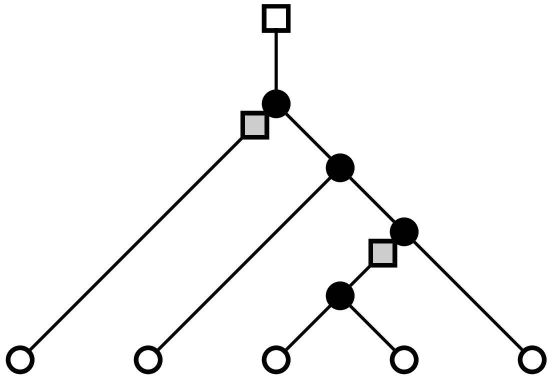
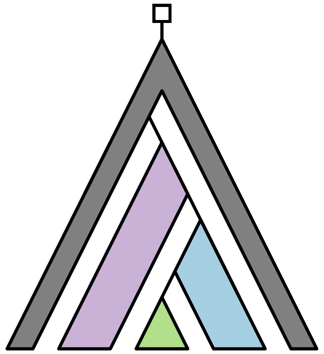
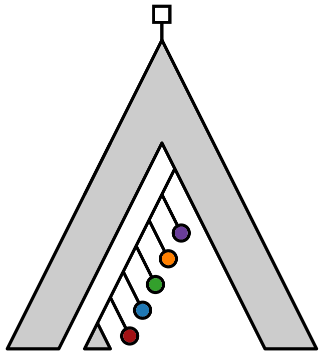
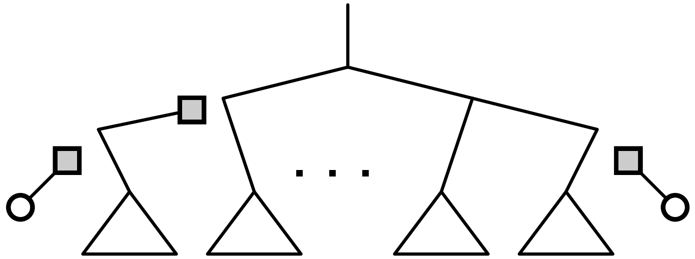
Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Advanced Algorithms

Rearrangement distance of phylogenetic trees

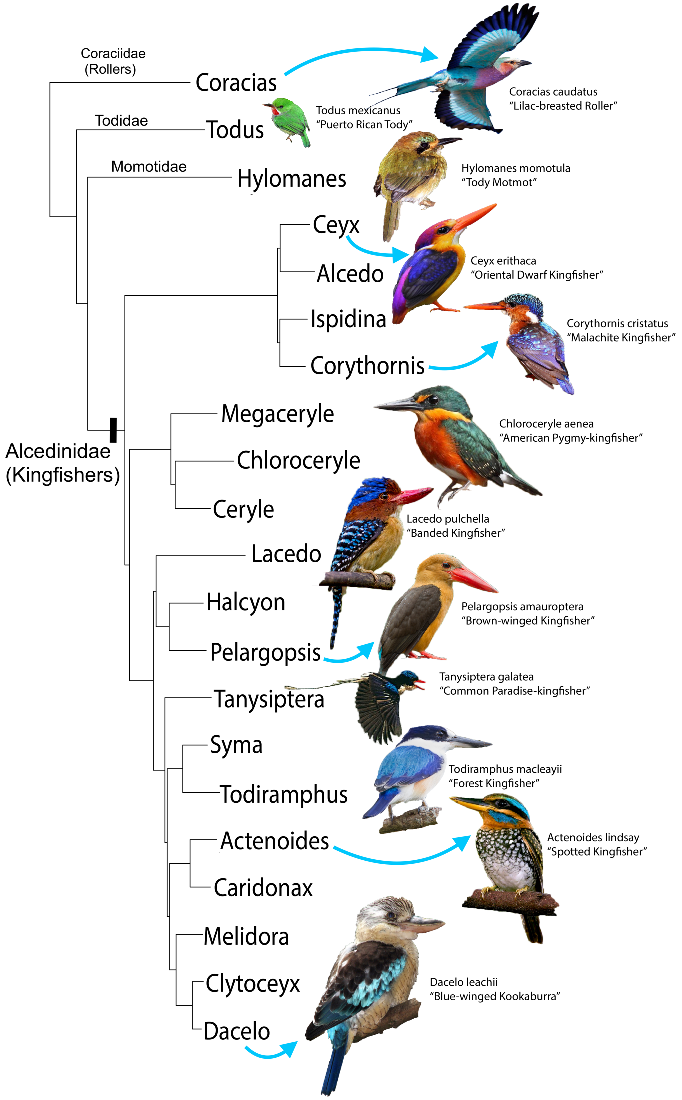
Kernelisation, fpt and approximation algorithm

Jonathan Klawitter · WS20

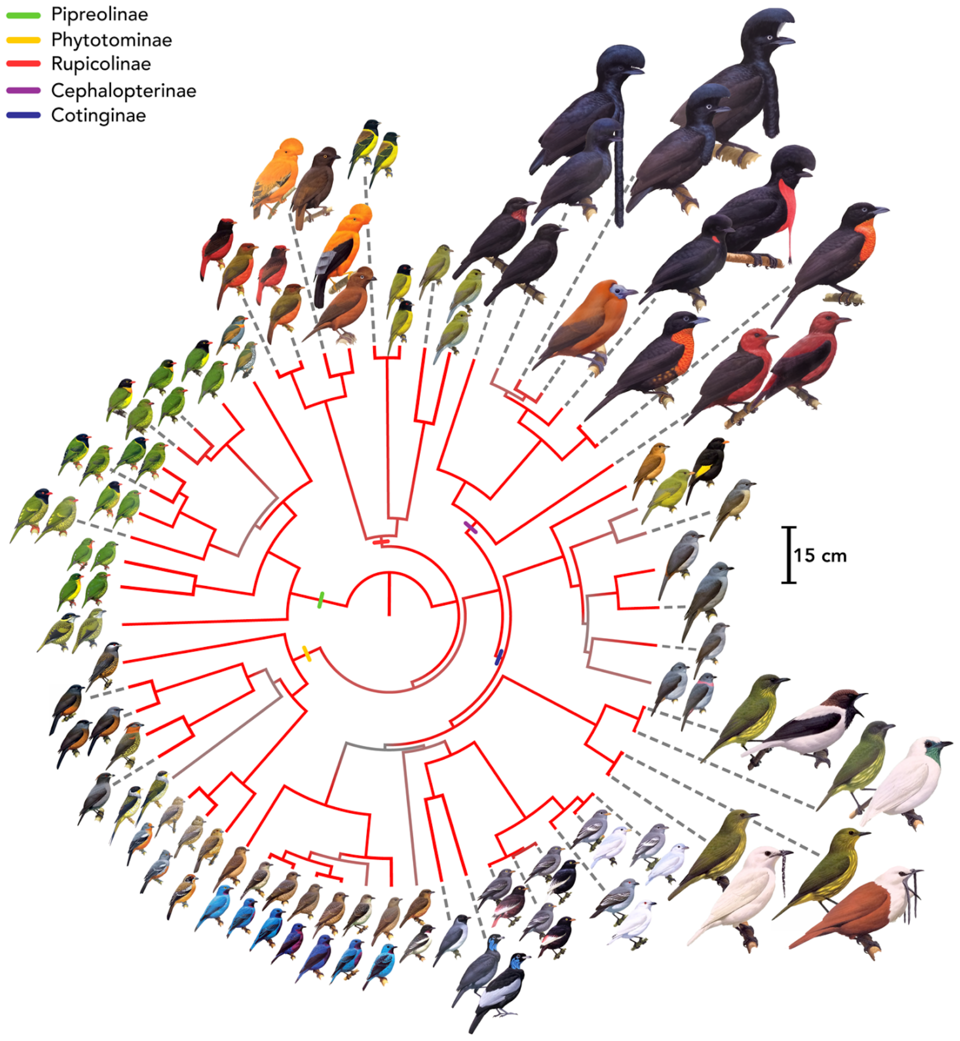





Phylogenetic trees

… represent the evolutionary history of a set of taxa.


Coraciidae (Rollers)
Coracias
Todidae
Todus
Momotidae
Hylomanes
Ceyx
Alcedo
Ispidina
Corythornis
Megaceryle
Chloroceryle
Ceryle
Lacedo
Halcyon
Pelargopsis
Tanysiptera
Syma
Todiramphus
Actenoides
Caridonax
Melidora
Clytoceyx
Dacelo
Alcedinidae (Kingfishers)
Coracias caudatus “Lilac-breasted Roller”
Todus mexicanus “Puerto Rican Tody”
Hylomanes momotula “Tody Motmot”
Ceyx erithaca “Oriental Dwarf Kingfisher”
Corythornis cristatus “Malachite Kingfisher”
Chloroceryle aenea “American Pygmy-kingfisher”
Lacedo pulchella “Banded Kingfisher”
Pelargopsis amauroptera “Brown-winged Kingfisher”
Tanysiptera galatea “Common Paradise-kingfisher”
Todiramphus macleayii “Forest Kingfisher”
Actenoides lindsay “Spotted Kingfisher”
Dacelo leachii “Blue-winged Kookaburra”

by Jenna McCullough 2016



by Berv & Prum 2014

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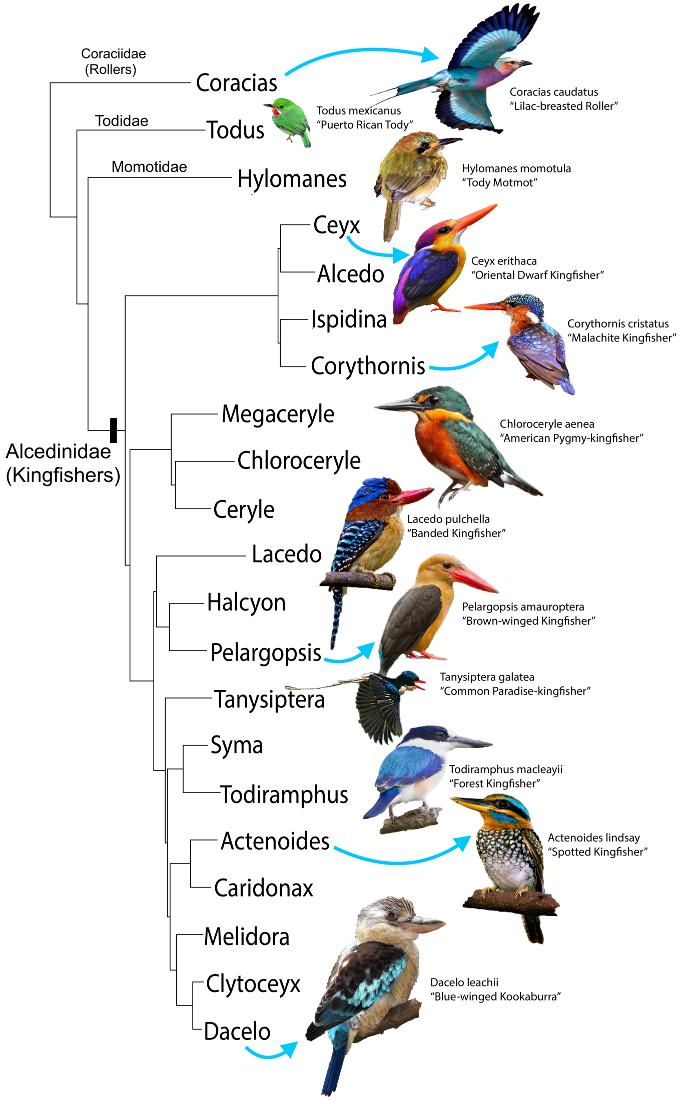

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- Leaves are labelled with taxa.
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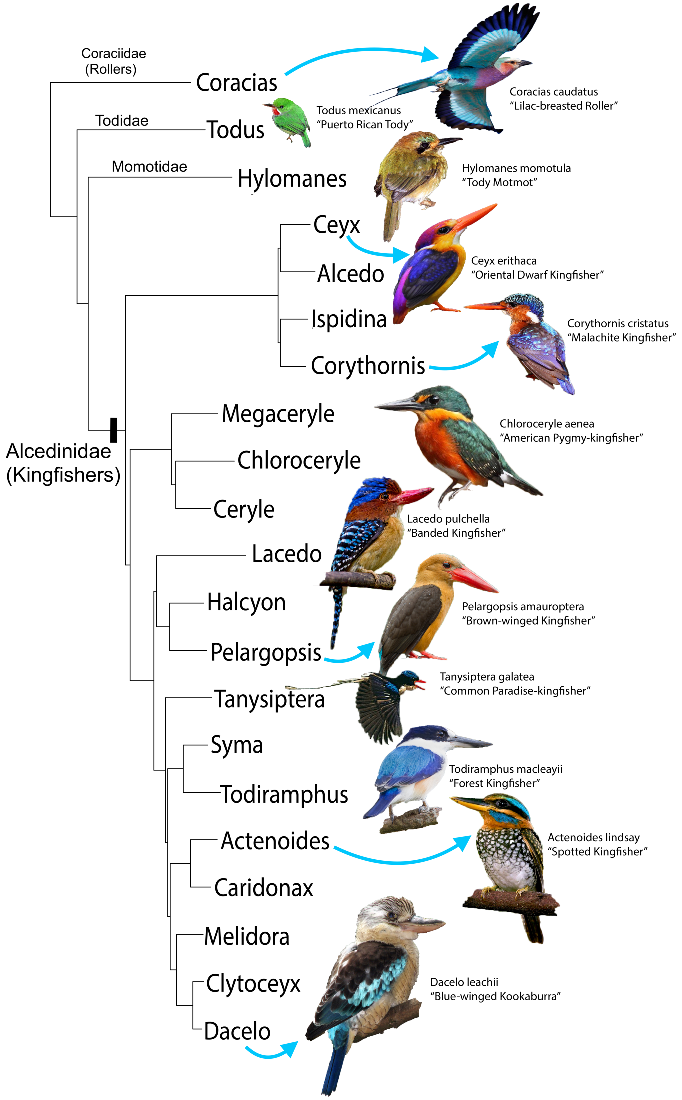

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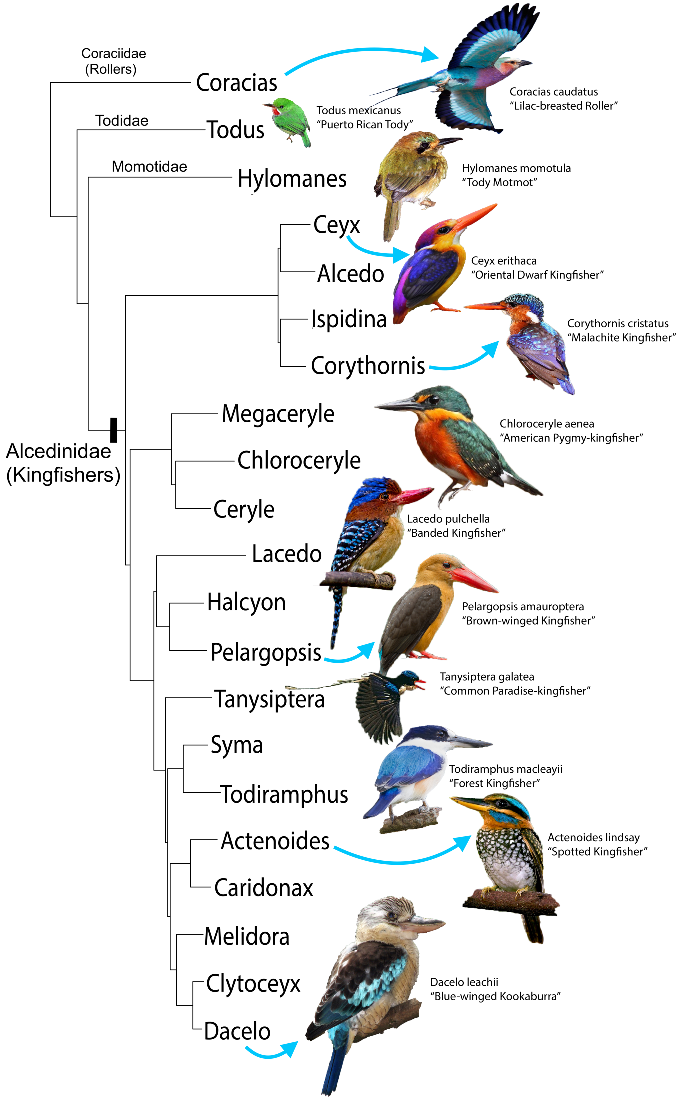

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- Edge lenghts represents amount of time passed or genetic distance.
- Inference methods compute a phylogenetic tree based on some model and data.

Phylogenetic trees

Let $X = \{1, 2, 3, \ldots n\}$.
A **(rooted, binary) phylogenetic tree** T
is a rooted tree with the following
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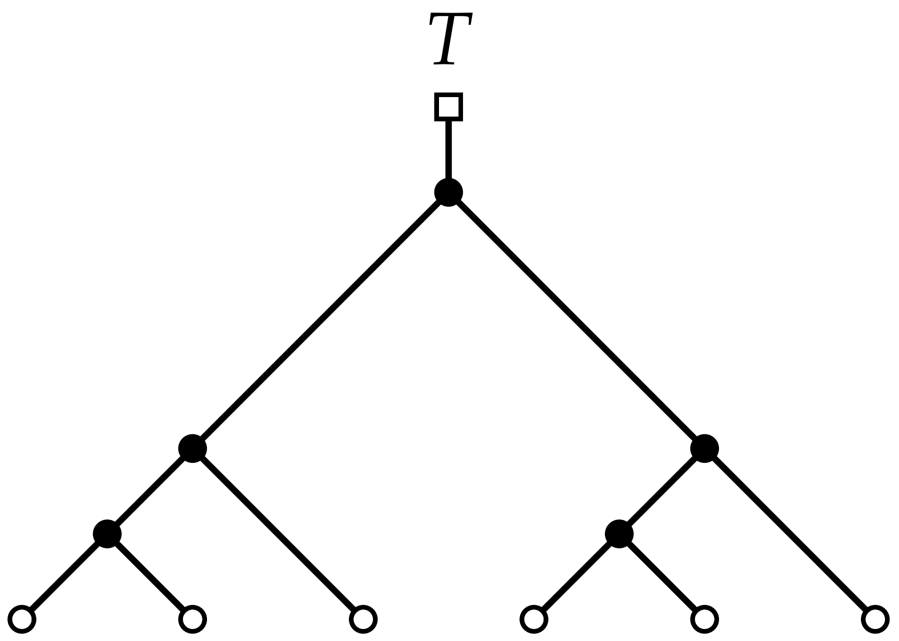

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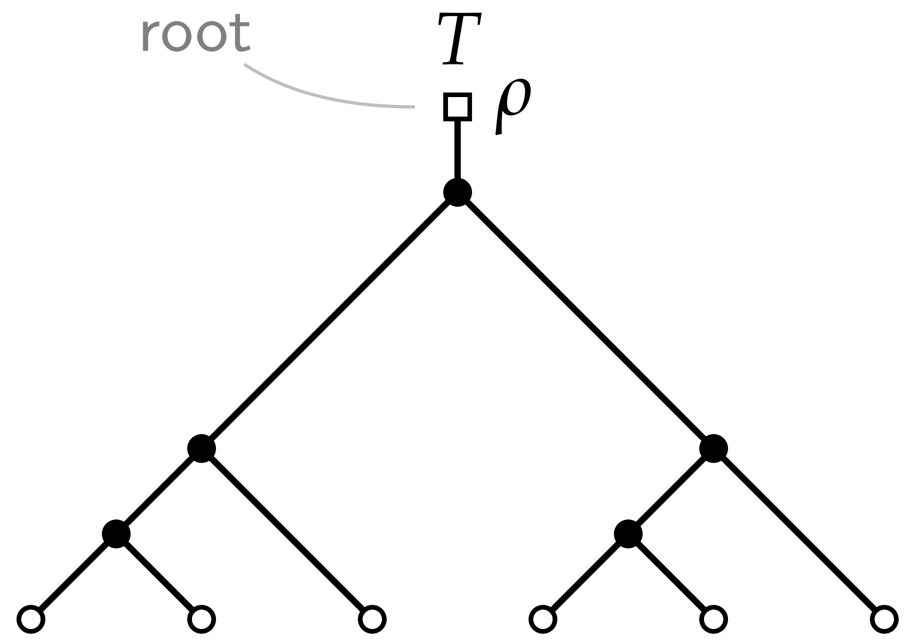

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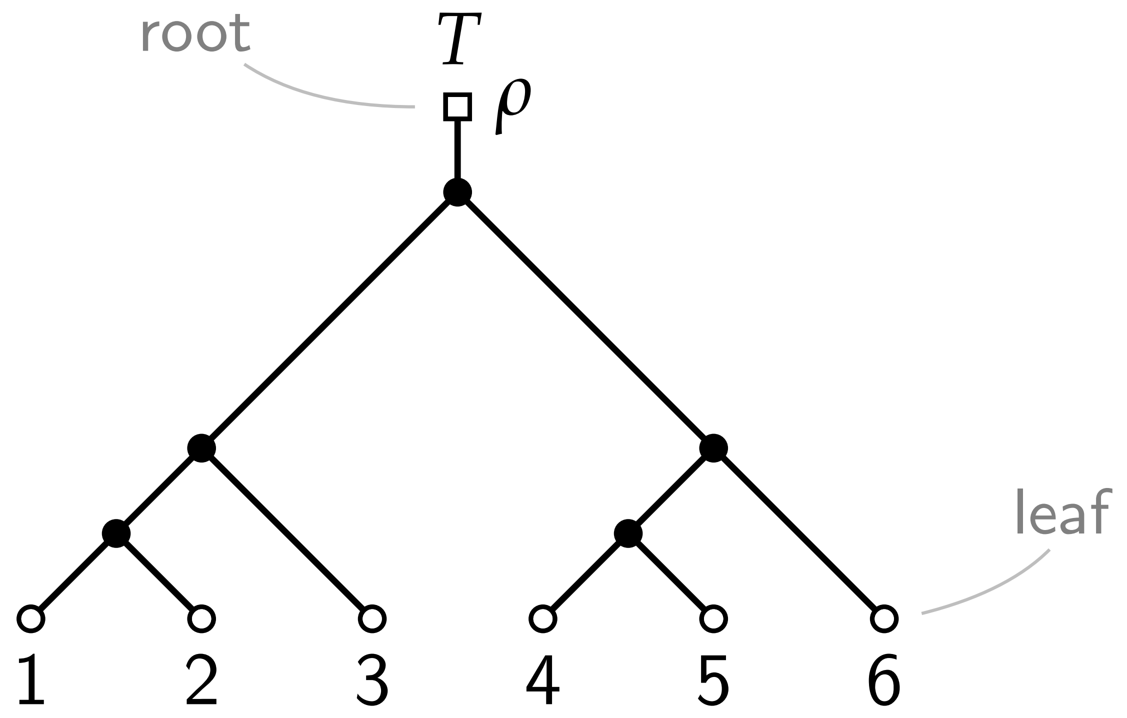

