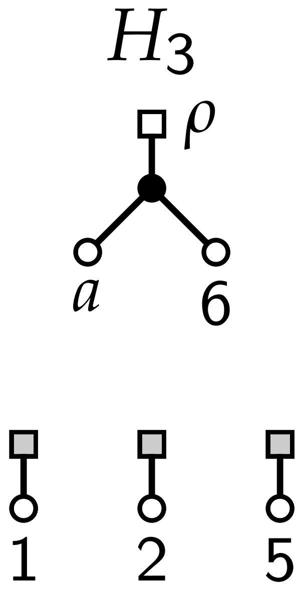



**Case 1**

- If the same "cherry" (i.e., pair of leaves) occurs in $G_i$ and $H_i$, we simply reduce it.

# Approximation Algorithm – Example

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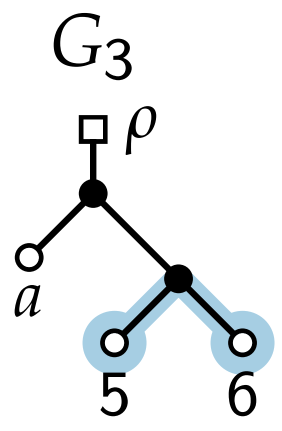
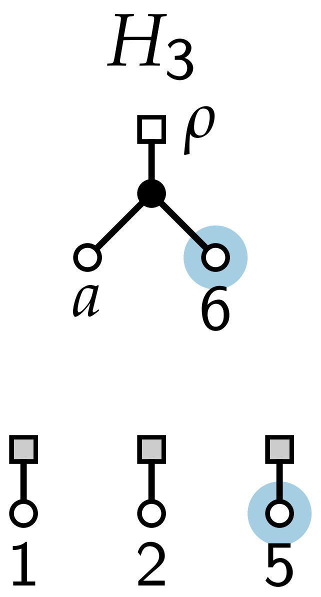
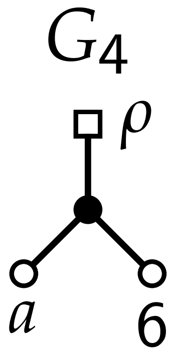


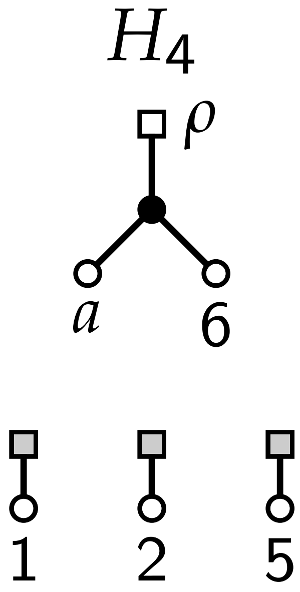




**Case 4**

- Leaf $b$ is the only leaf of a tree in $H_i$.
- Cut off $b$ in $G_i$.

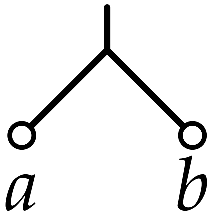
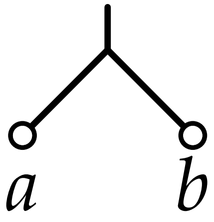
# Approximation Algorithm – Example



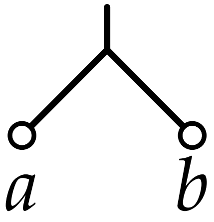
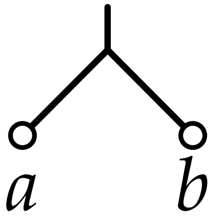
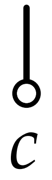




- Return 3.