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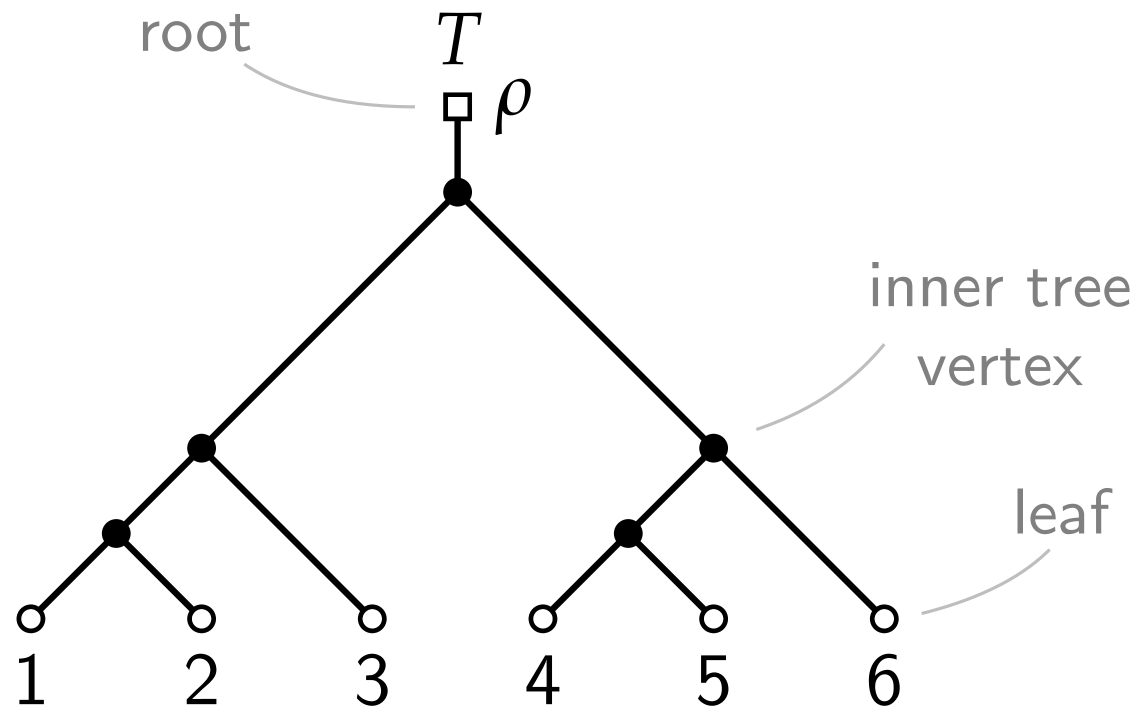

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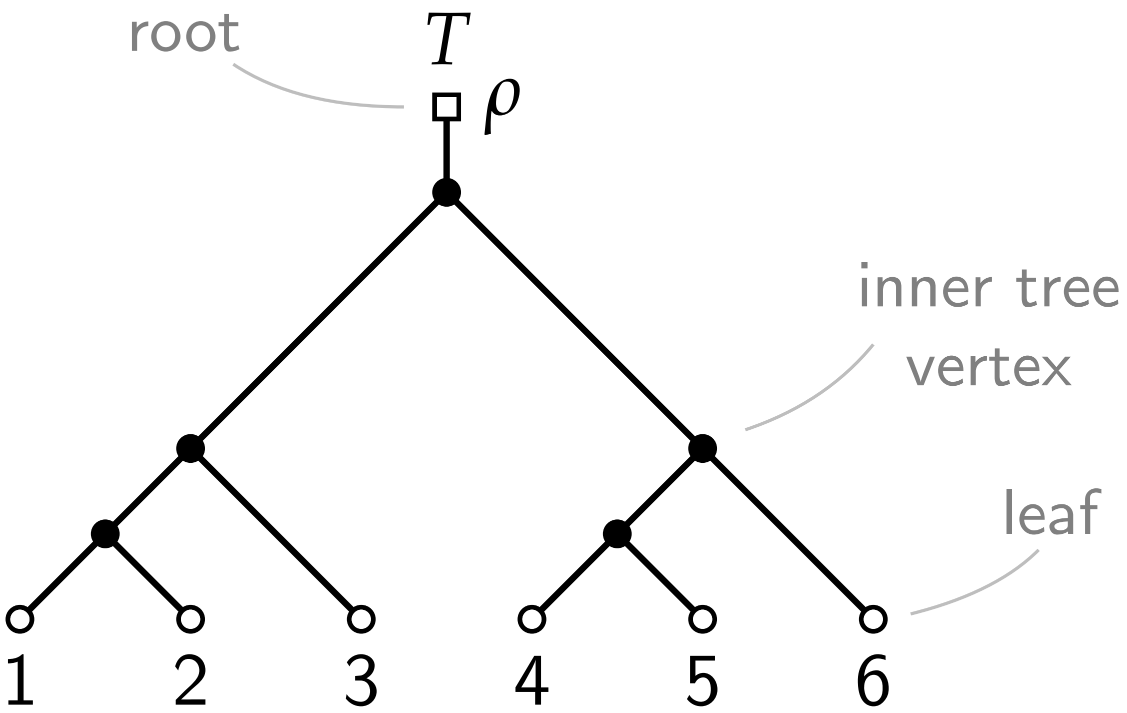
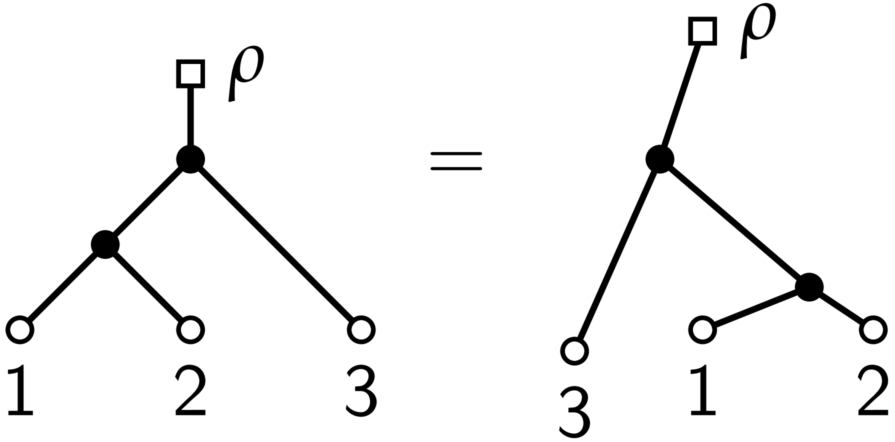


Remarks.
Here, in our definition

- vertices have **no heights** and
- the order of leaves does not matter.



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

- different inference methods,
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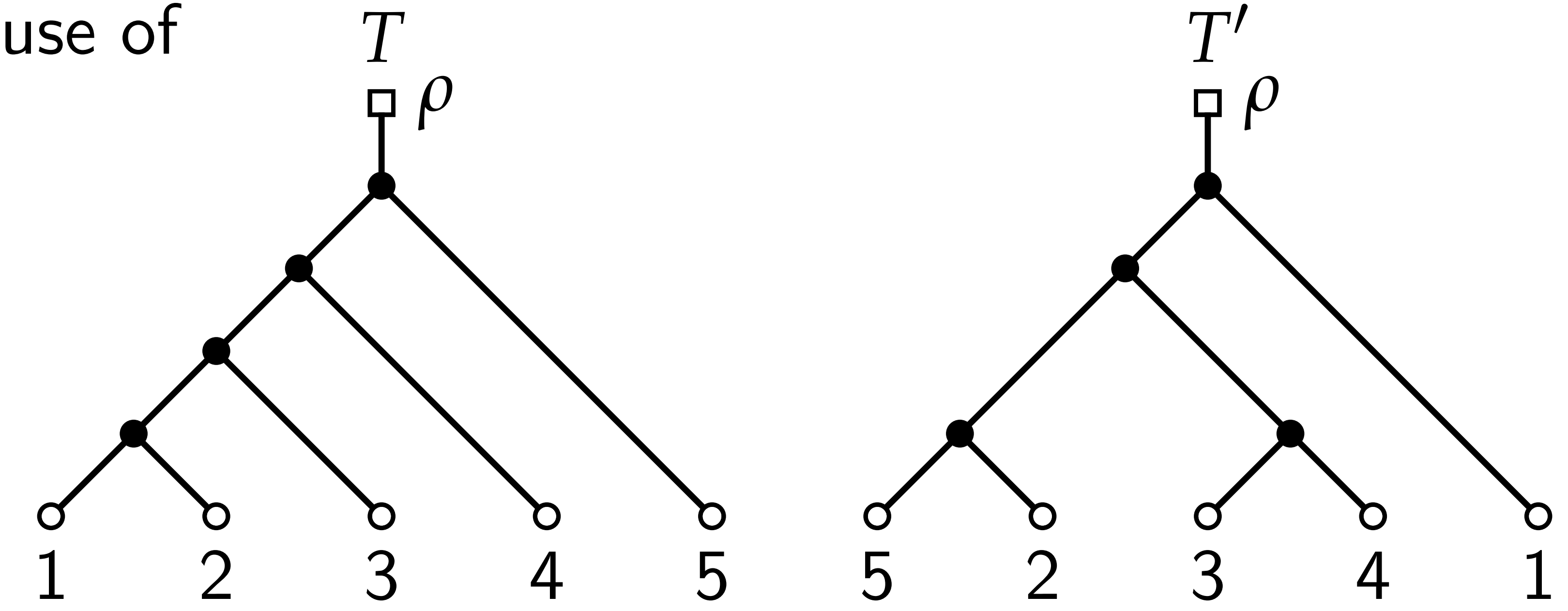

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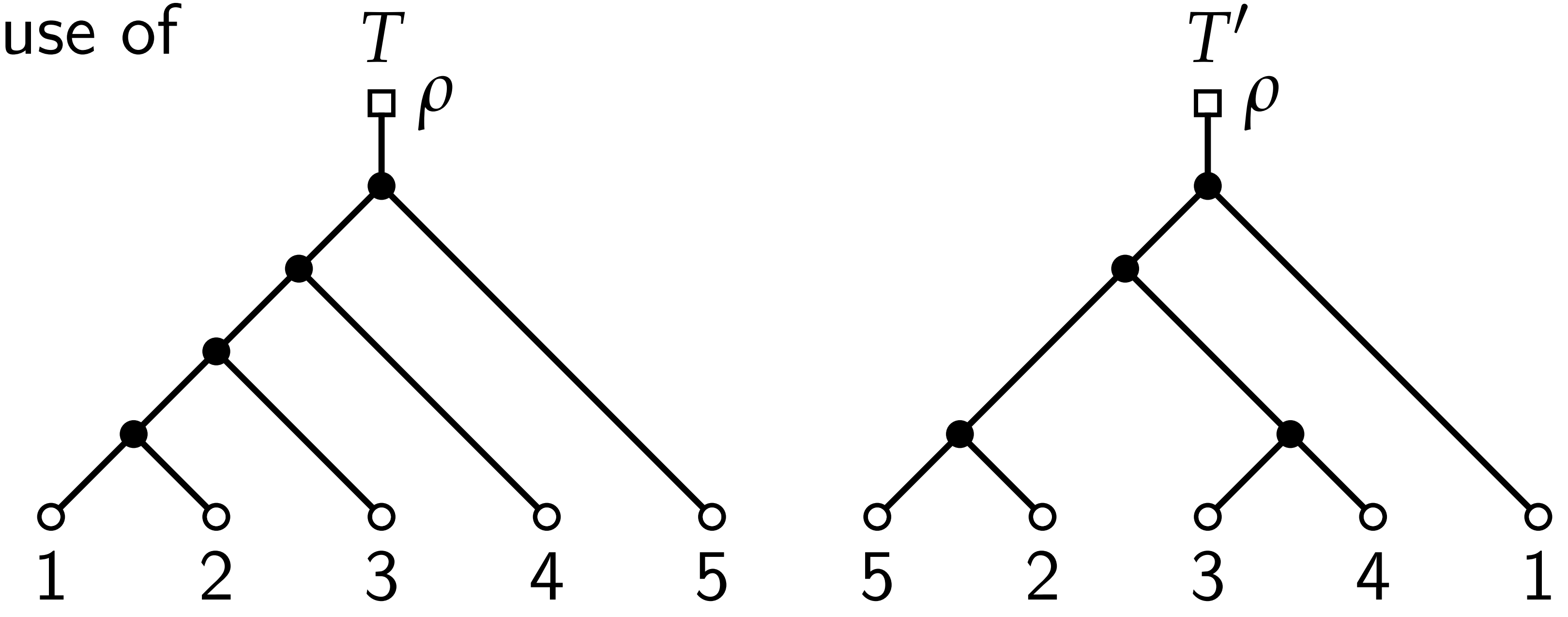

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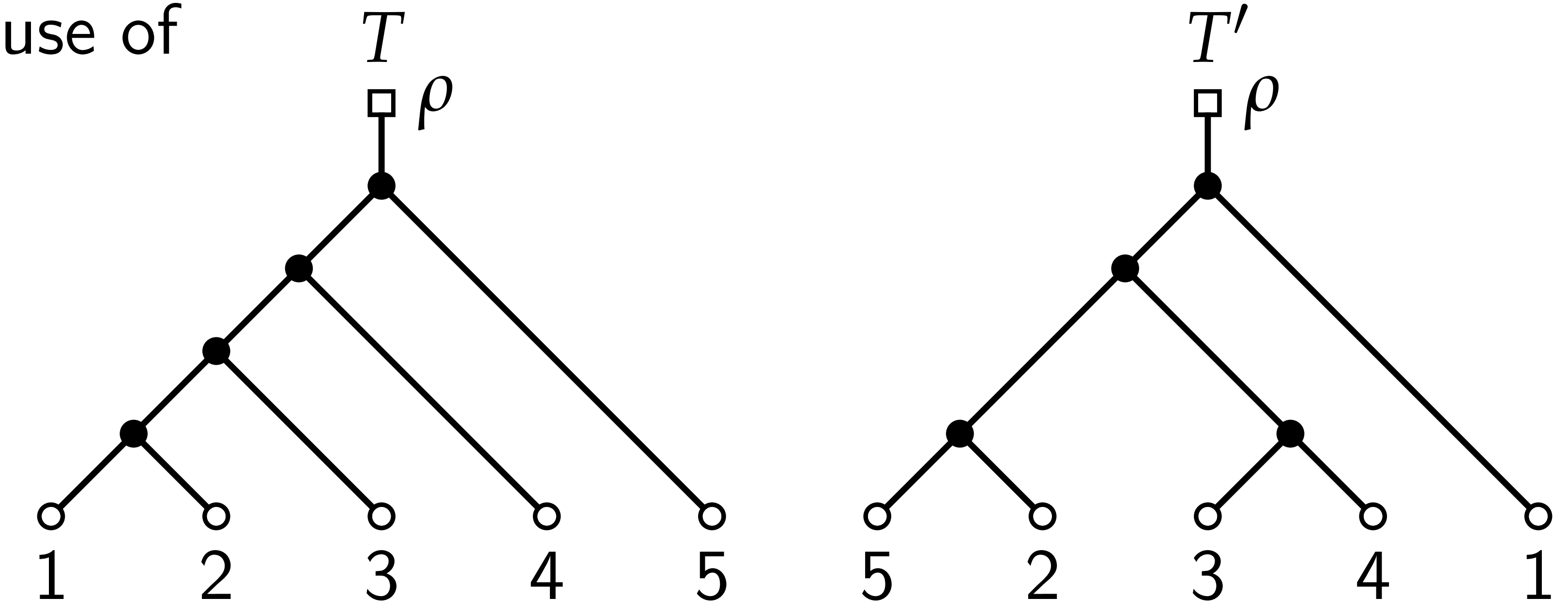

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Define a **metric** on phylogenetic trees on X and devise algorithms to compute it.

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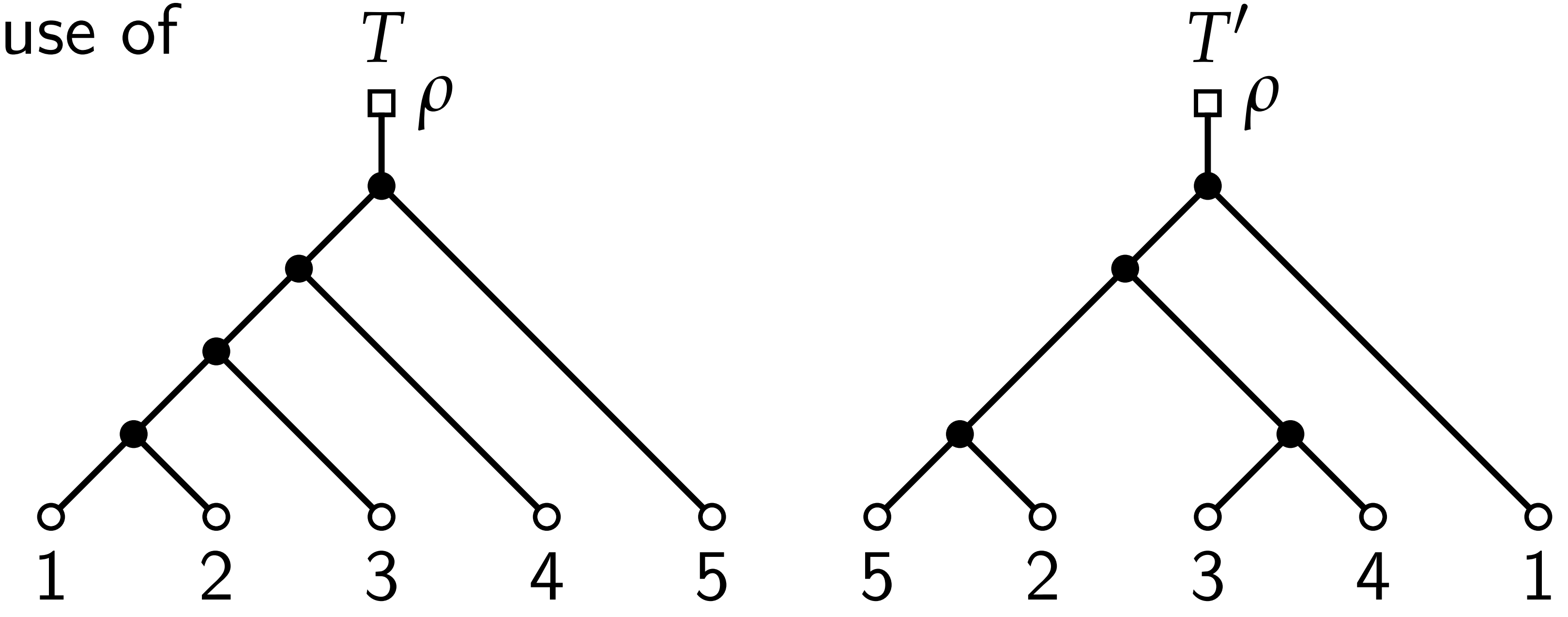

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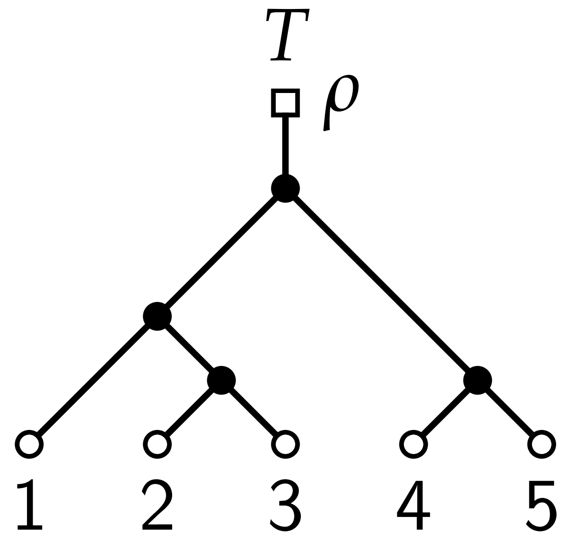
Idea.
Count the number of **rearrangement operations** that are necessary to transform T into T'.

Subtree Prune & Regraft (SPR)

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



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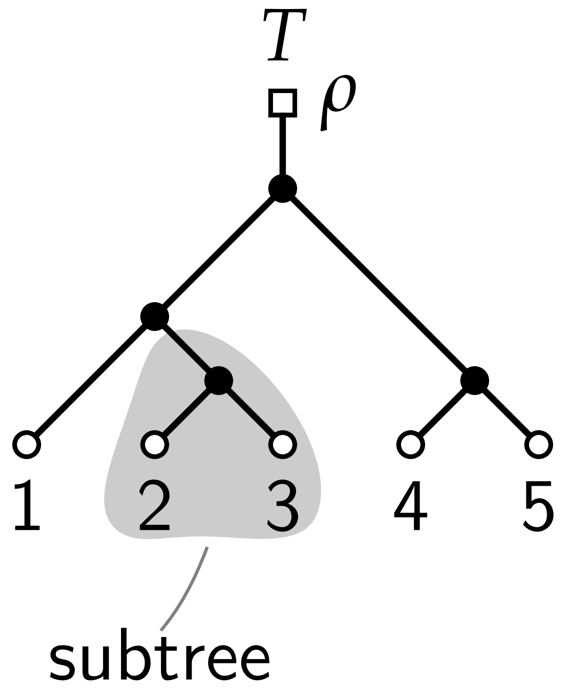

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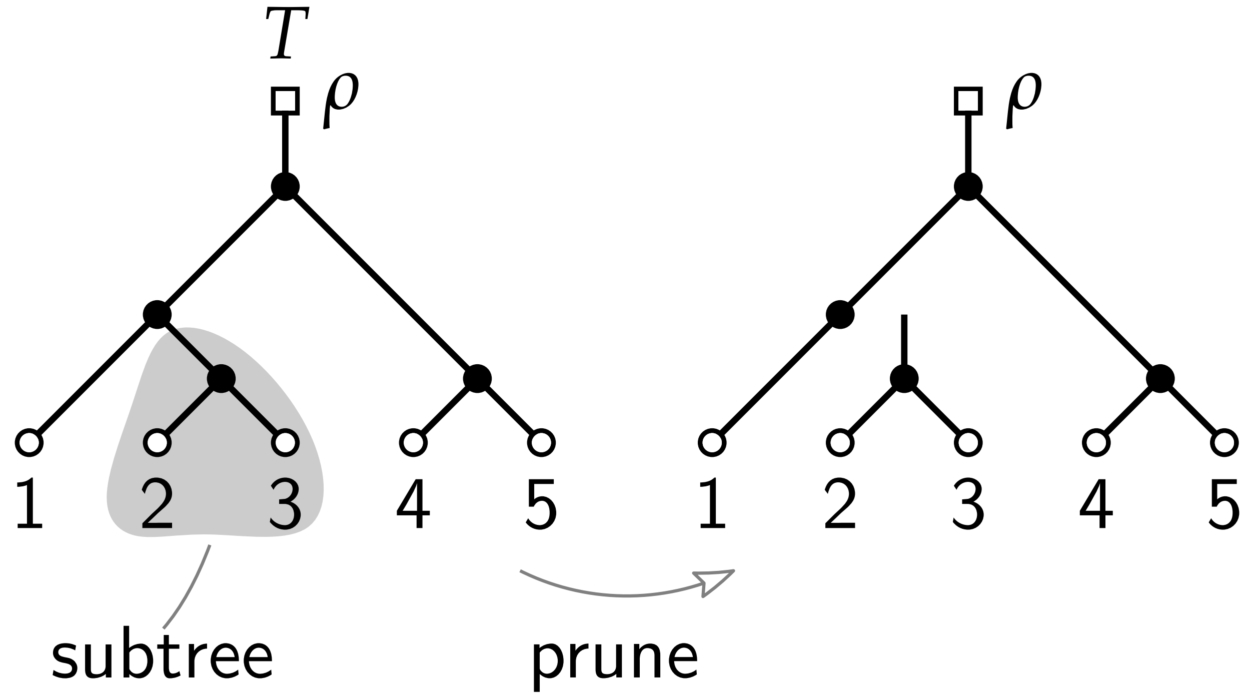

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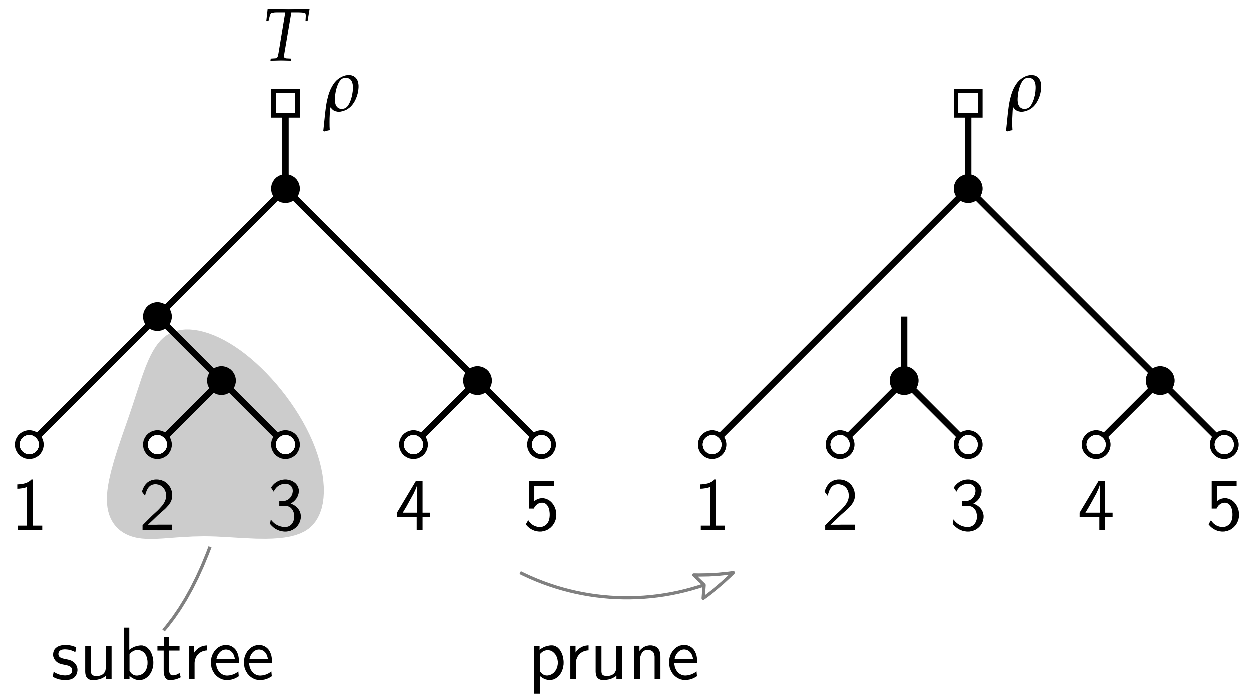

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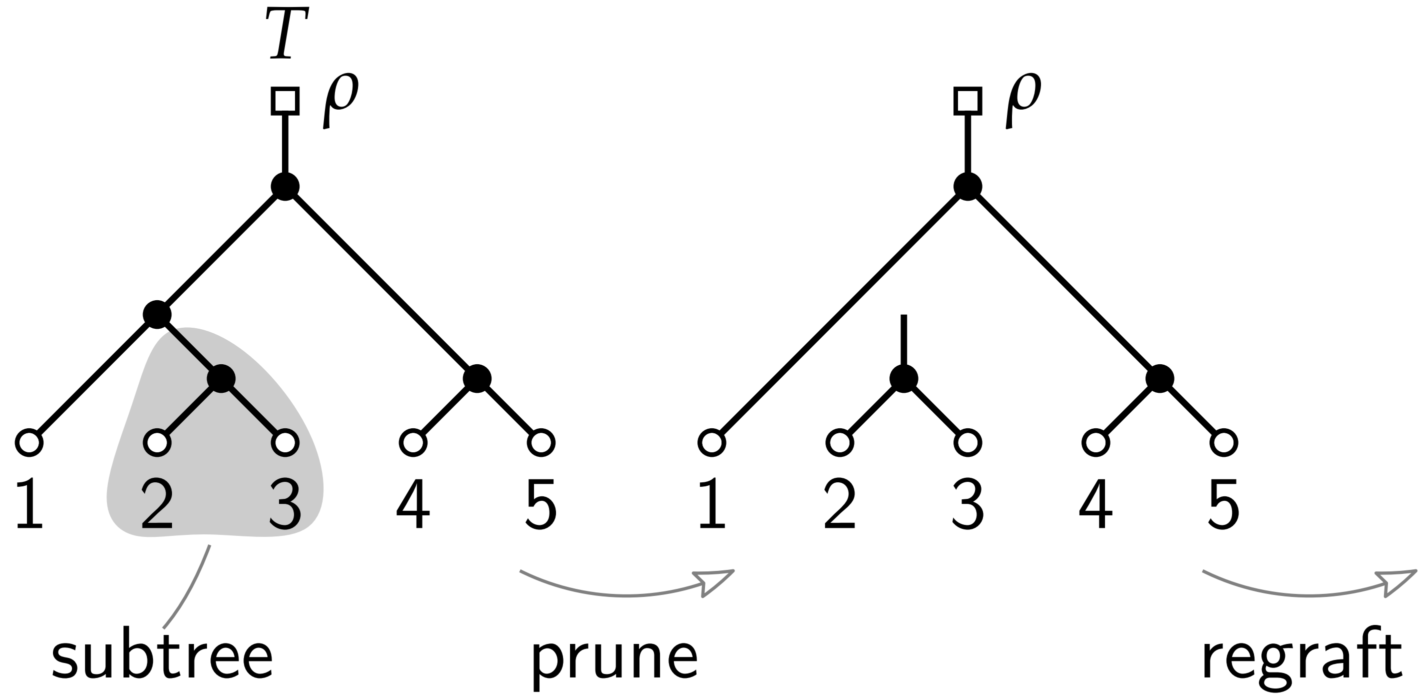

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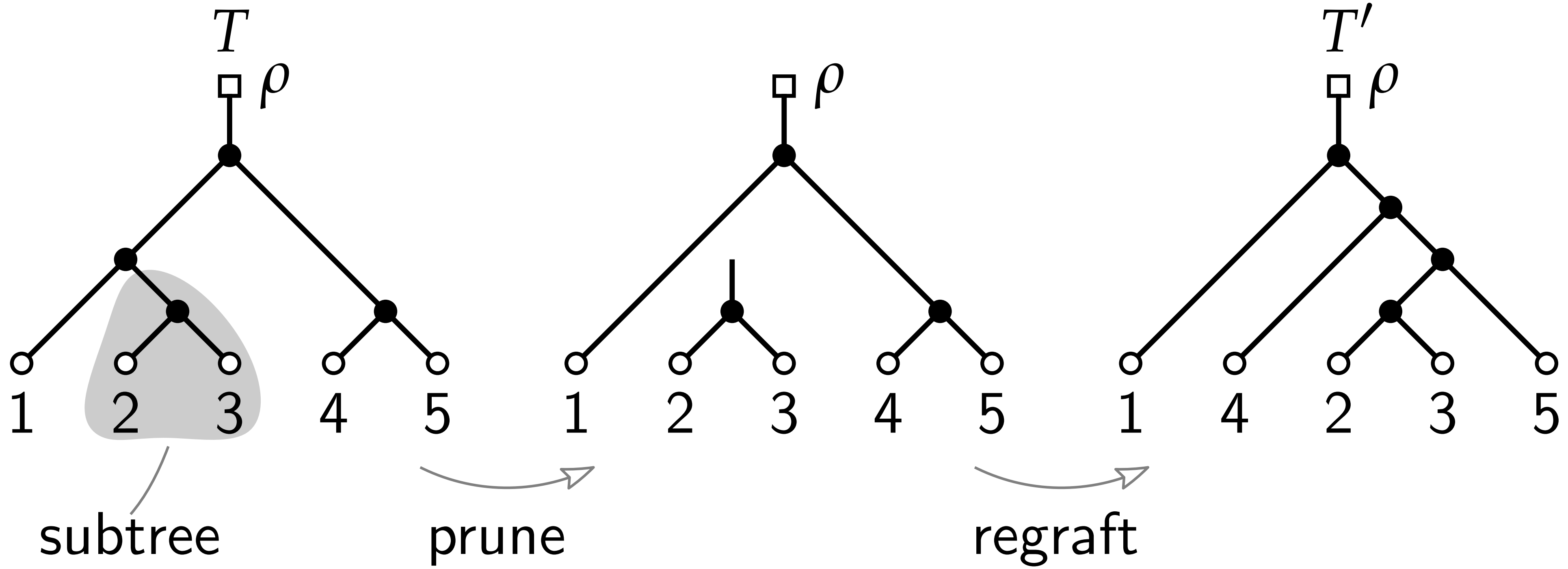

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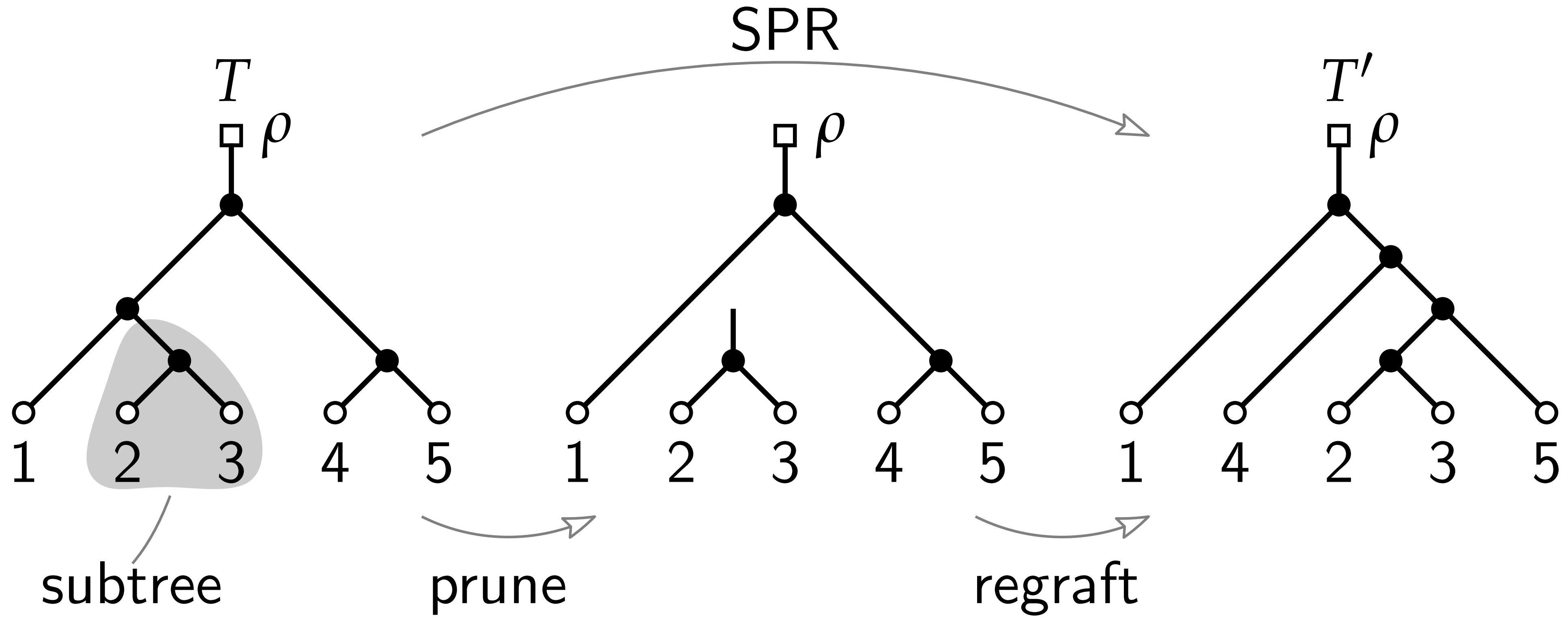

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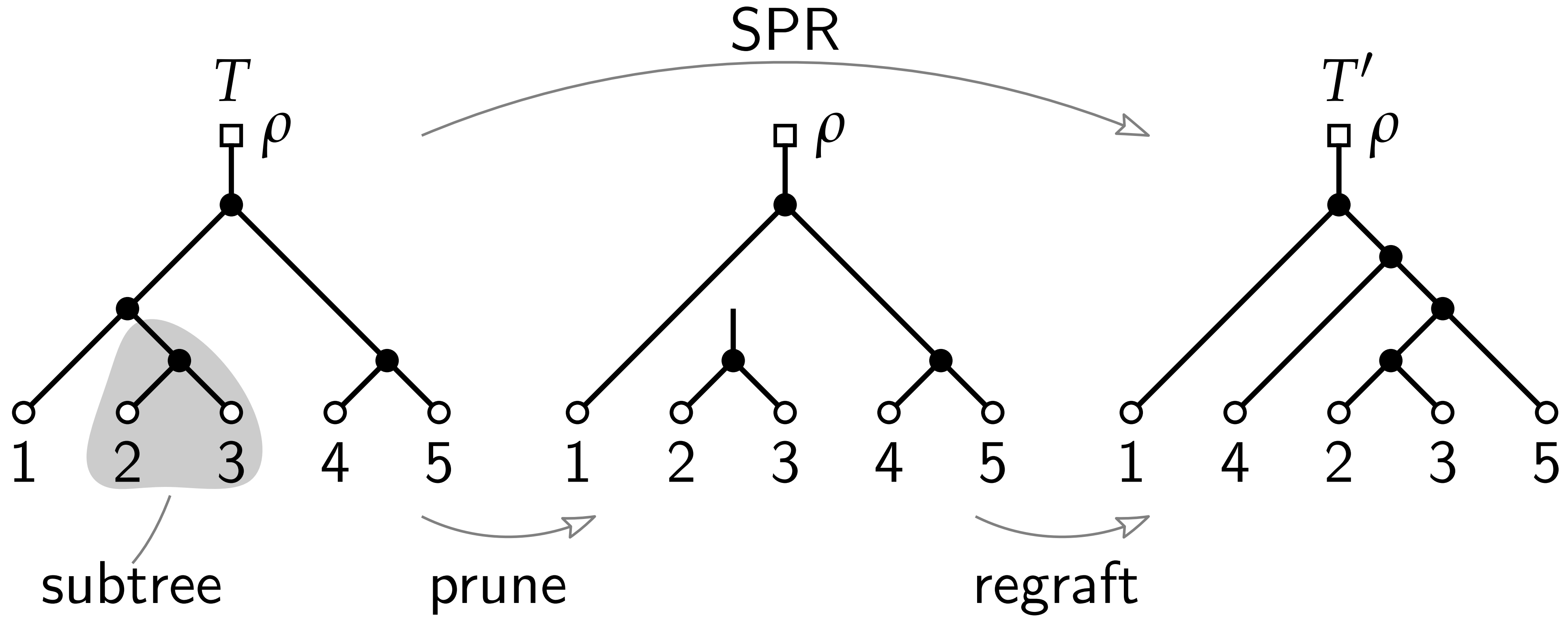

- Note that an SPR operation is reversible.

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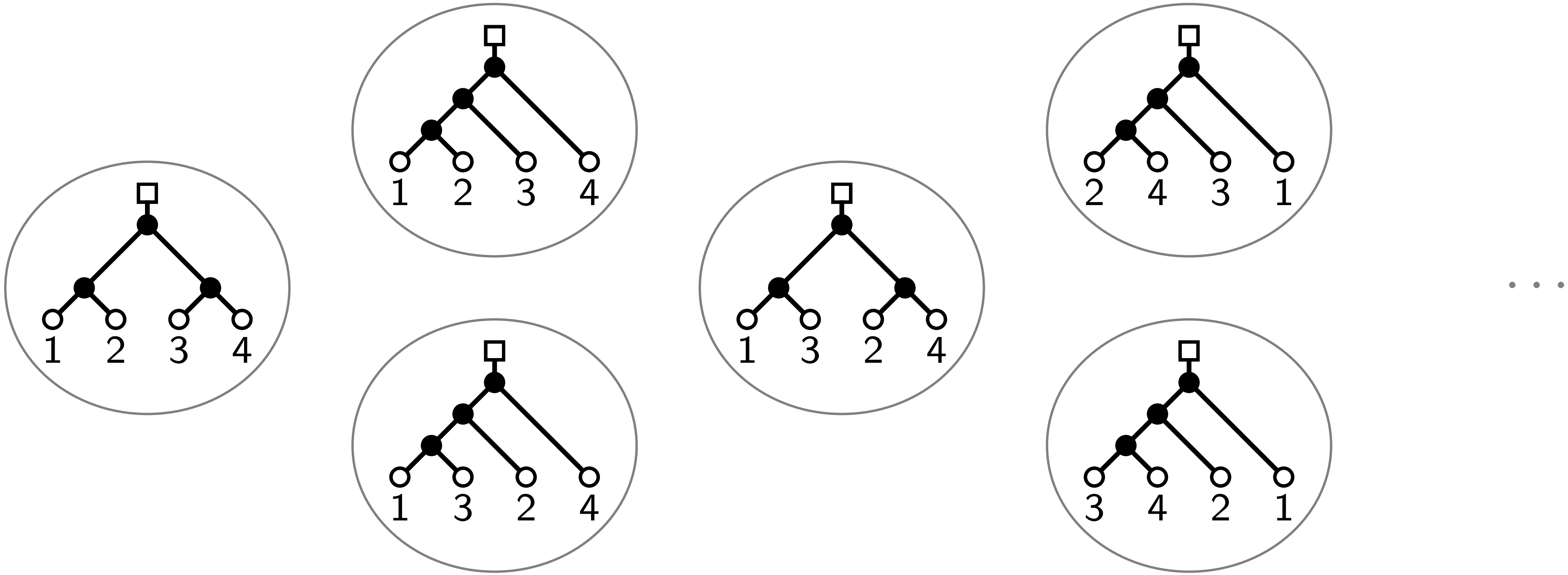

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SPR induces the **SPR-graph** $G = (V, E)$:

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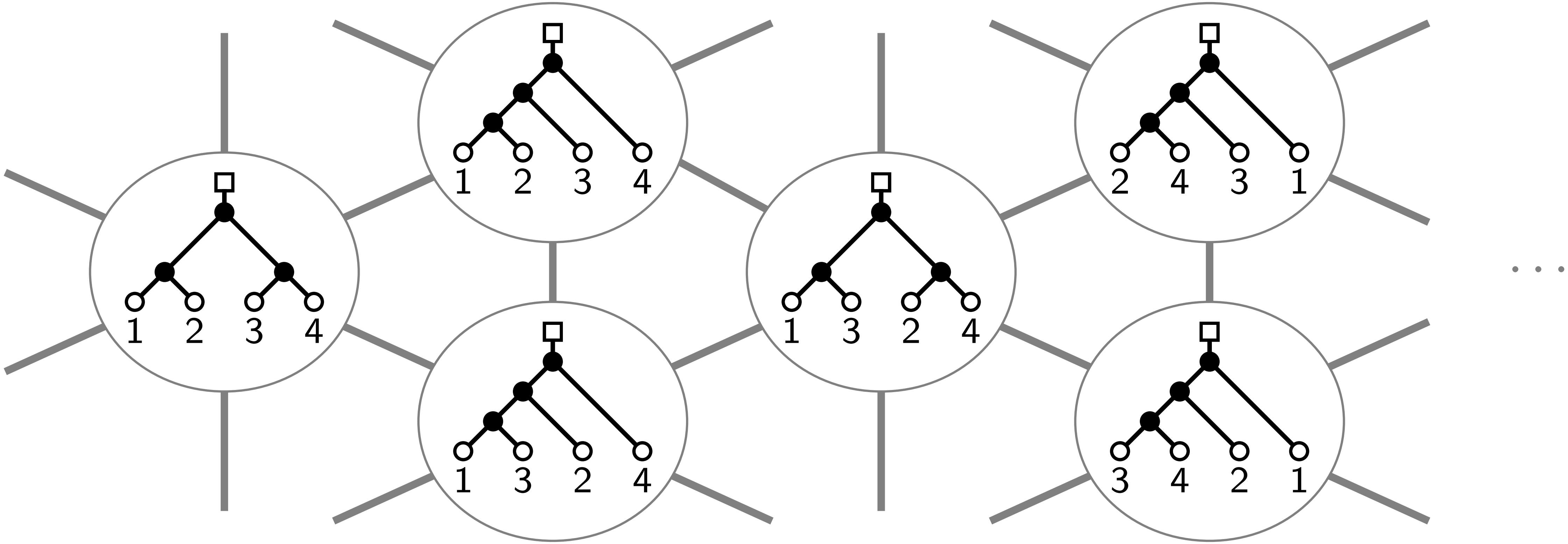
- $\{T, T'\} \in E$ if T can be transformed into T' with a single SPR operation