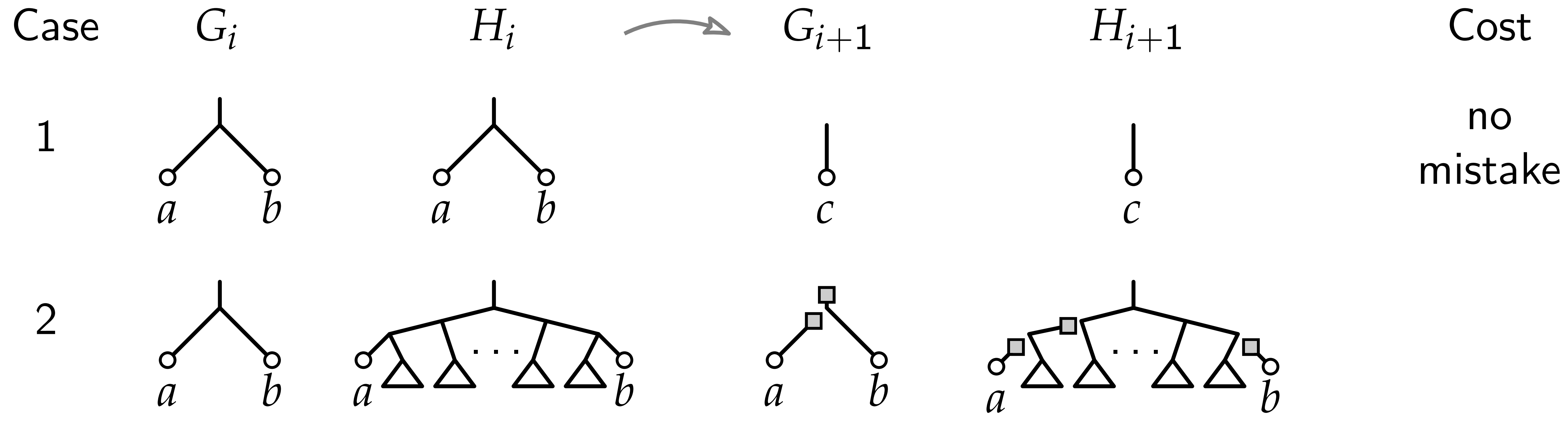
# Approximation Algorithm – Analysis

| Case | $G_i$ | $H_i$ | → | $G_{i+1}$ | $H_{i+1}$ | Cost |
|---|---|---|---|---|---|---|
| 1 |  |  | |  |  | |

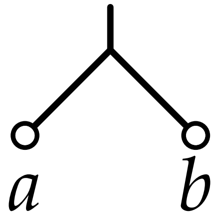
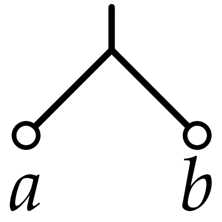
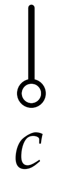
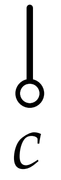
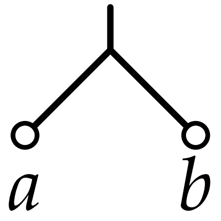
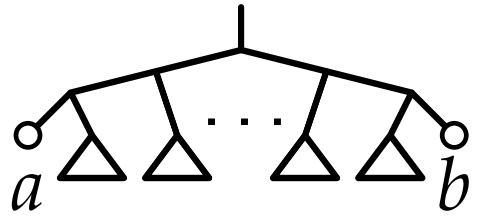
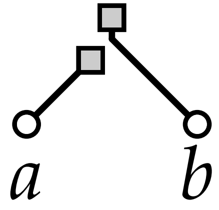
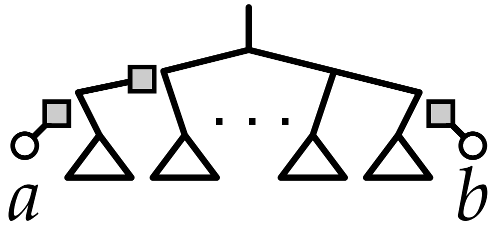
# Approximation Algorithm – Analysis

| Case | $G_i$ | $H_i$ | $G_{i+1}$ | $H_{i+1}$ | Cost |
|---|---|---|---|---|---|
| 1 |   |   |   |   | no mistake |