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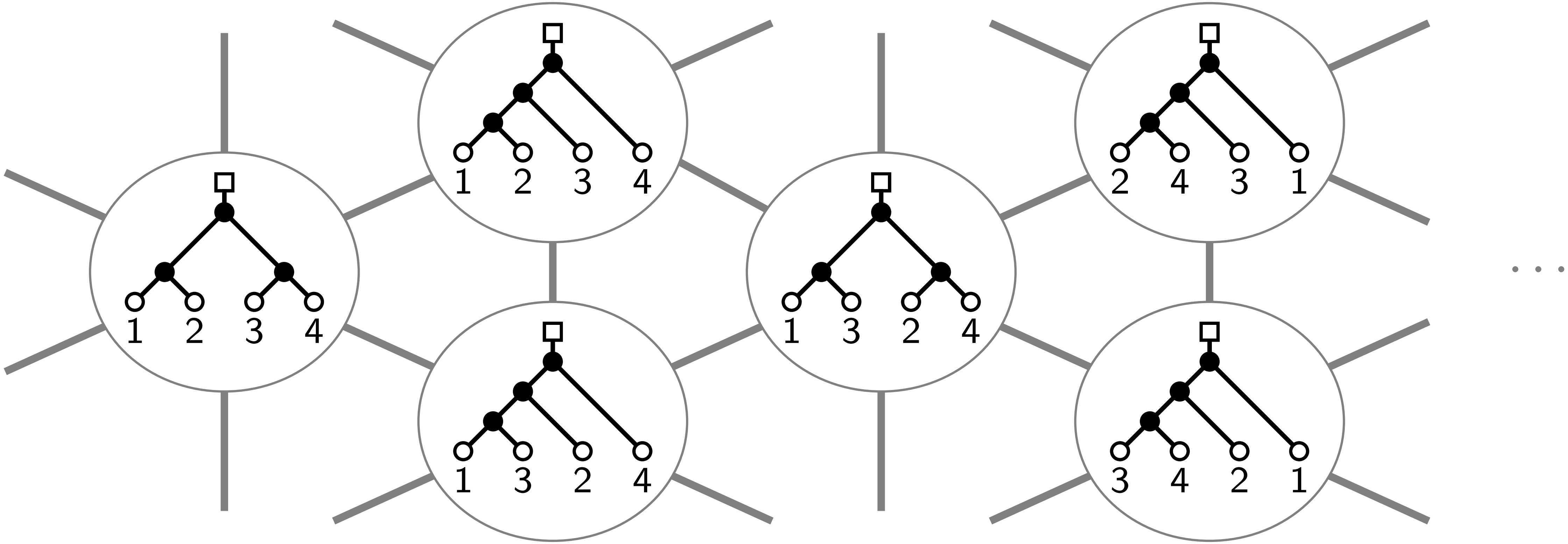

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$$|V(G)| = (2n-3)!! = (2n-3) \cdot (2n-5) \cdot \ldots \cdot 5 \cdot 3$$

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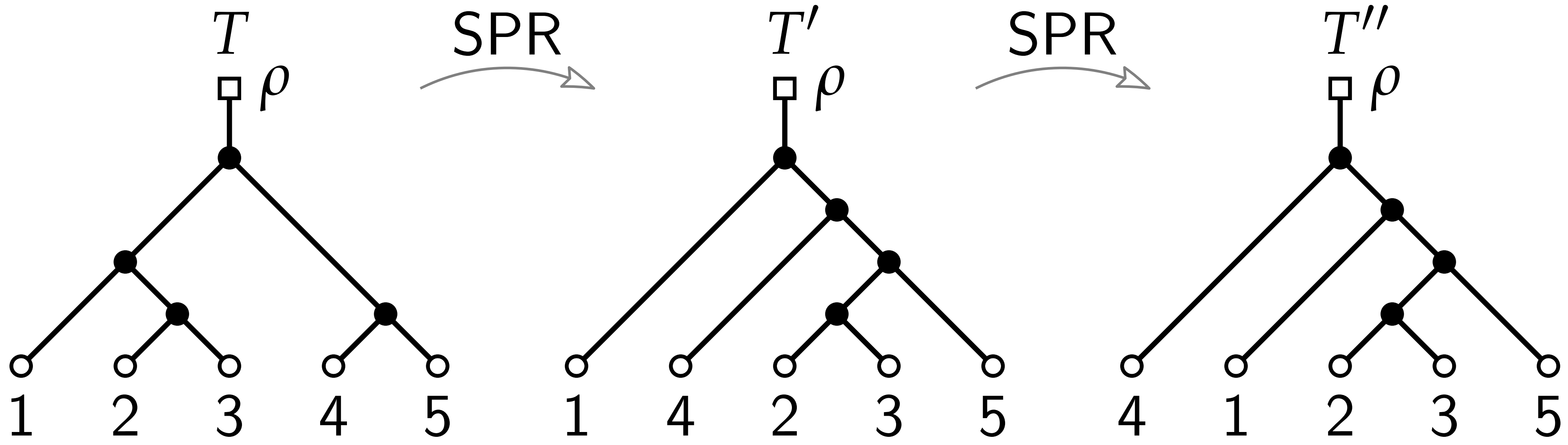
- Can we rephrase the problem?

Maximum agreement forests



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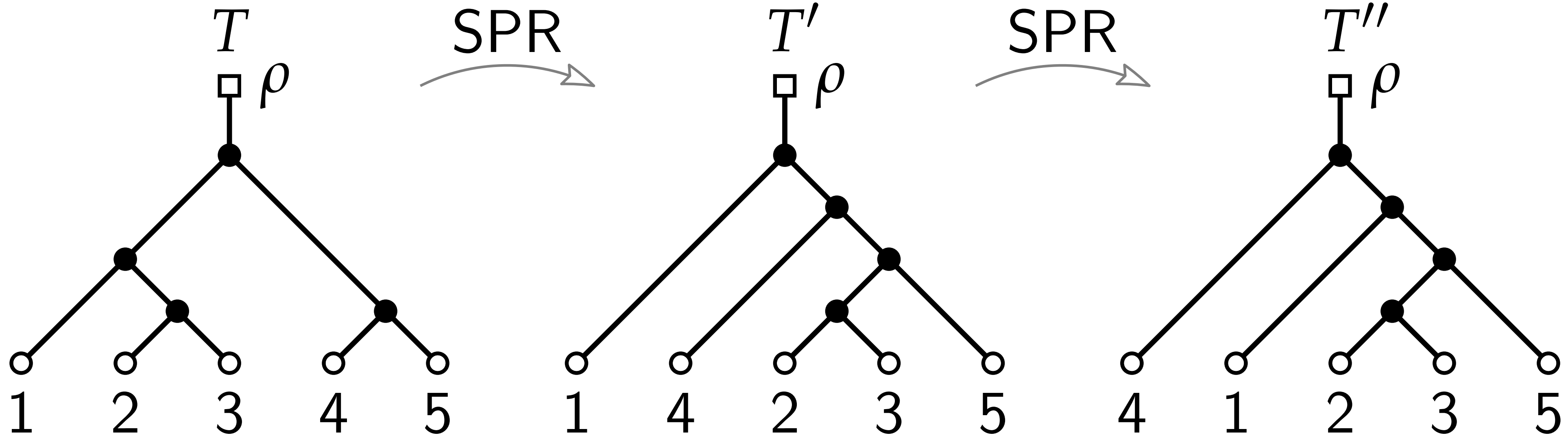

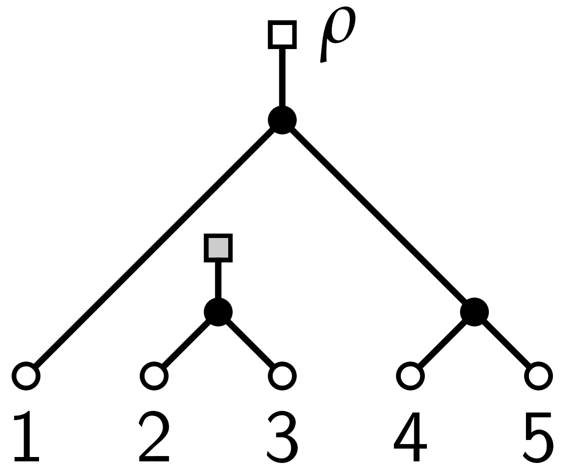

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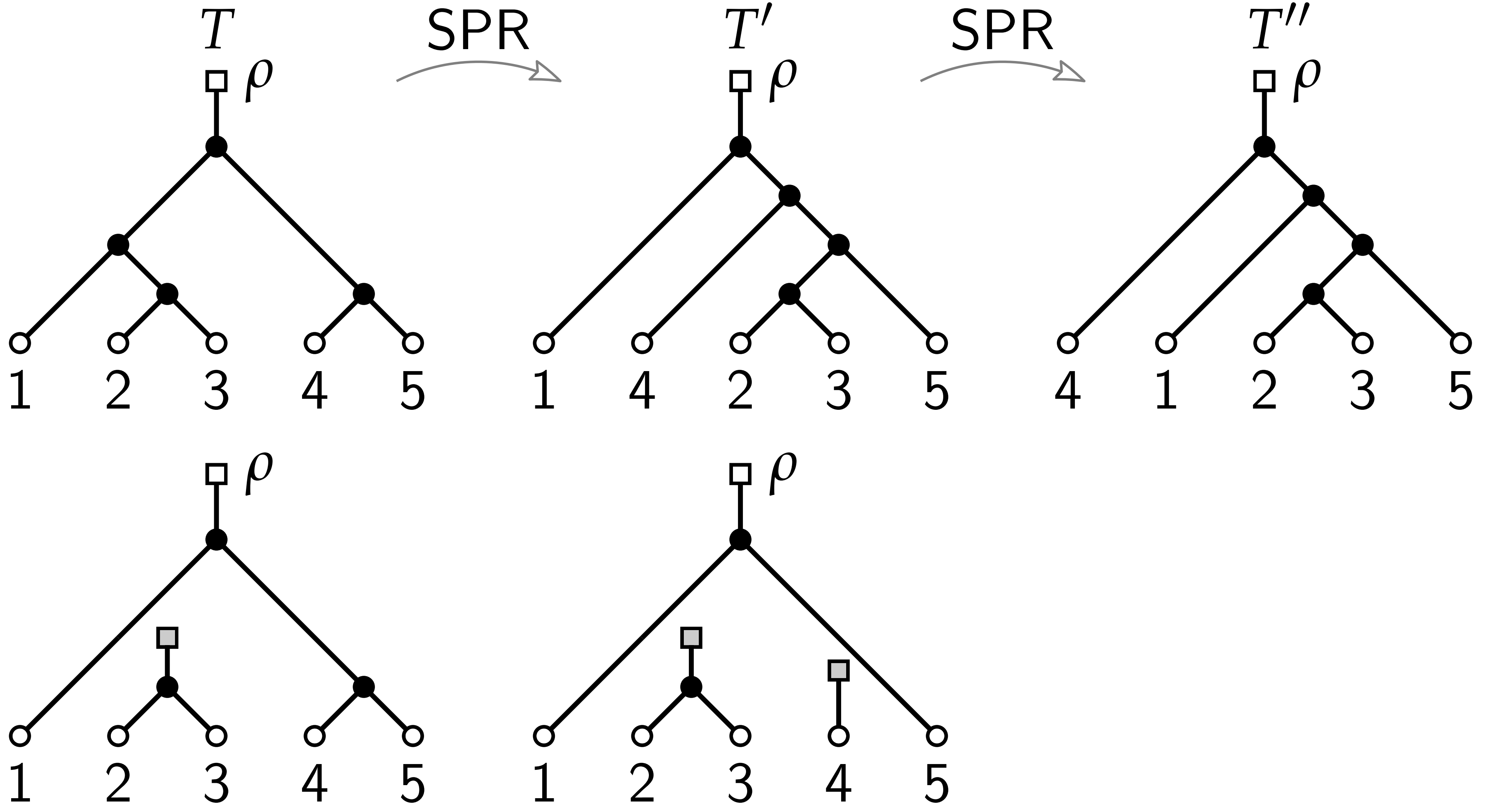

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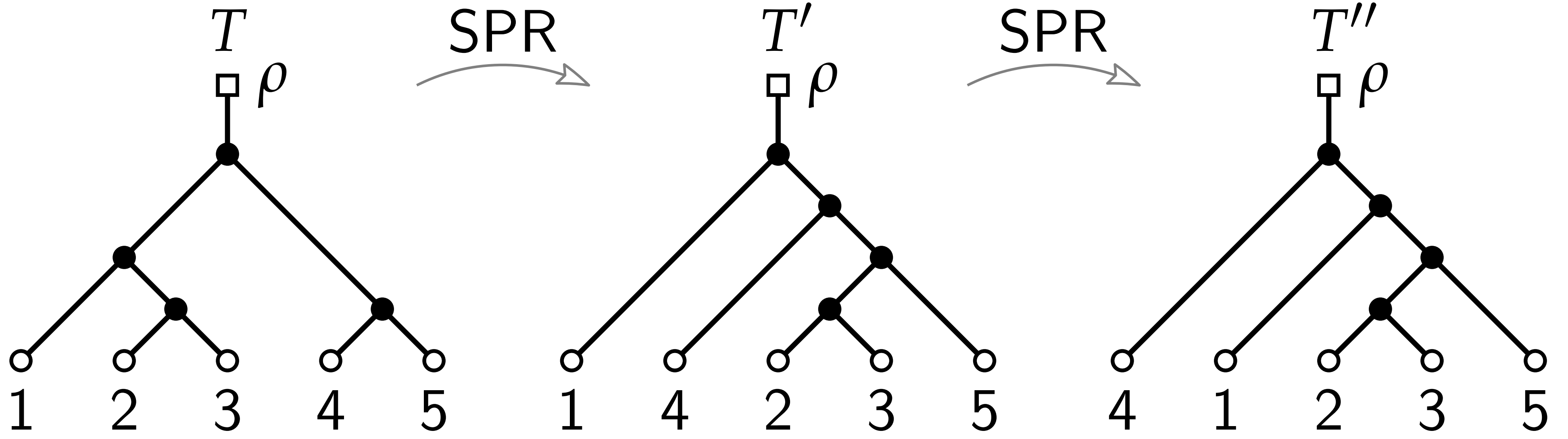

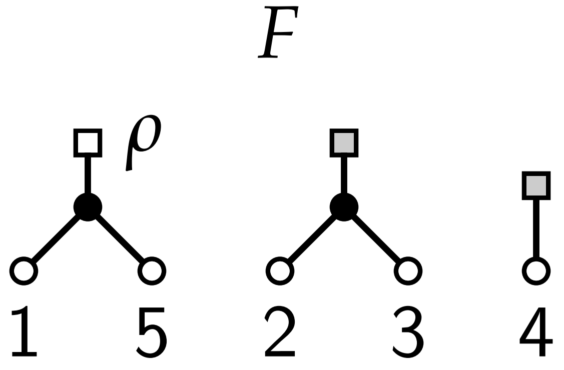

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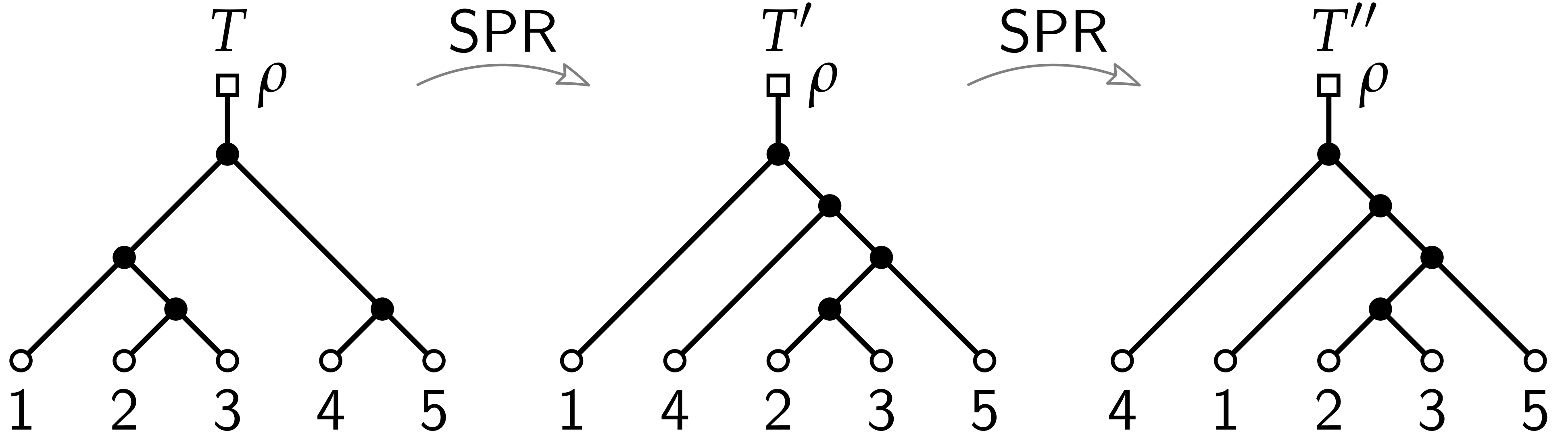

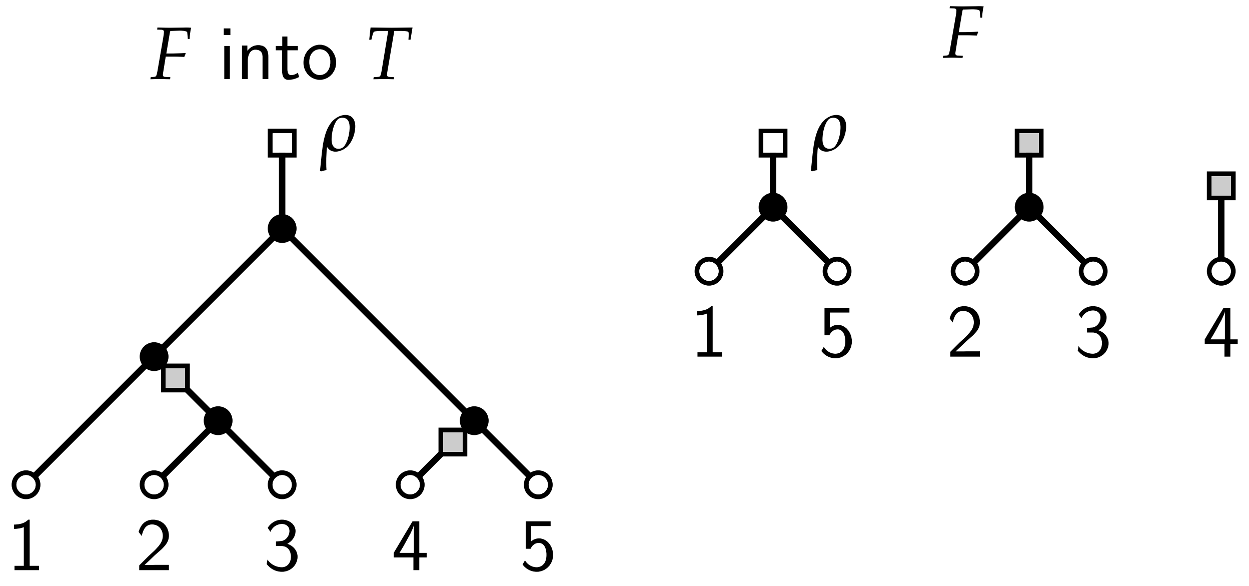

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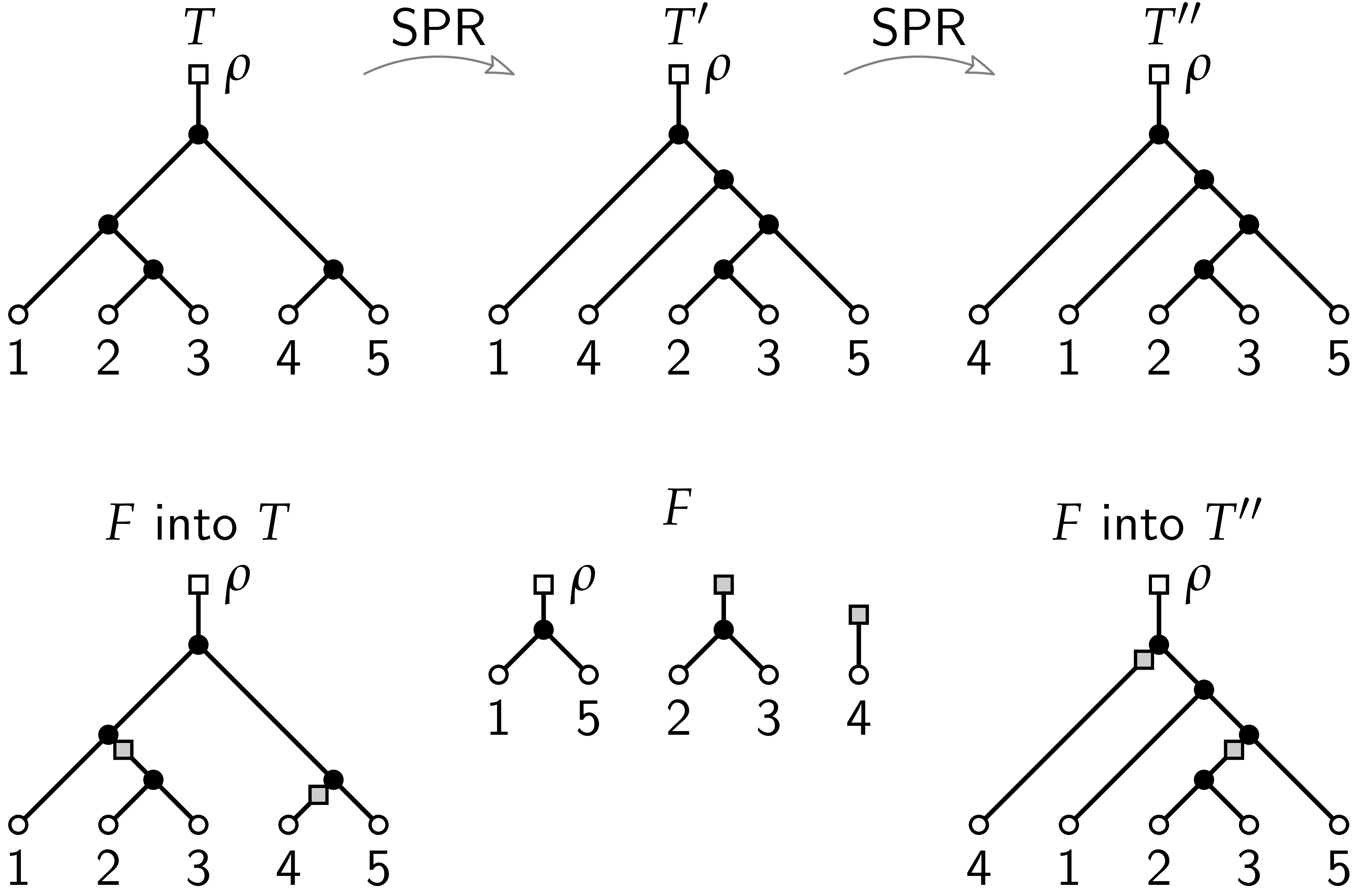

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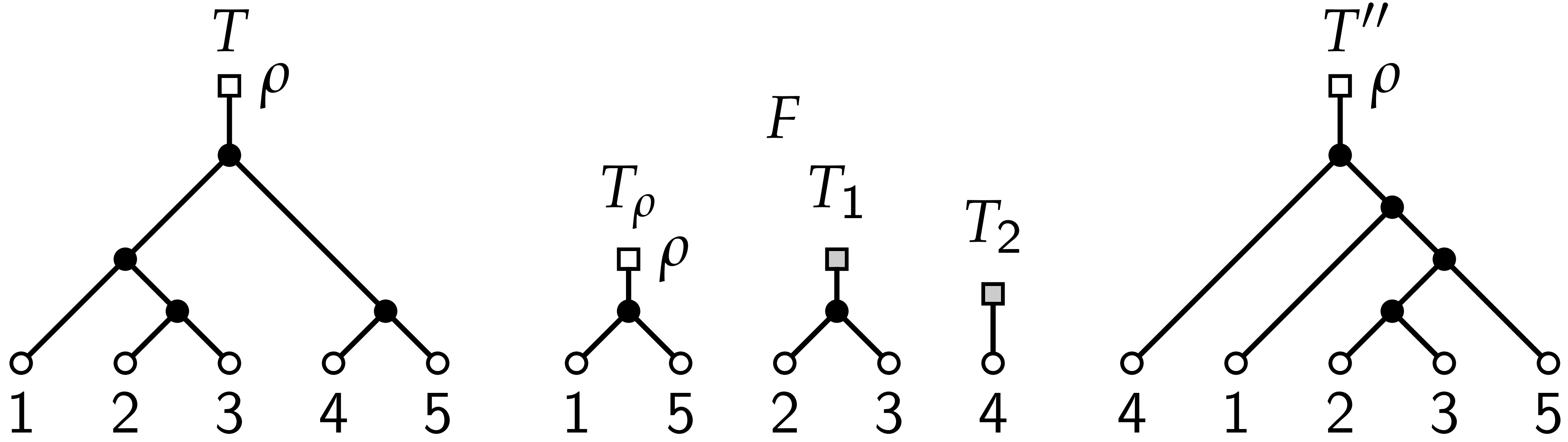

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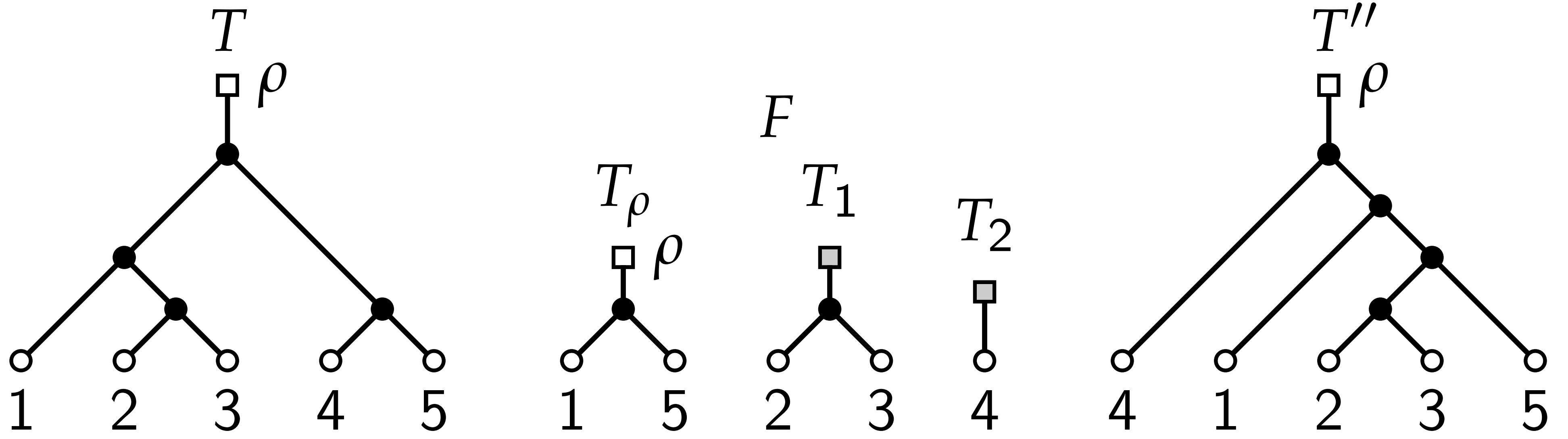

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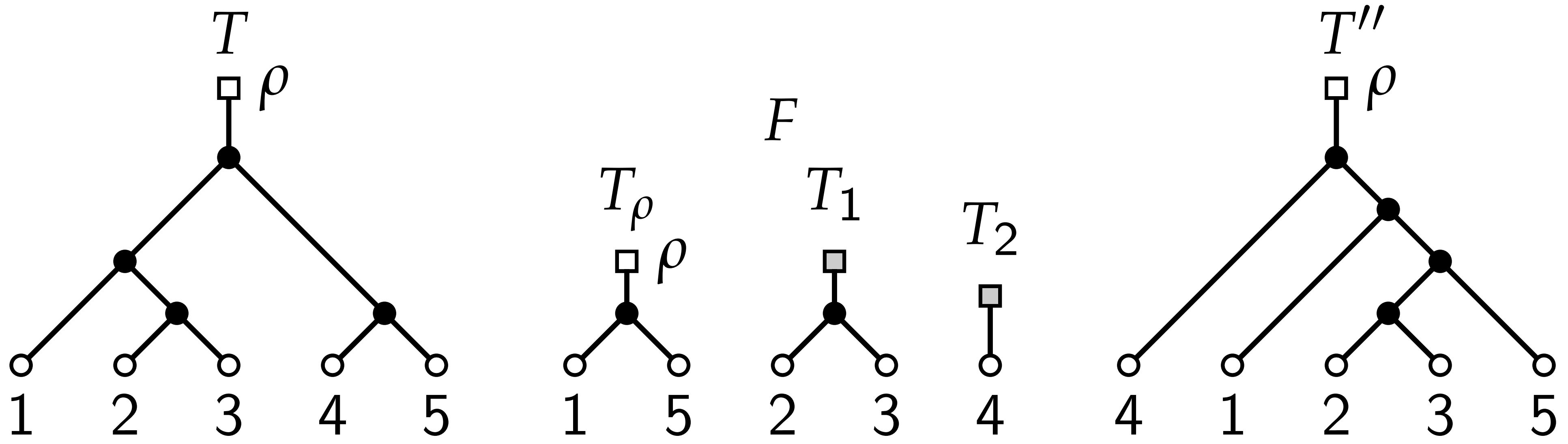

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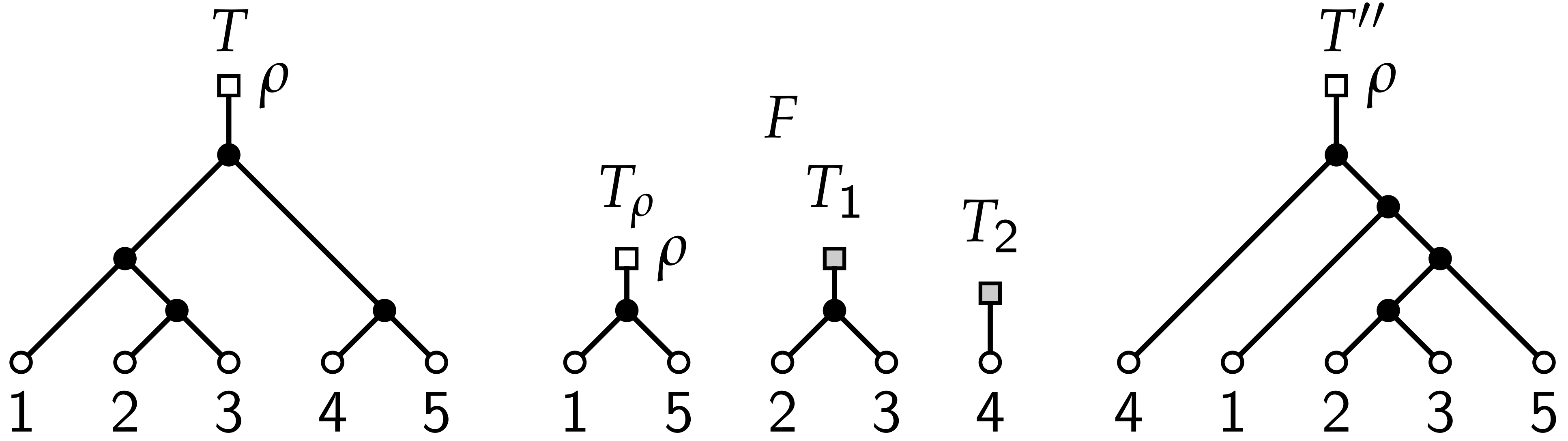

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If k is minimal, F is a **maximum agreement forest (MAF)**.

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Let T and T' be two phylogenetic trees on X.
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Define

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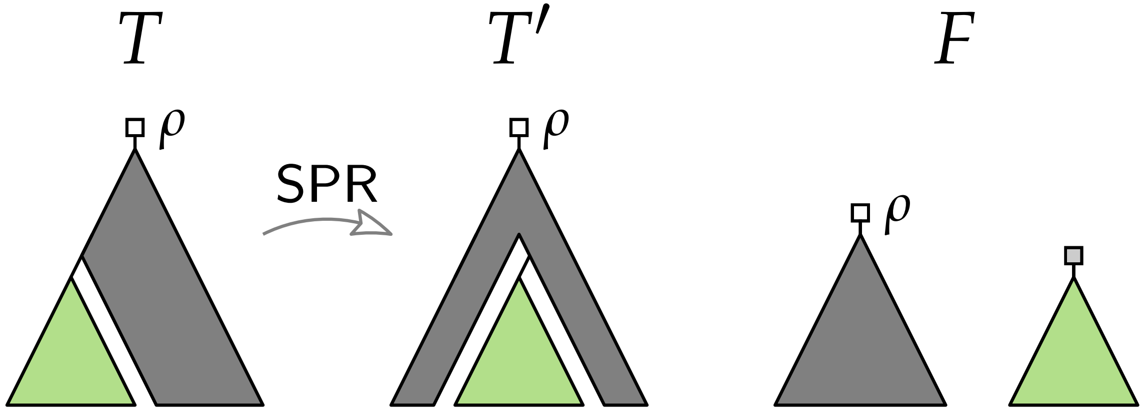
- Case $d = 1$ is easy. ✓



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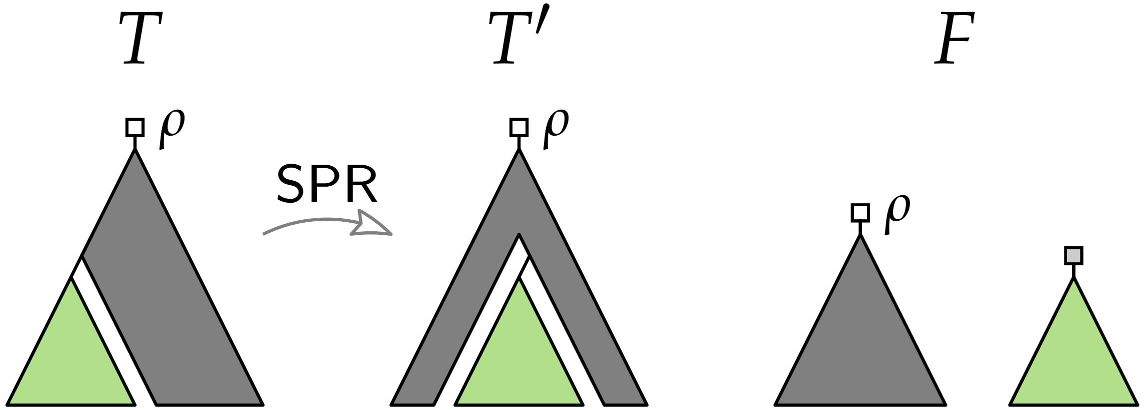

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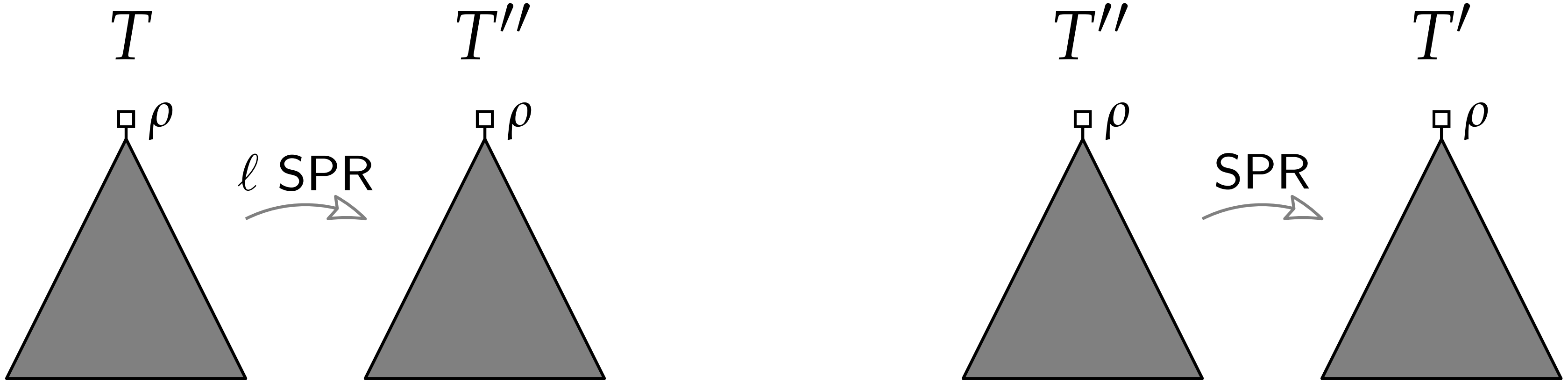

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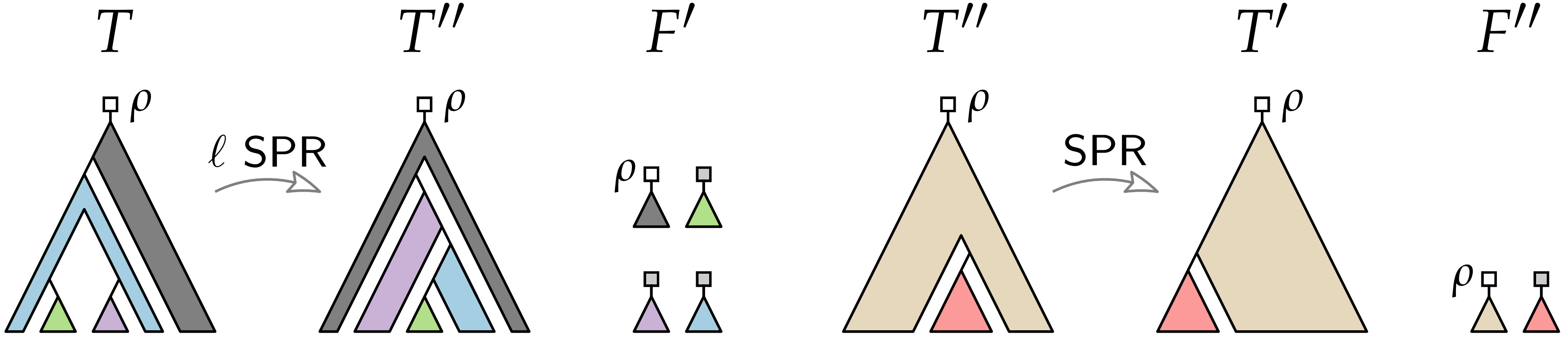

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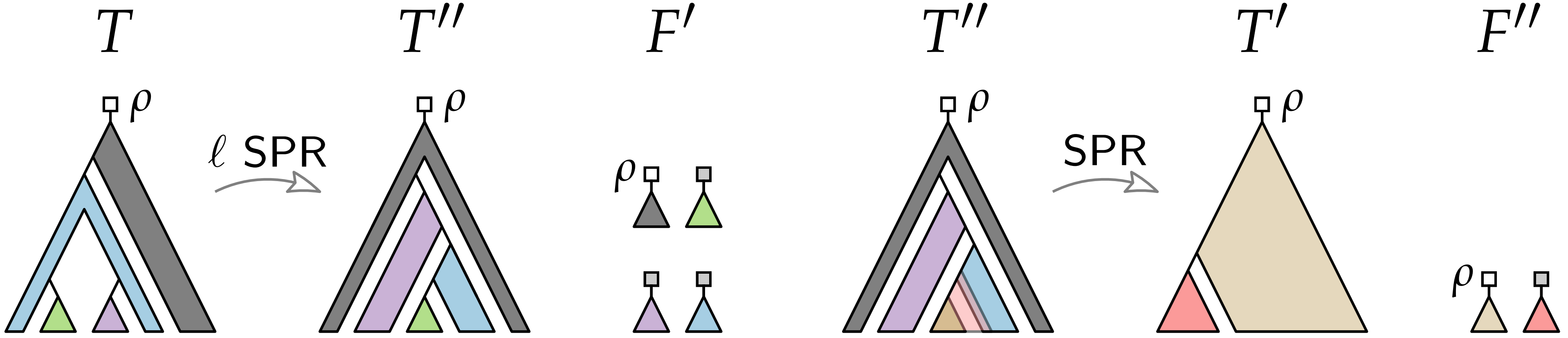

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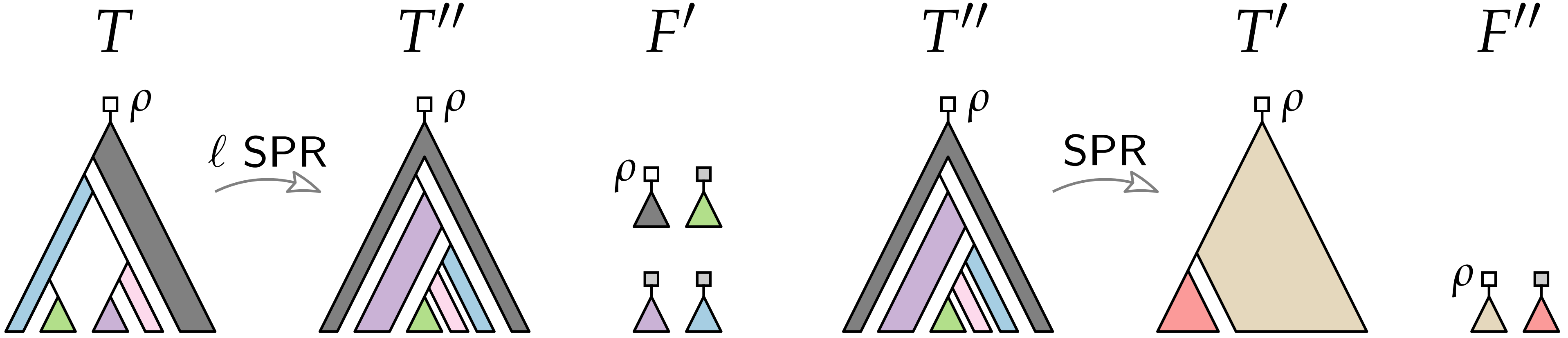

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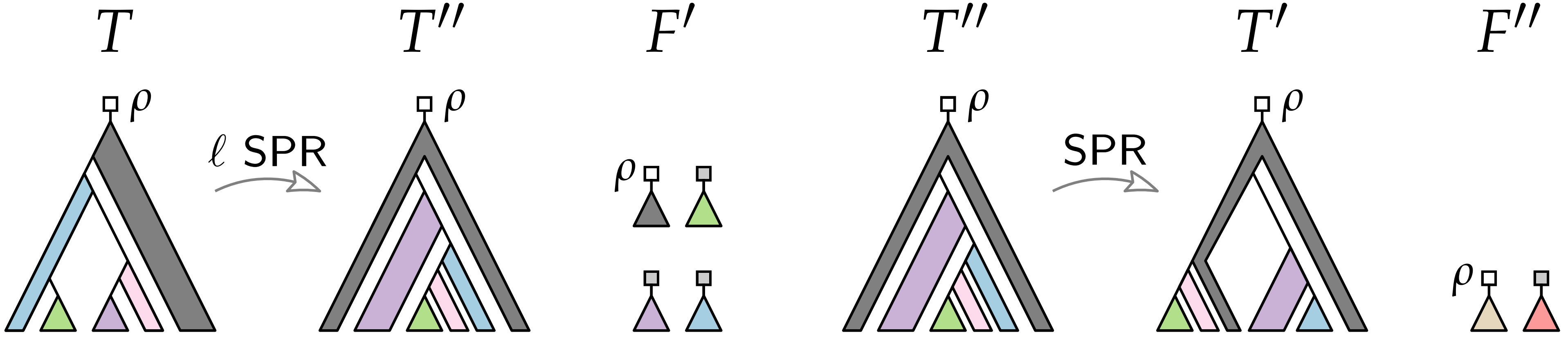

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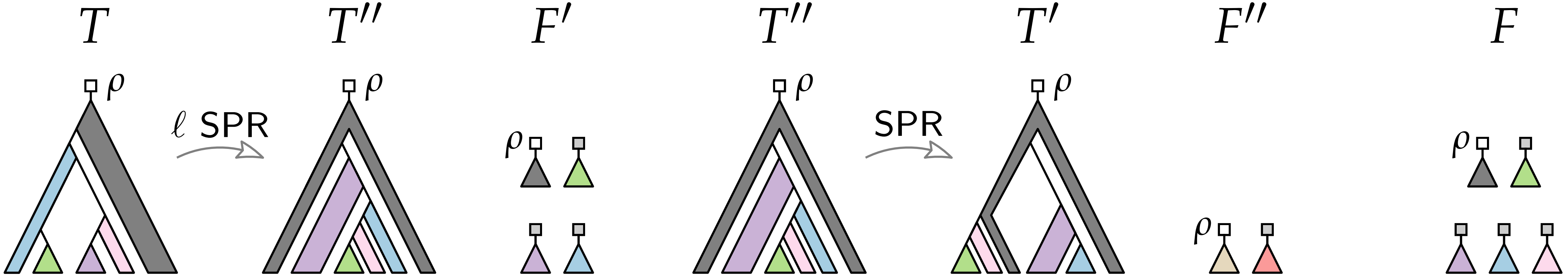

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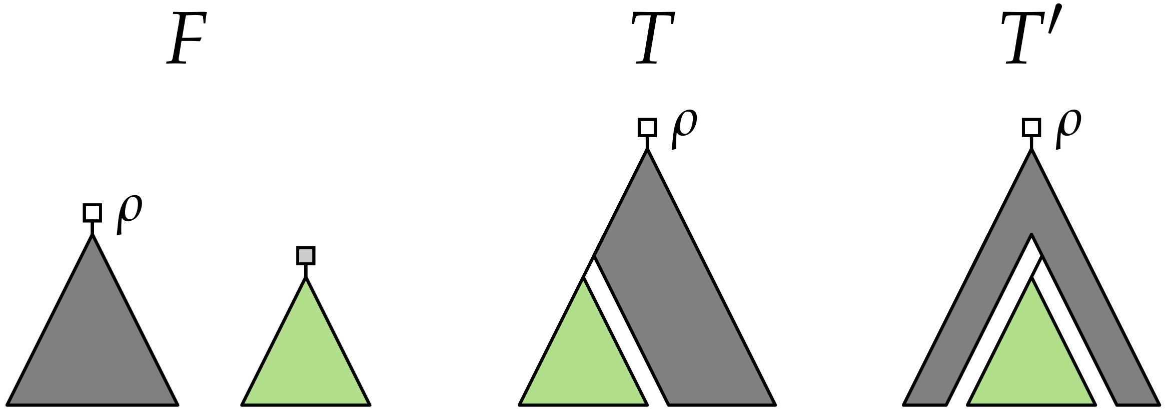