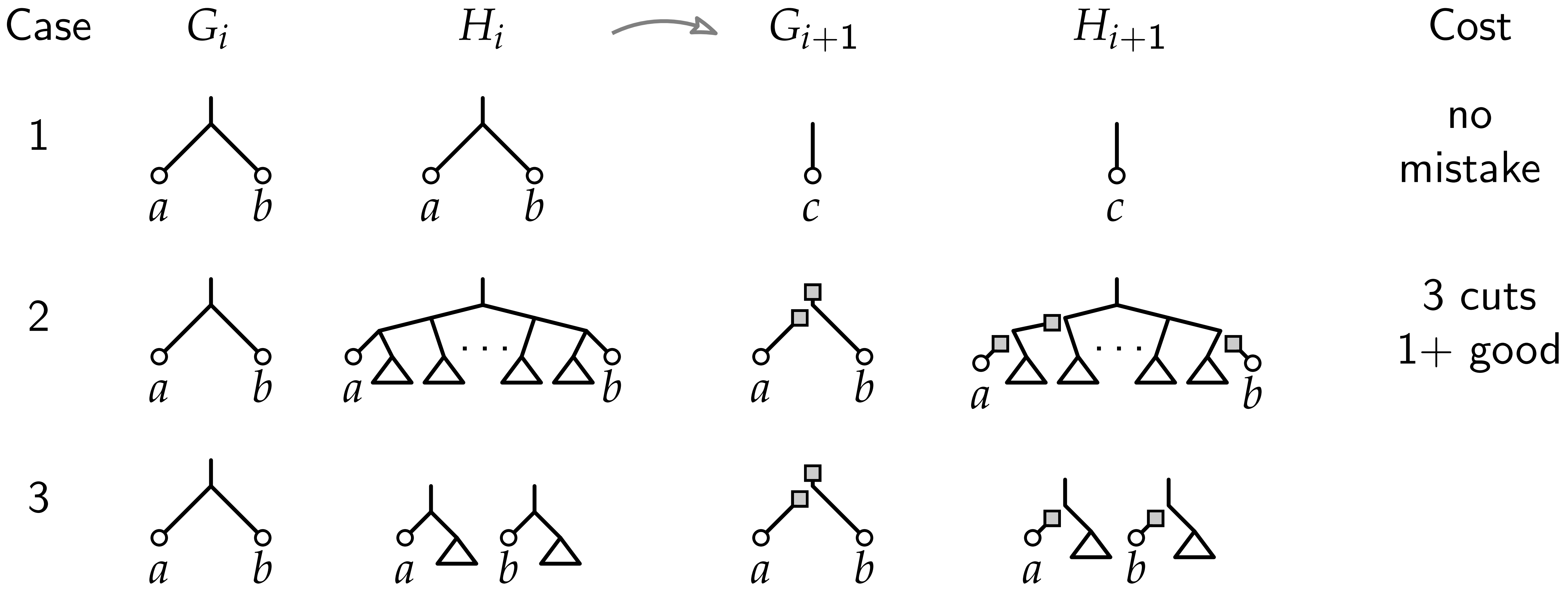
# Approximation Algorithm – Analysis



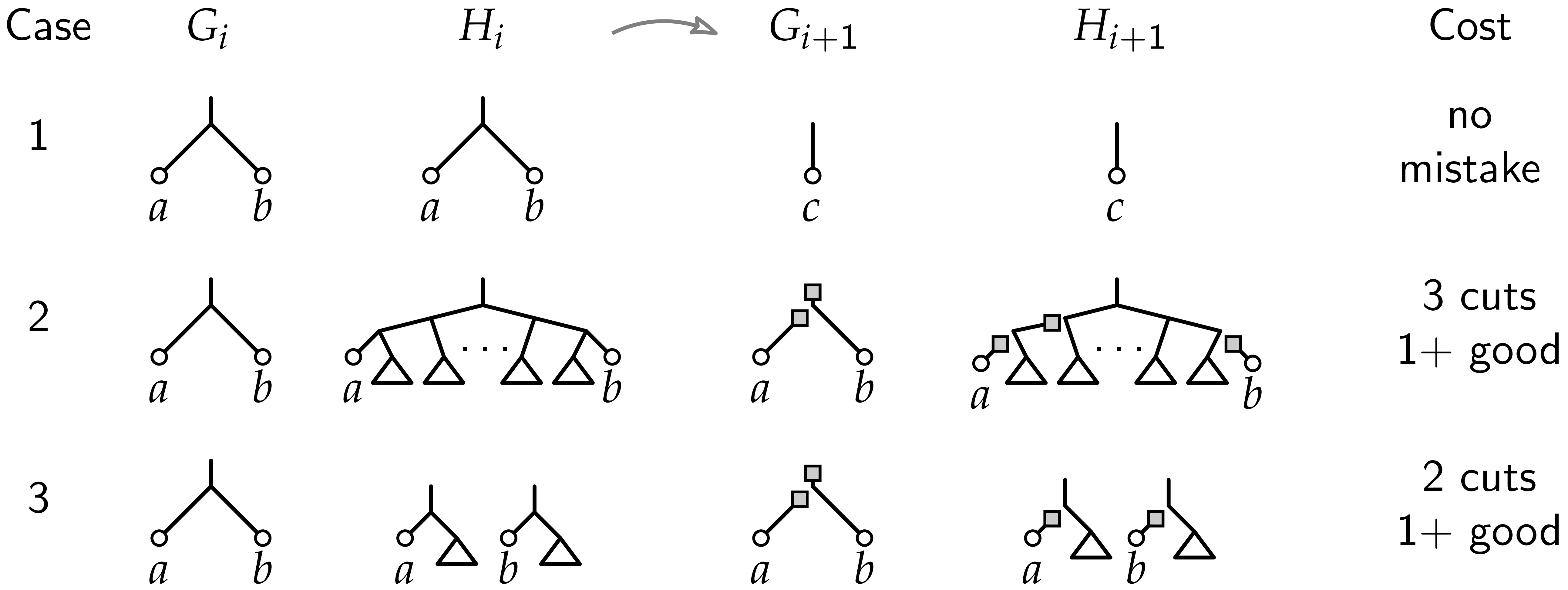
# Approximation Algorithm – Analysis

| Case | $G_i$ | $H_i$ | $G_{i+1}$ | $H_{i+1}$ | Cost |
|---|---|---|---|---|---|