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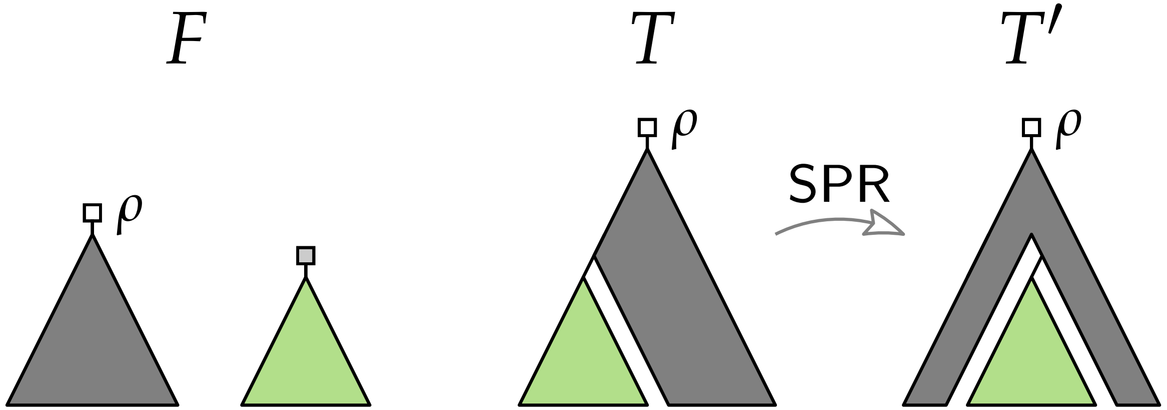

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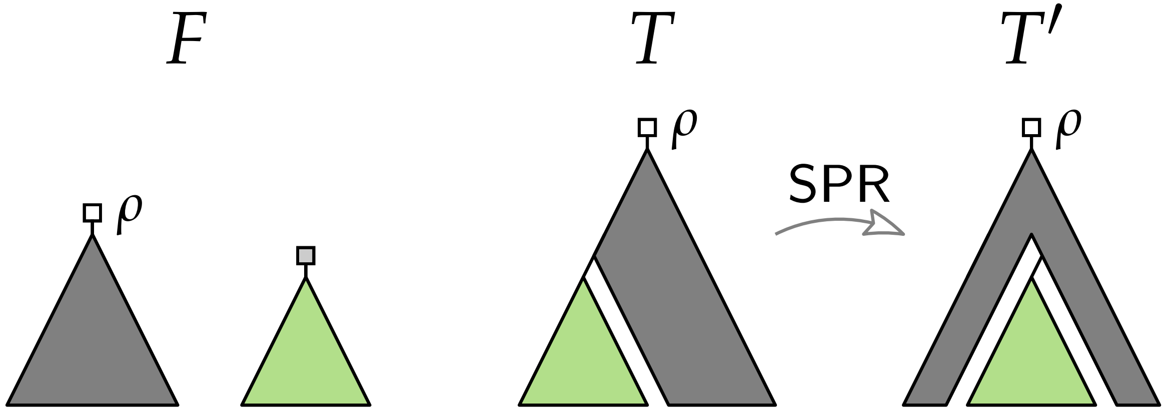

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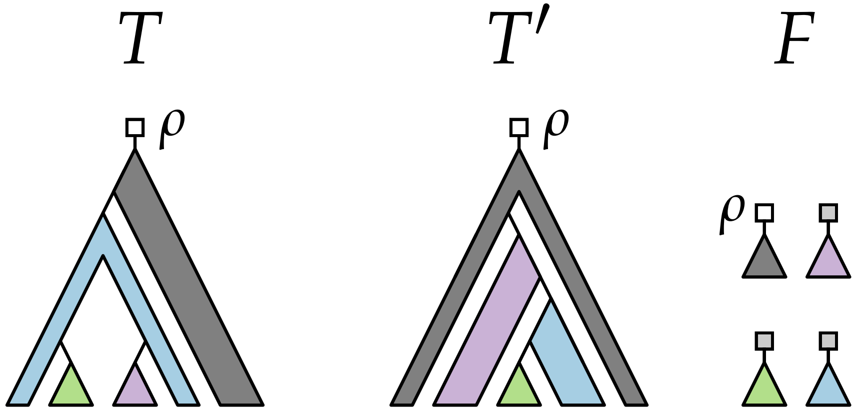

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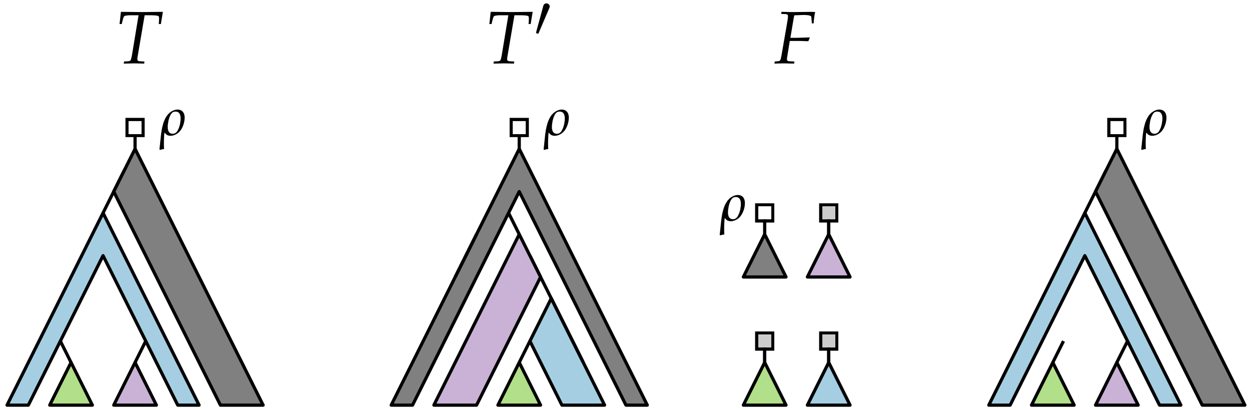

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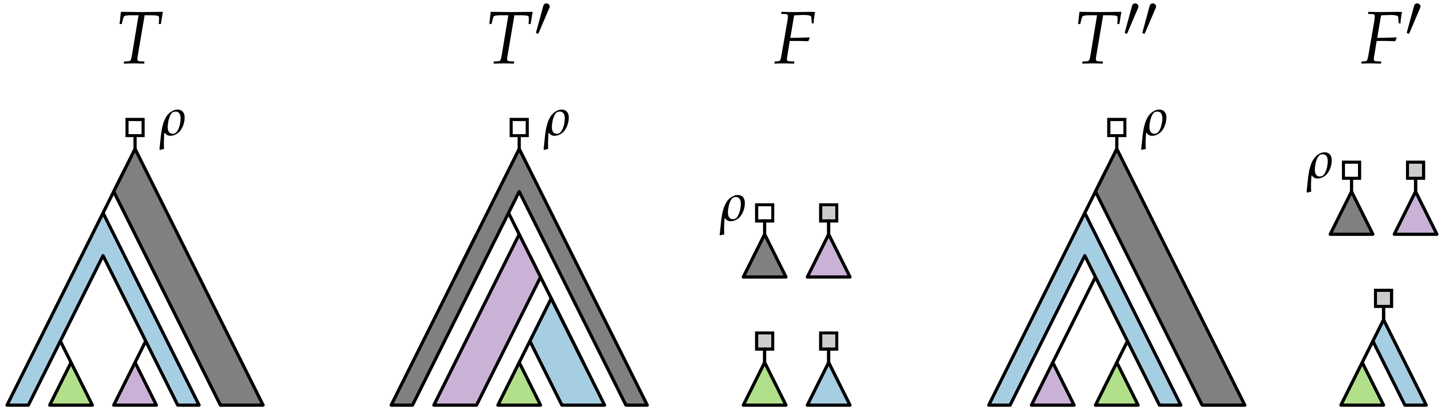

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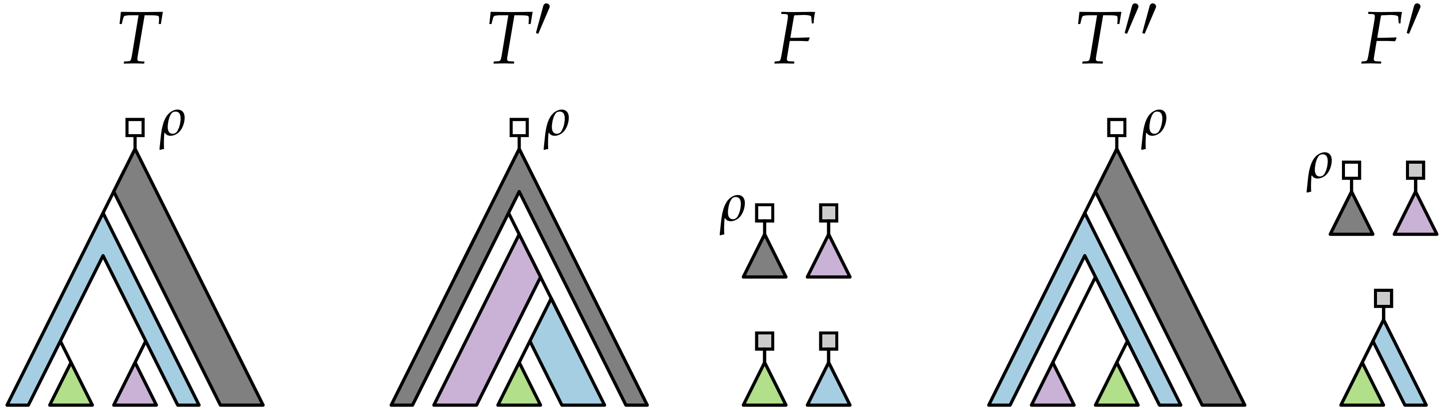

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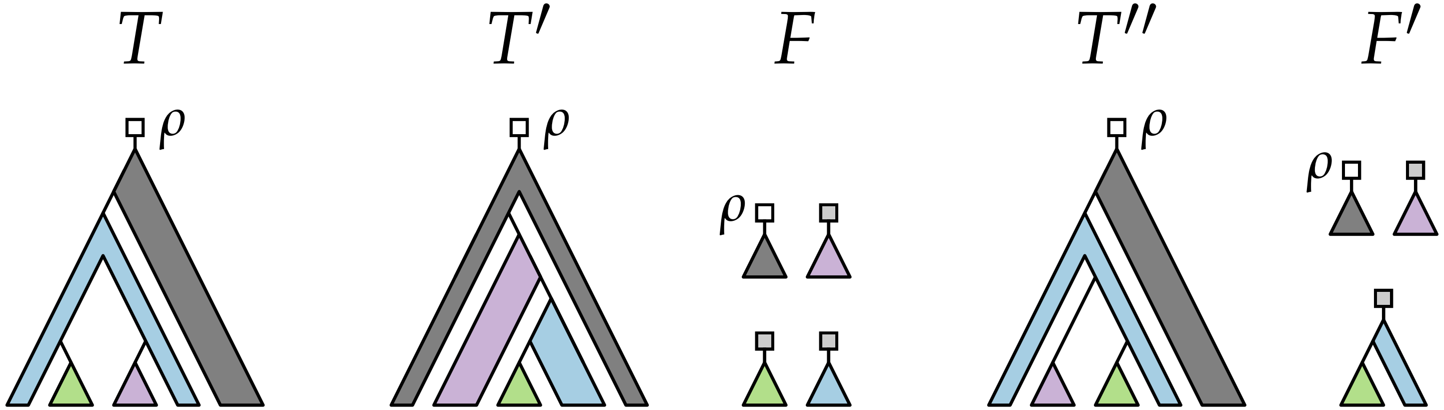

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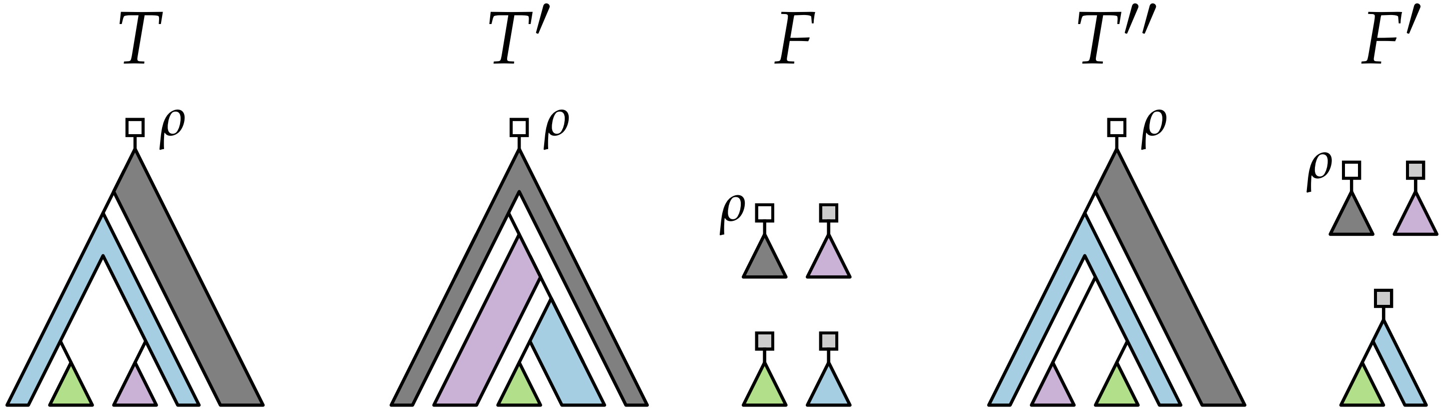

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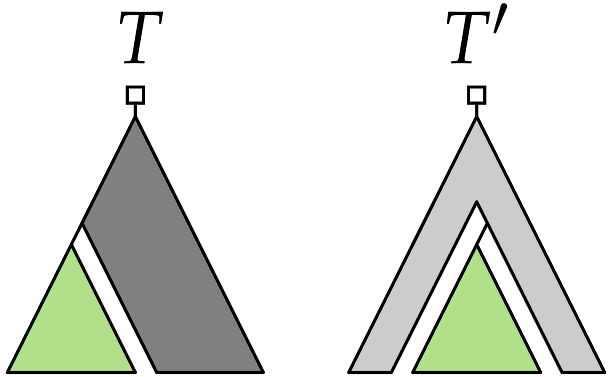

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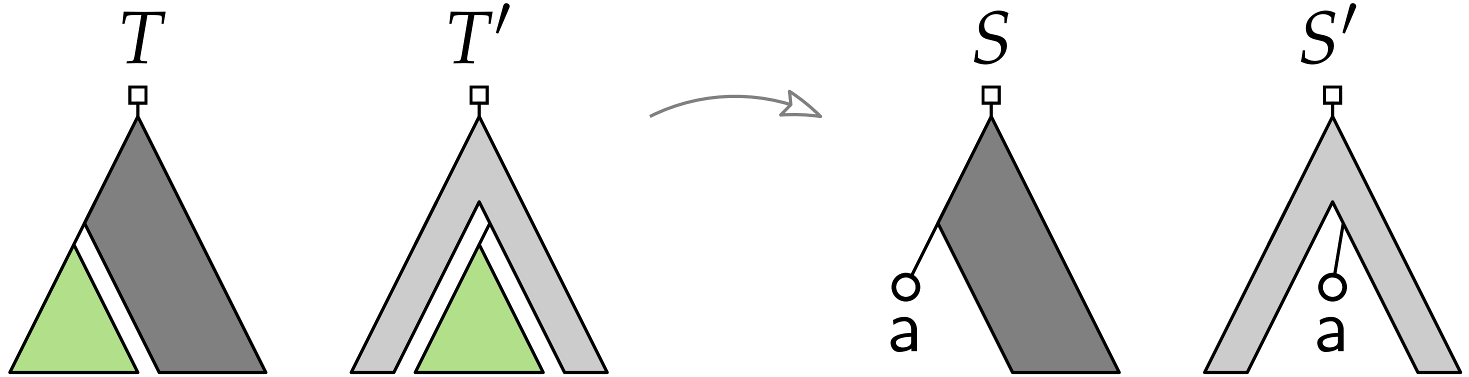

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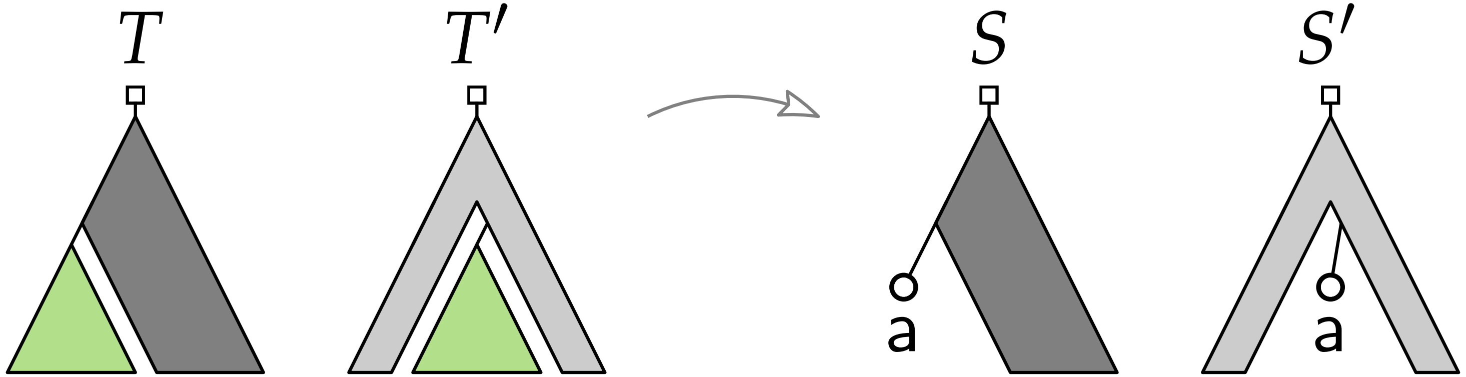

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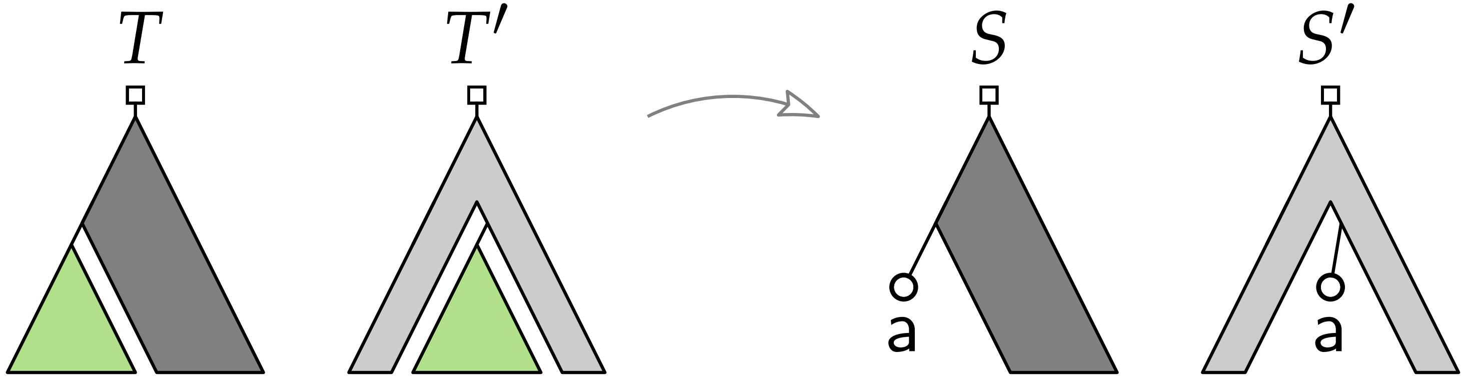

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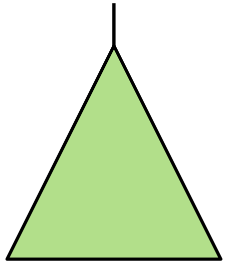

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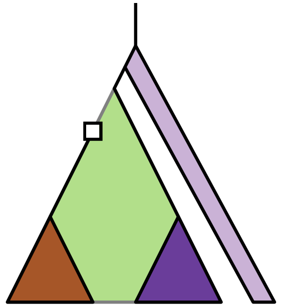

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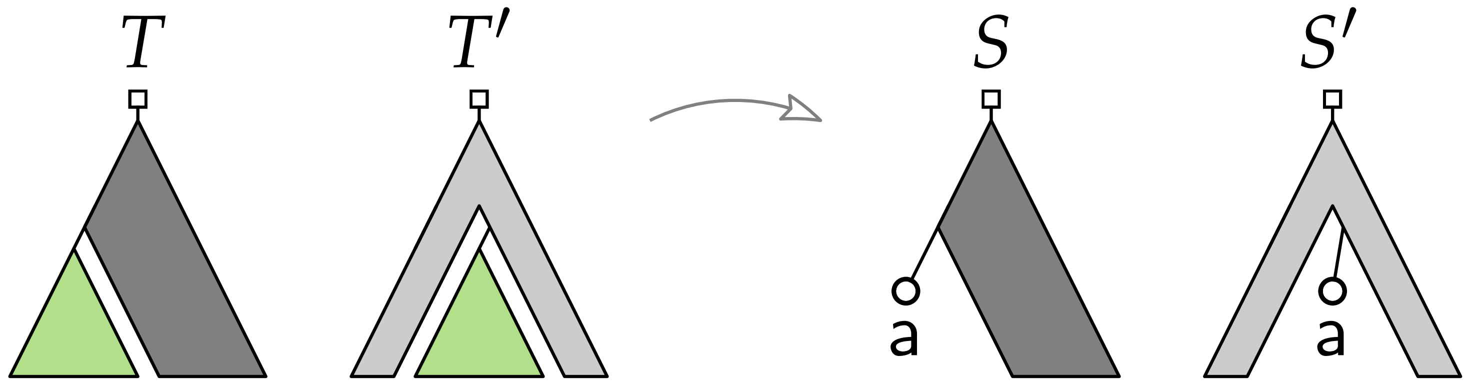

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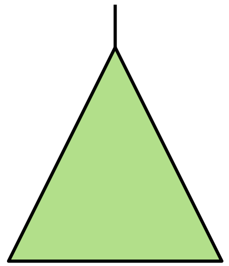