| 1 |  |  |  |  | no mistake |
| 2 |  |  |  |  | 3 cuts<br>1+ good |

# Approximation Algorithm – Analysis



# Approximation Algorithm – Analysis



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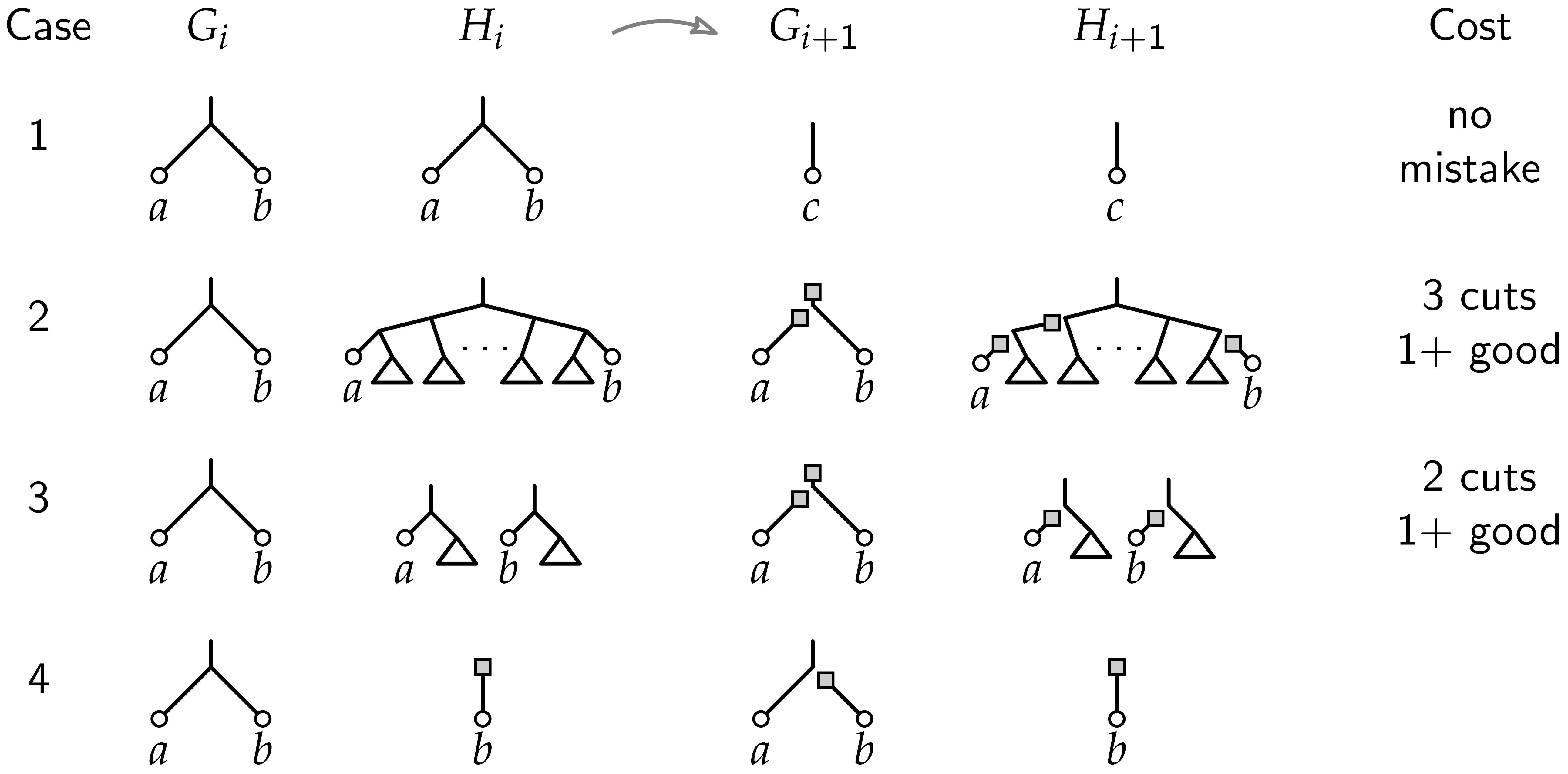

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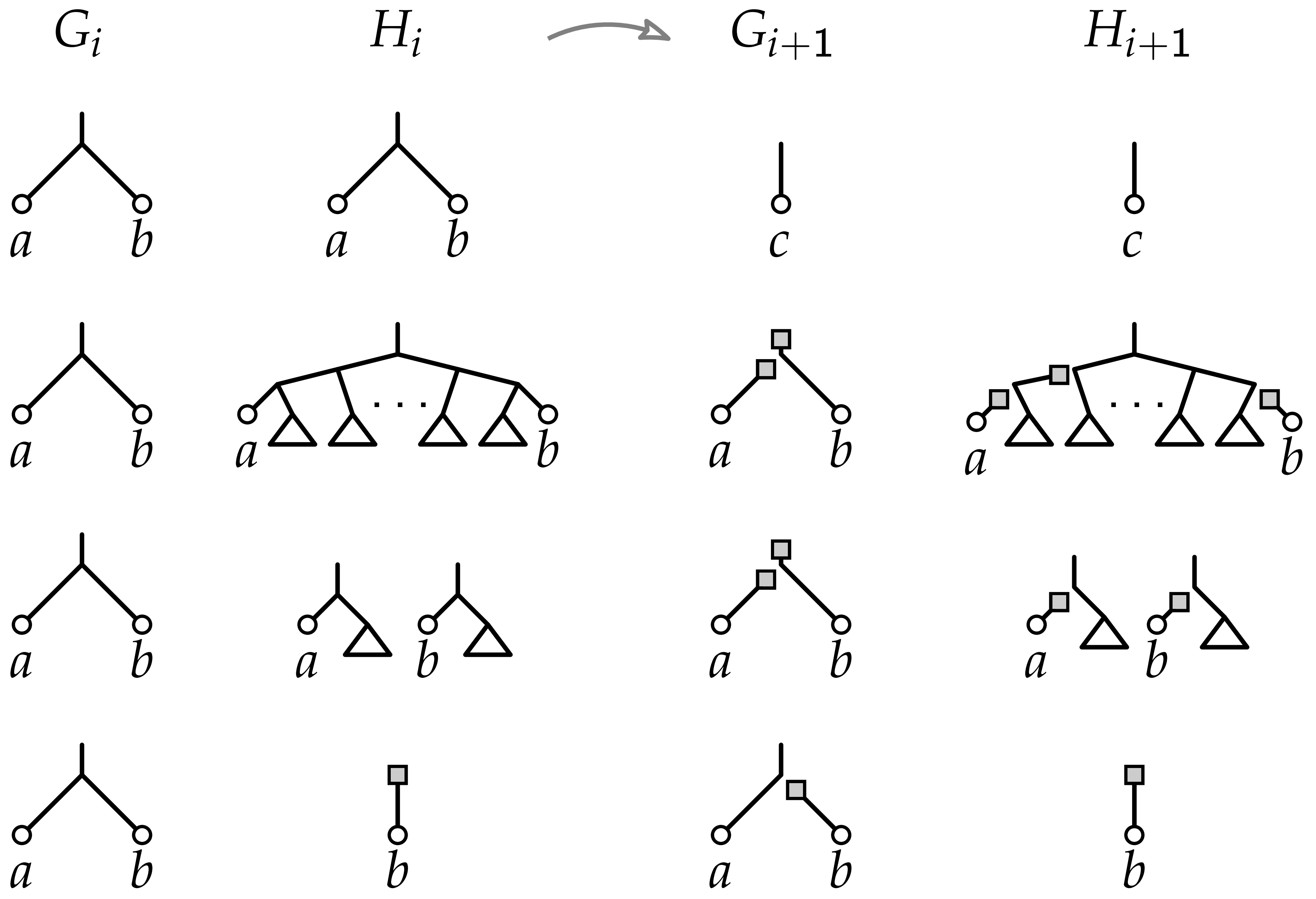
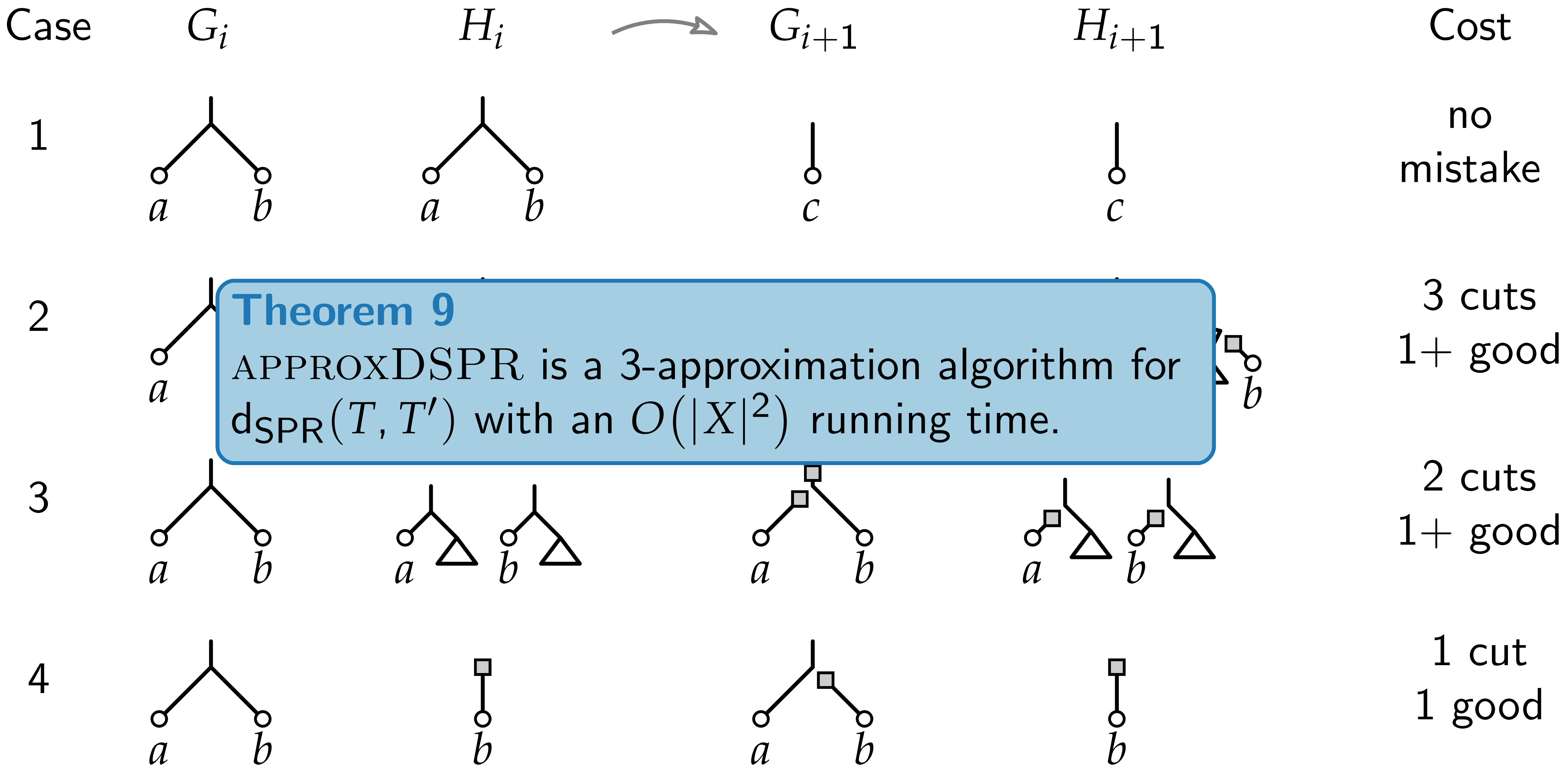