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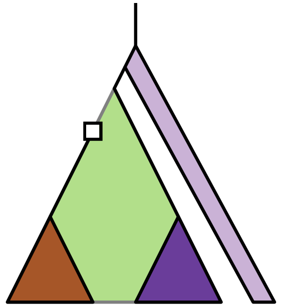
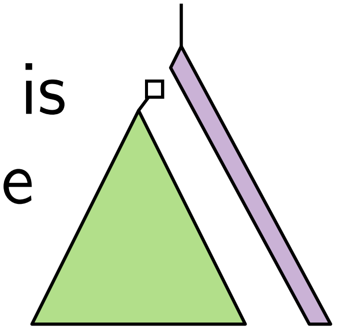


then there is alternative MAF



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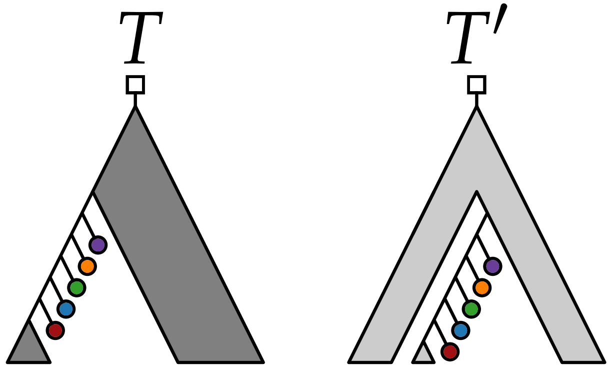

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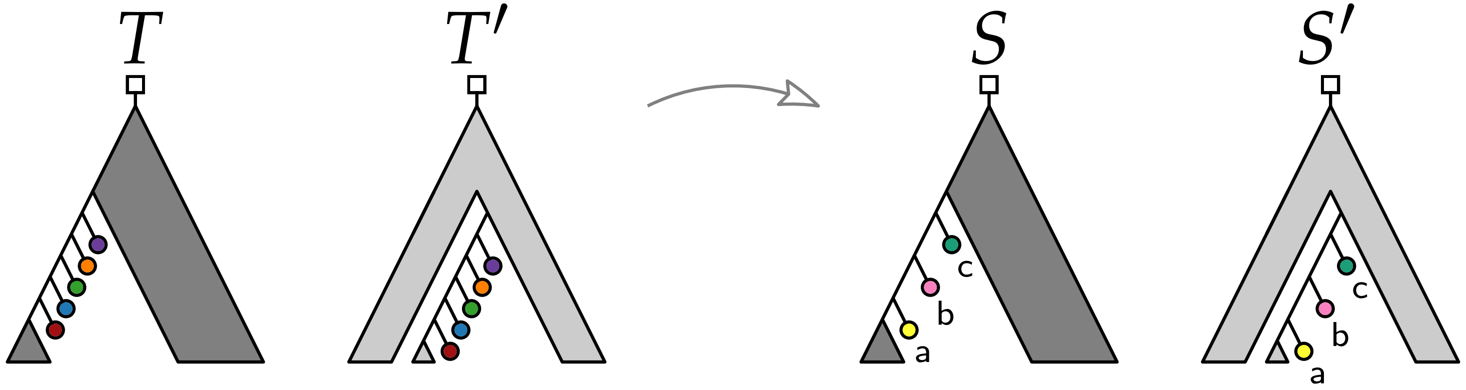

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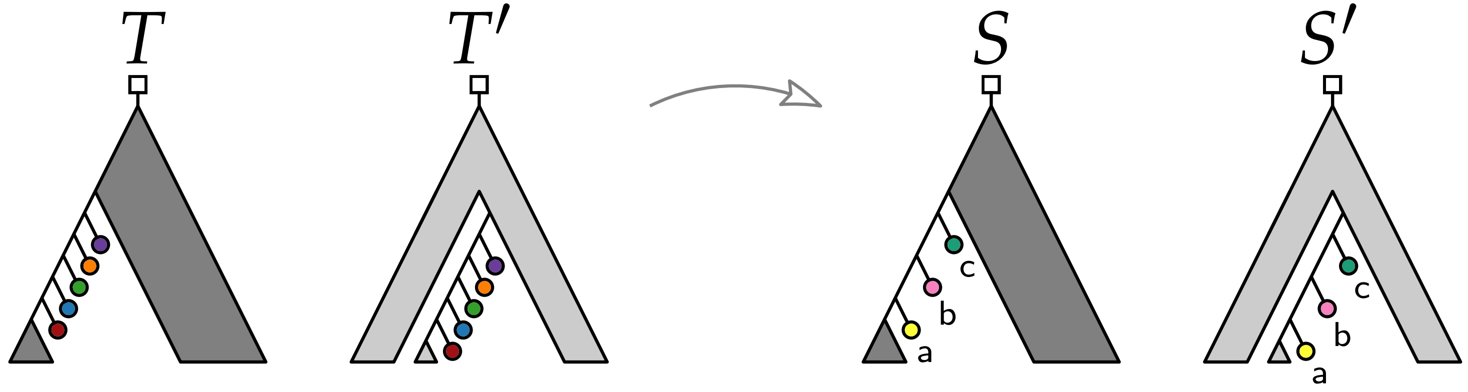

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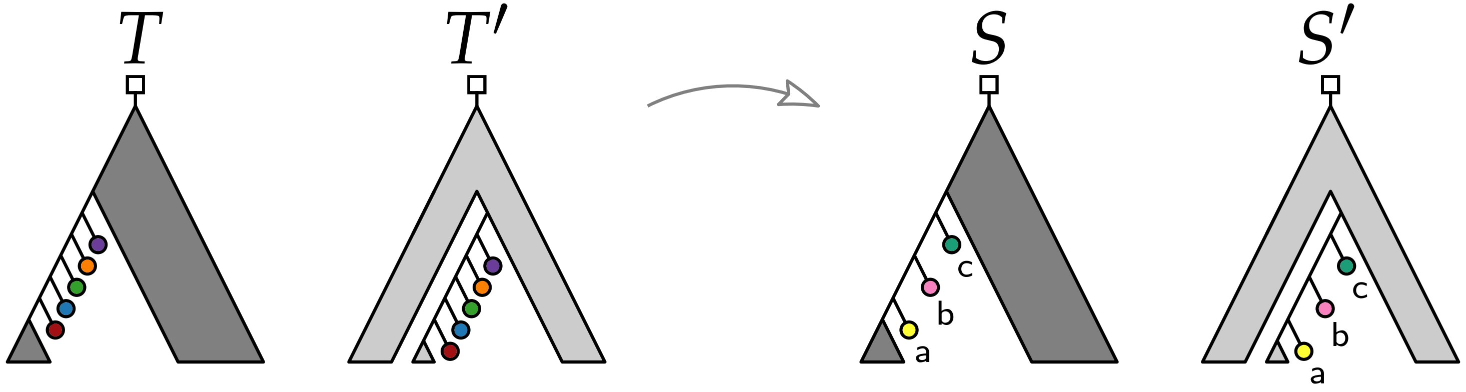

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Proof.

- 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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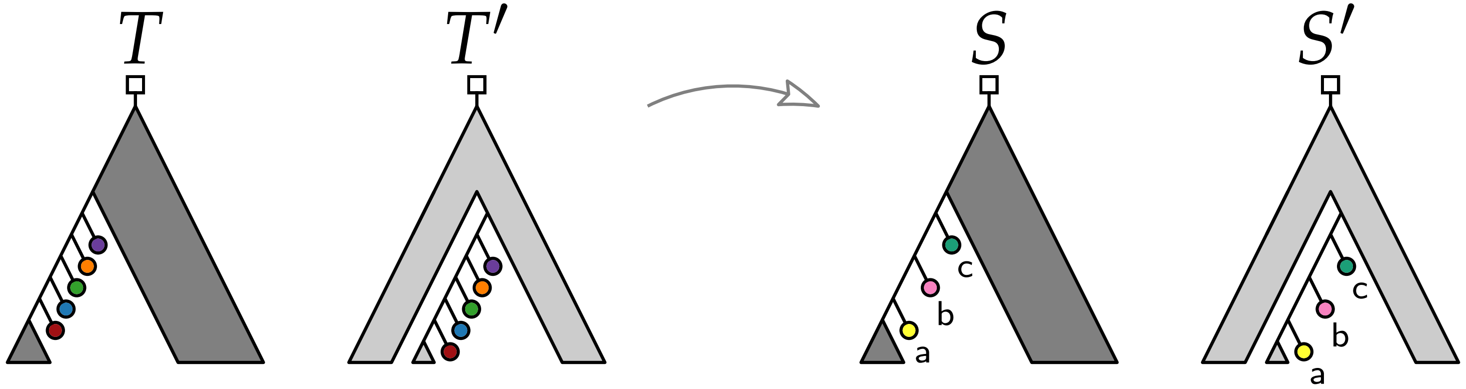

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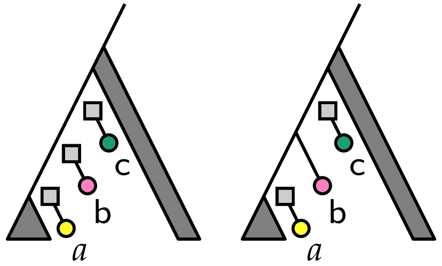
- Consider embedding of a MAF F into S.

Case 1



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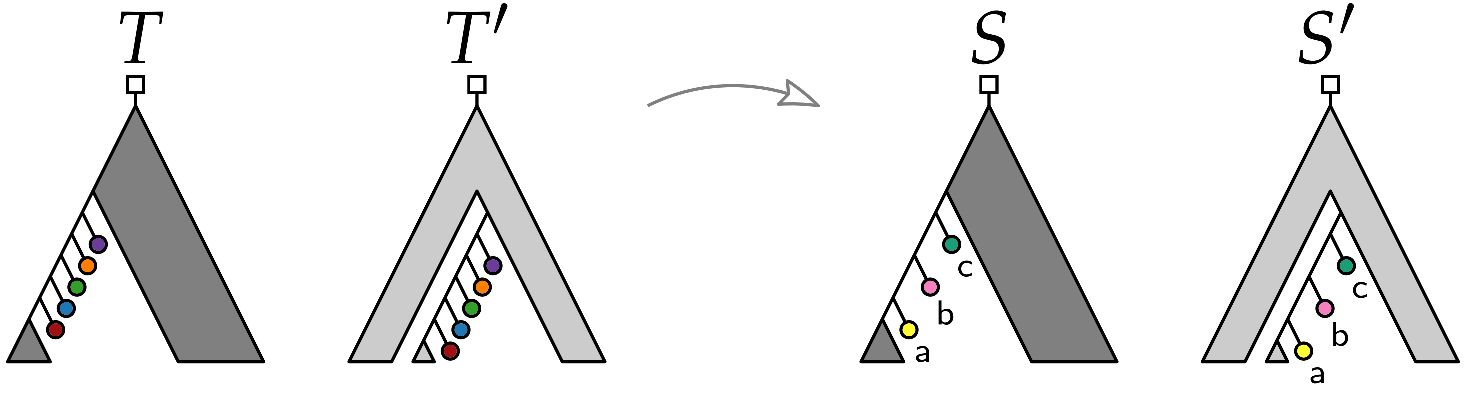
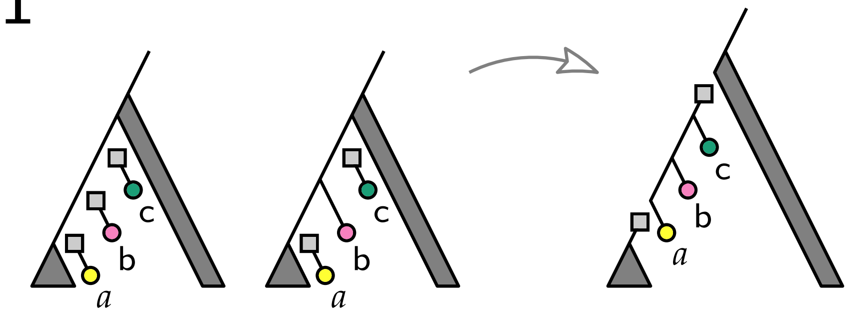


Lemma 6. Applying chain reduction is safe; i.e. $\mathrm{d_{SPR}}(T, T') = \mathrm{d_{SPR}}(S, S')$.

Proof.

- Consider embedding of a MAF F into S.

Case 1



Kernelisation – Chains

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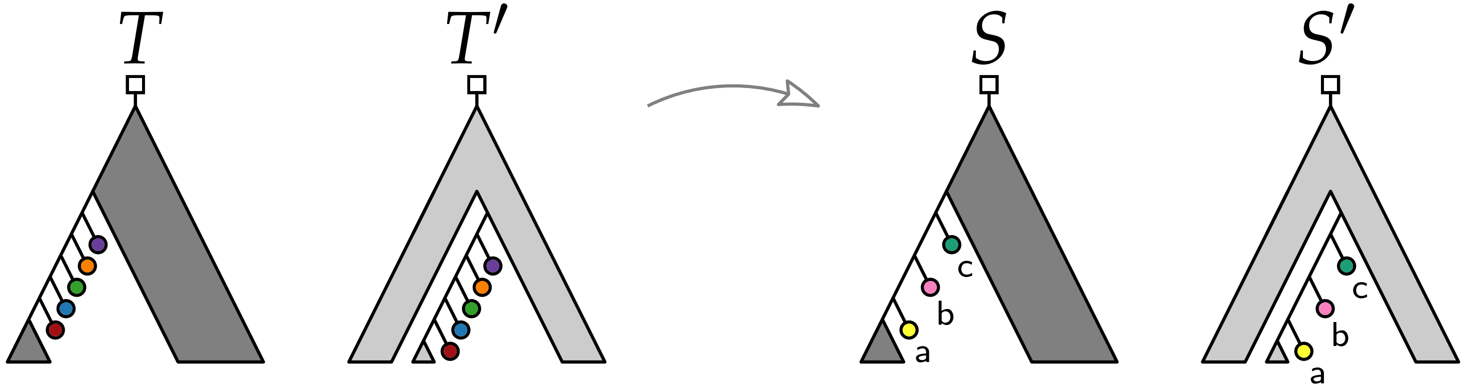

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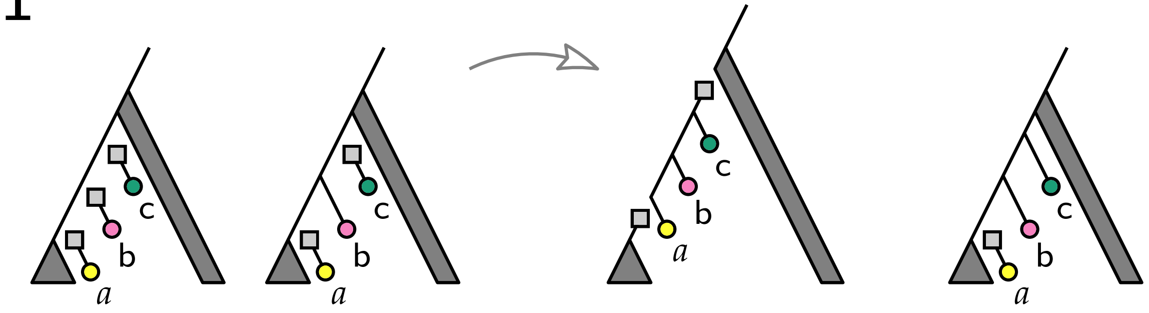

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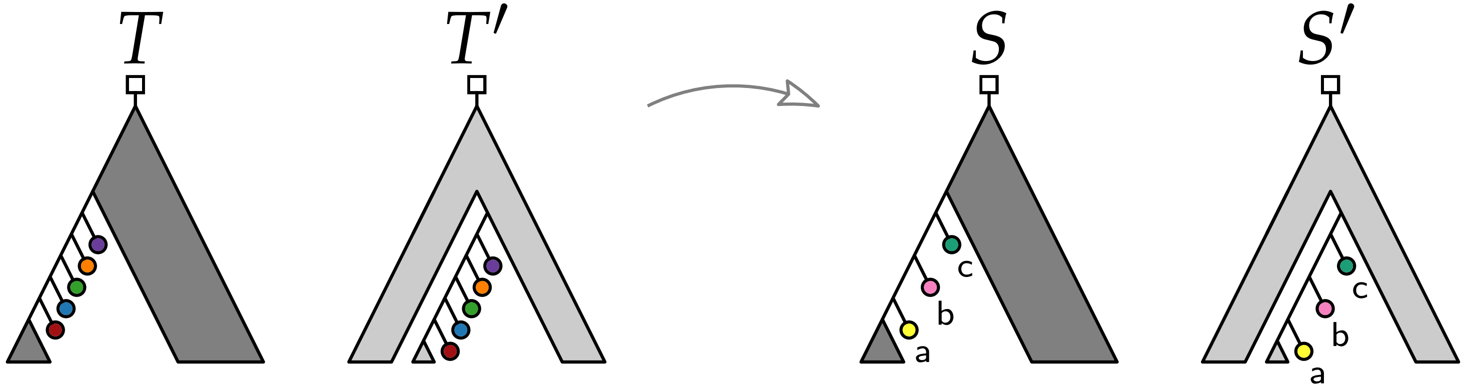

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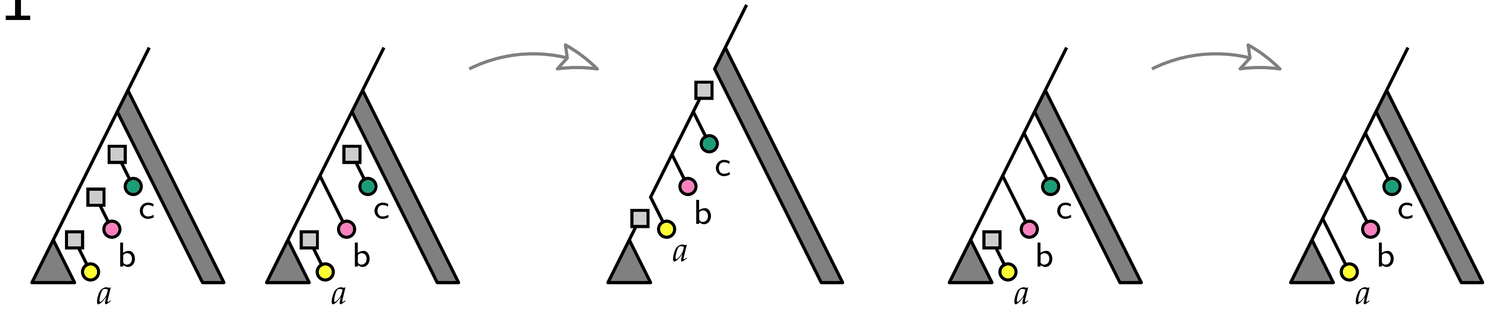

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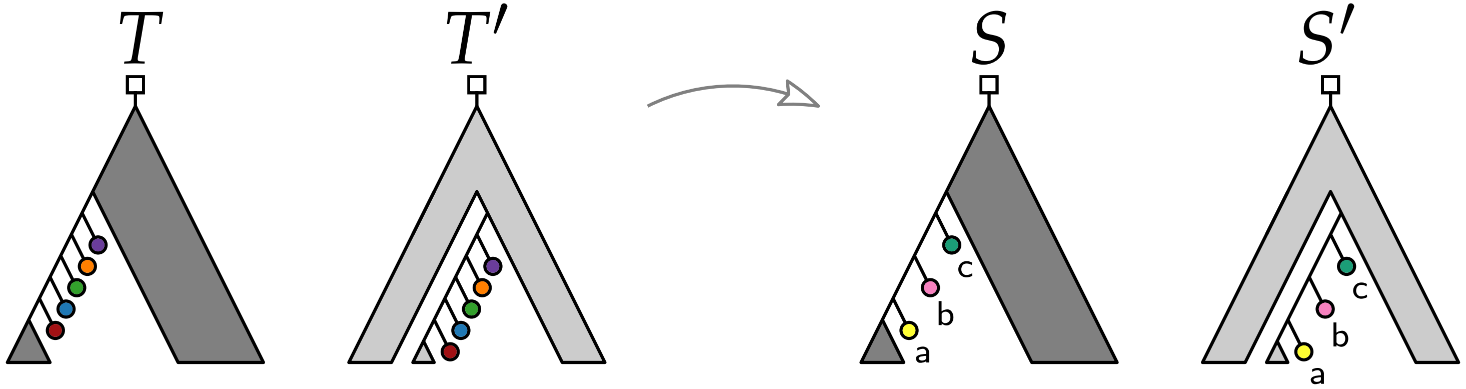

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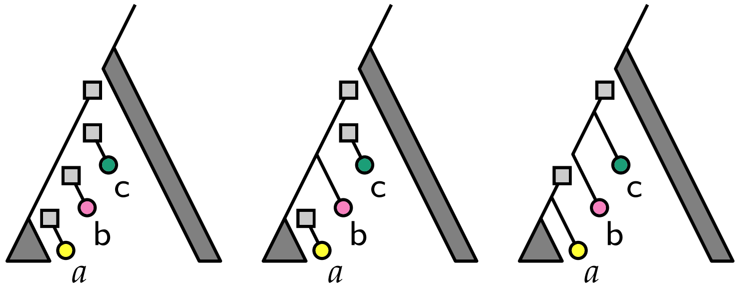

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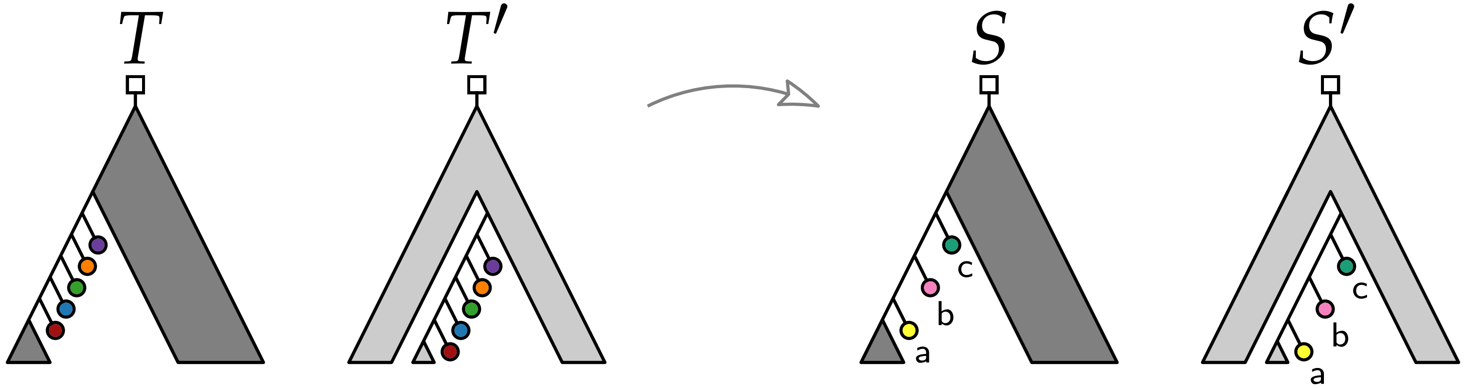