| Case | Cost |
|---|---|
| 1 | no mistake |
| 2 | 3 cuts<br>1+ good |
| 3 | 2 cuts<br>1+ good |
| 4 | 1 cut<br>1 good |

# Approximation Algorithm – Analysis




**Theorem 9**

ApproxDSPR is a 3-approximation algorithm for $d_{\mathsf{SPR}}(T, T')$ with an $O(|X|^2)$ running time.

# Discussion

**Kernelization.**

- Kernelization is an important technique to construct FPT algorithms.
- Result important since SPR-distance small in practice.
- Reduction rules actually give a kernel of size at most $15k - 9$ (we have shown $28k$).
- With further reduction rules, we can get a size below $11k - 9$. [KL '18]
- Divide & conquer techniques can (in practice) further reduce the problem sizes. [LS '11]

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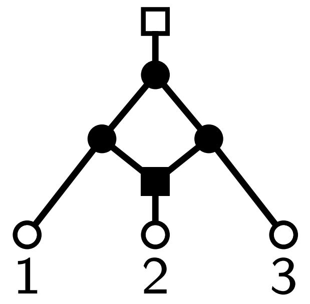
## Approximation algorithm.

- There exists a 2-approximation algorithms for the SPR-distance with a running time in $\mathcal{O}(n^3)$. [CHW '17]

# Discussion

## Phylogenetic trees.

- There are other classes of phylogenetic trees: unrooted, non-binary, ranked, . . .
- Trees can be generalized to **phylogenetic networks**, which can also have indegree 2 outdegree 1 vertices.



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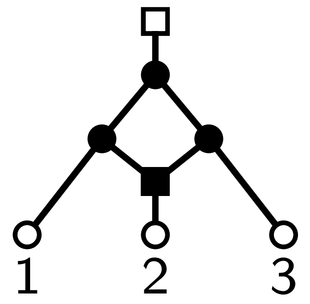


## Maximum Agreement Forests.

- Reframing (characterizing) a problem in a different way, can sometimes make your life a lot easier.
- MAF can be generalized to Maximum Agreement Graphs, but these do not characterize the SPR-distance of networks anymore. [K '20]

# Literature

Original papers:


- [BS '05] Semple C., Bordewich M.: *On the computational complexity of the rooted subtree prune and regraft distance* (for SPR, MAF, characterisation, fpt, divide & conquer)
- [HJWZ '96] Hein J., Jiang T., Wang L., Zhang K.: *On the complexity of comparing evolutionary trees* (for NP-hardness proof)
- [RSW '06] Rodrigues E. M., Sagot M.-F., Wakabayashi Y.: *The maximum agreement forest problem: Approximation algorithms and computational experiments* (for approx. algorithm)


Referenced papers:


- [CHW '17] Chen Z., Harada Y., Wang L.: *A new 2-approximation algorithm for rSPR distance*
- [K '20] Klawitter J.: *The agreement distance of unrooted phylogenetic networks*
- [KL '19] Kelk S., Linz. S.: *New reduction rules for the tree bisection and reconnection distance*
- [LS '11] Linz S., Semple C.: *A cluster reduction for computing the subtree distance between phylogenies*