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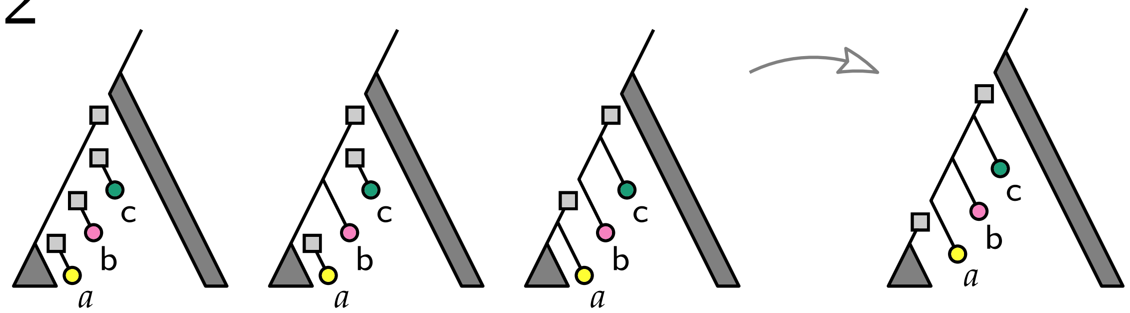

Kernel size

Theorem 7.
Reduce T and T' to S and S' by exhaustively applying the reduction rules. Let S and S' be on X'. Then

$$|X'| \leq 28\, \mathsf{d}_{\mathsf{SPR}}(T, T').$$

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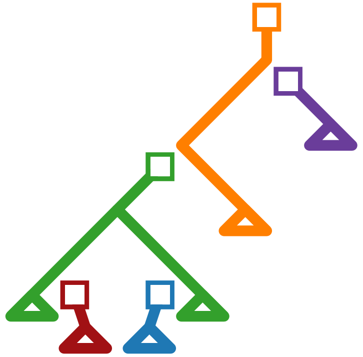

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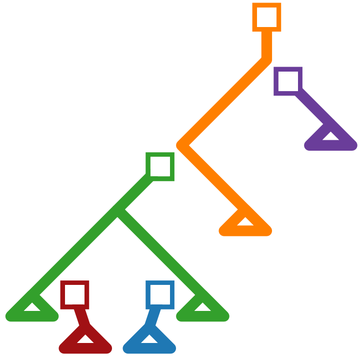

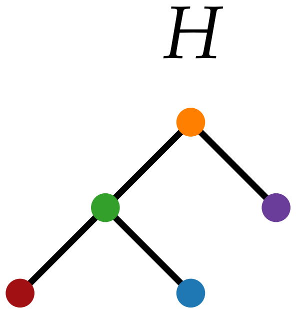

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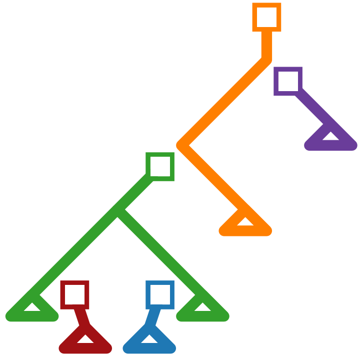

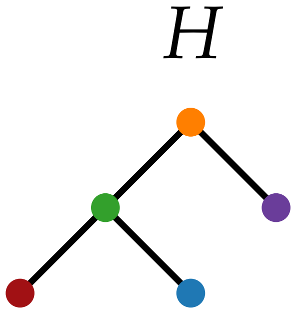

$|V(H)| = k + 1$

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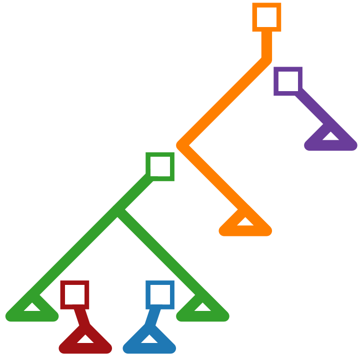

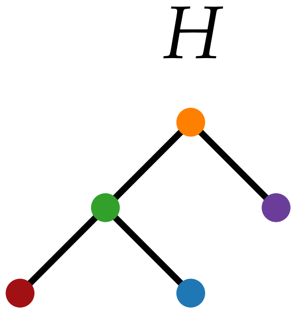

$$|V(H)| = k+1$$
$$= |E(H)| + 1$$

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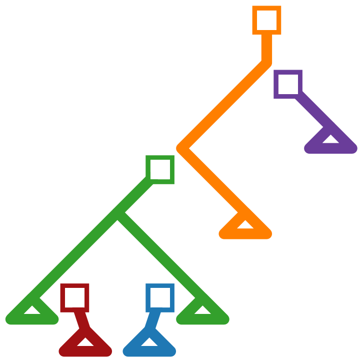

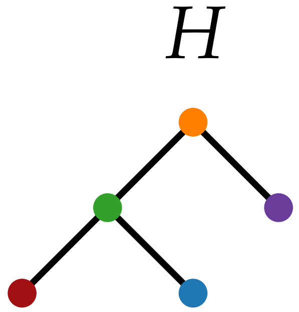

$$\begin{aligned}|V(H)| &= k + 1\\ &= |E(H)| + 1\end{aligned}$$

$$\sum n(T_i) = 2|E(H)| \le 2k$$

Kernel size

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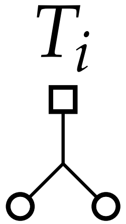

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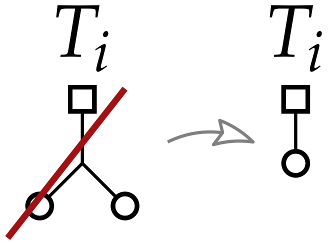

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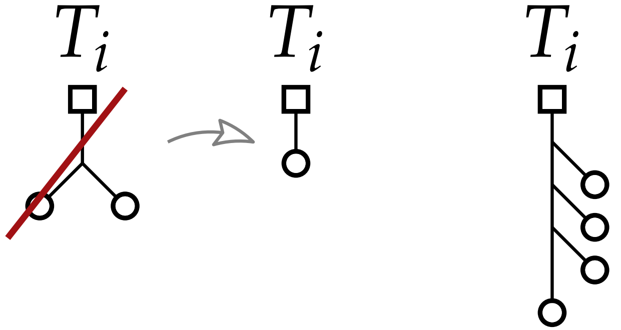

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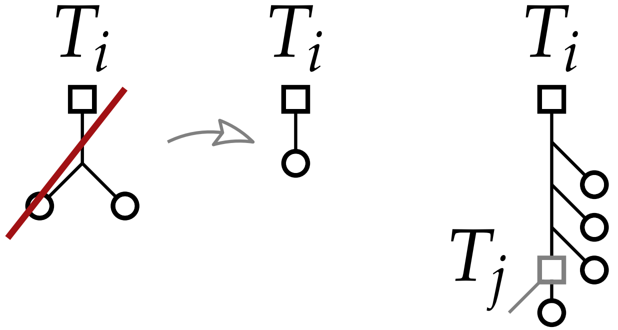

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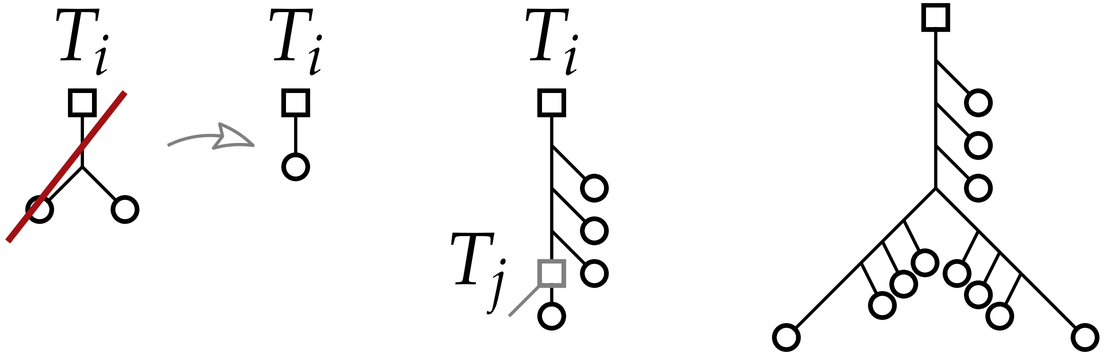

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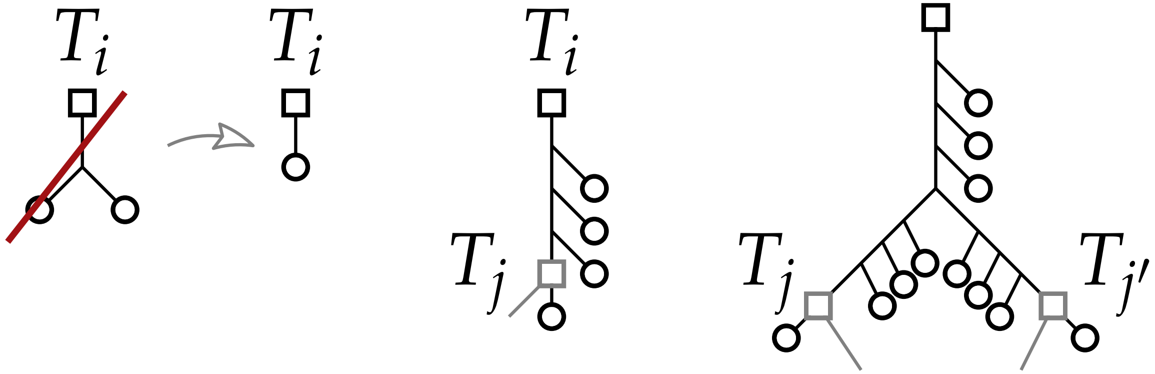

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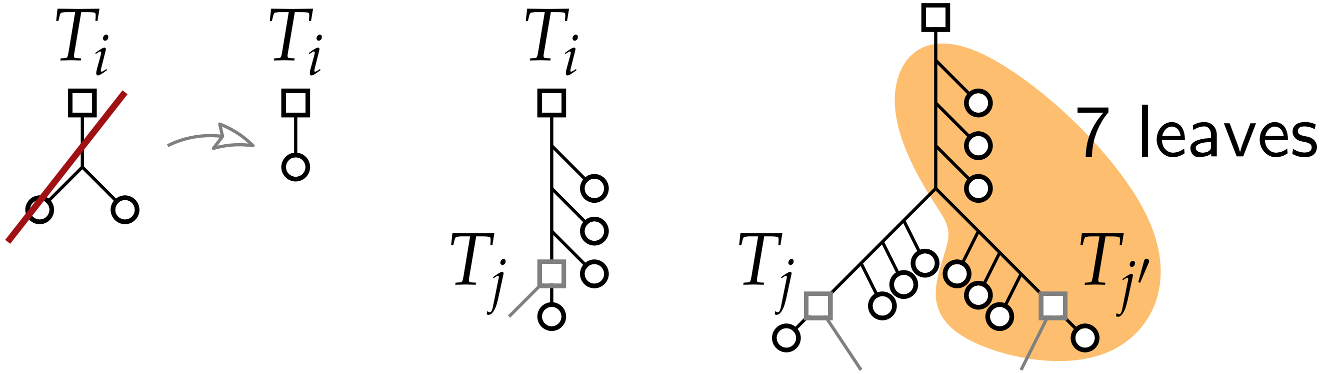

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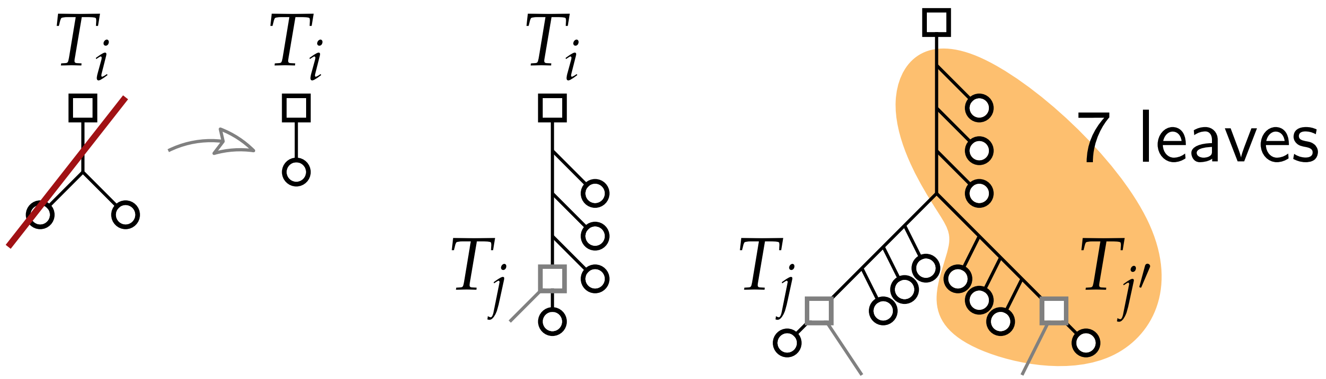

$\sum_{i=\rho}^{k}$ # leaves of T_i

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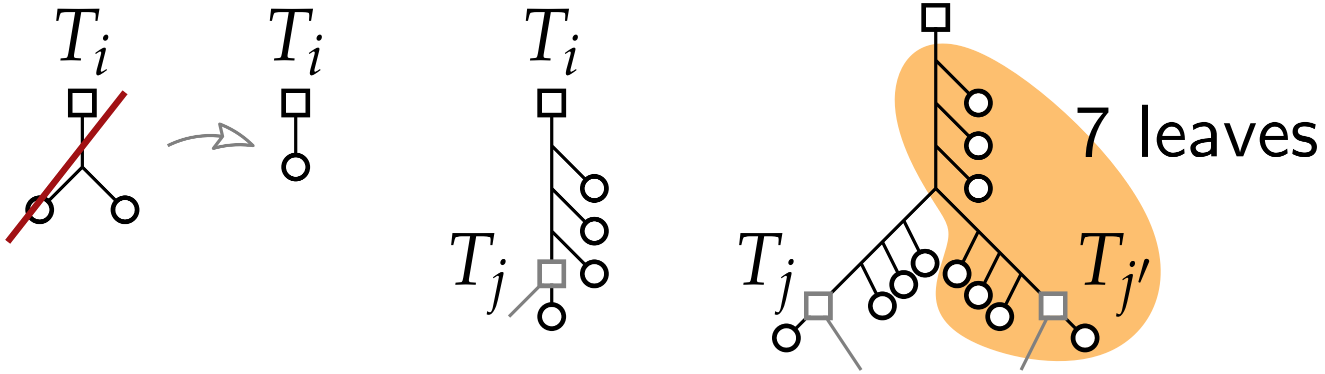

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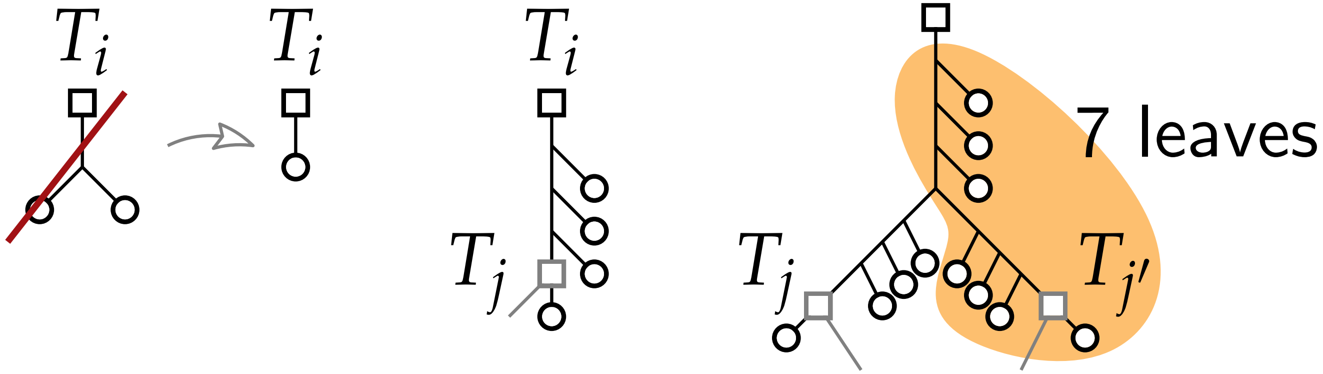

$\sum_{i=\rho}^{k}$ # leaves of T_i

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$\leq 28k$

FPT algorithm

Theorem 8.
Computing $\mathsf{d}_{\mathsf{SPR}}(T, T')$ is fixed-parameter tractable when parameterized by $\mathsf{d}_{\mathsf{SPR}}(T, T')$.

FPT algorithm

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FPT algorithm

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  - S has less than $2|X'|$ edges to cut and to attach to.
- Length-k BFS from S visits at most $O\Big(\big(4|X'|^2\big)^k\Big) = O\big((56k)^{2k}\big)$ trees.

by Theorem 7

- Since $k = \mathsf{d}_{\mathsf{SPR}}(S, S') = \mathsf{d}_{\mathsf{SPR}}(T, T')$, this yields an fpt algorithm.

Approximation algorithm

Idea.

- Given reduced trees T and T' we compute an agreement forest F by
- successively making "cuts" and "eliminations".
- This shrink T and T' further and further.
- Show that $|F|$ is at most $3|F'|$, where F' is a MAF of T and T'.

Approximation algorithm

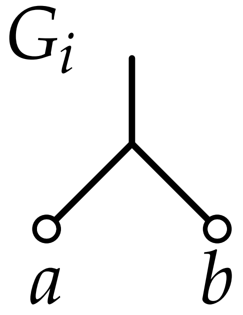
```
APPROXDSPR$(T, T')$
    $i \leftarrow 1$
    $G_i \leftarrow T$
    $H_i \leftarrow T'$
    while $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ do

    return $|H_i| - 1$
```

Approximation algorithm

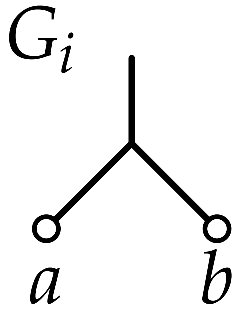
```
approxDSPR($T, T'$)
    $i \leftarrow 1$
    $G_i \leftarrow T$
    $H_i \leftarrow T'$
    while $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ do

    return $|H_i| - 1$
```



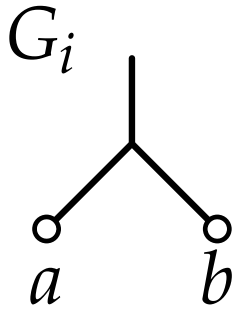
Approximation algorithm

```
$\textsc{approxDSPR}(T, T')$
    $i \leftarrow 1$
    $G_i \leftarrow T$
    $H_i \leftarrow T'$
    while $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ do
        find the case that applies to $a$ and $b$ in $H_i$
    return $|H_i| - 1$
```

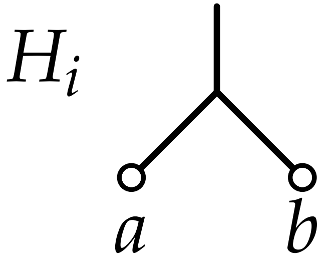


Approximation algorithm

```
$\textsc{approx}\mathrm{DSPR}(T, T')$
  $i \leftarrow 1$
  $G_i \leftarrow T$
  $H_i \leftarrow T'$
  while $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ do
      find the case that applies to $a$ and $b$ in $H_i$
  return $|H_i| - 1$
```

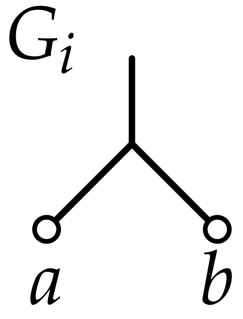


Case 1

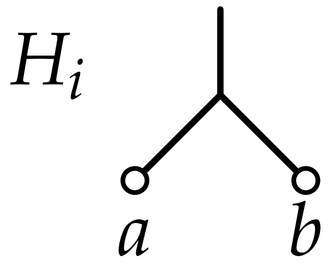


Approximation algorithm

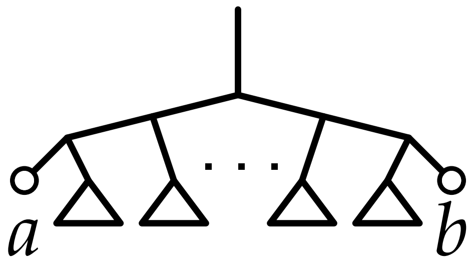
```
$\textsc{approx}\mathrm{DSPR}(T, T')$
    $i \leftarrow 1$
    $G_i \leftarrow T$
    $H_i \leftarrow T'$
    while $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ do
        find the case that applies to $a$ and $b$ in $H_i$
    return $|H_i| - 1$
```



Case 1

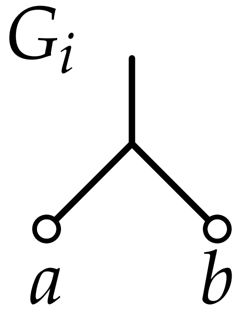


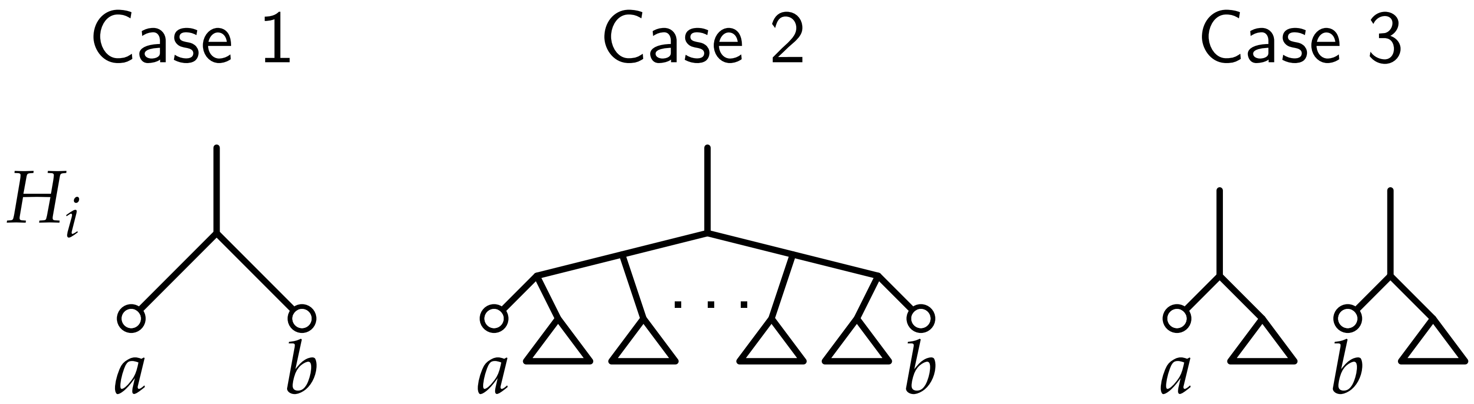
Case 2



Approximation algorithm

```
APPROXDSPR($T, T'$)
  $i \leftarrow 1$
  $G_i \leftarrow T$
  $H_i \leftarrow T'$
  while $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ do
      find the case that applies to $a$ and $b$ in $H_i$
  return $|H_i| - 1$
```



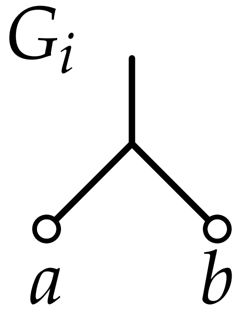

Case 1

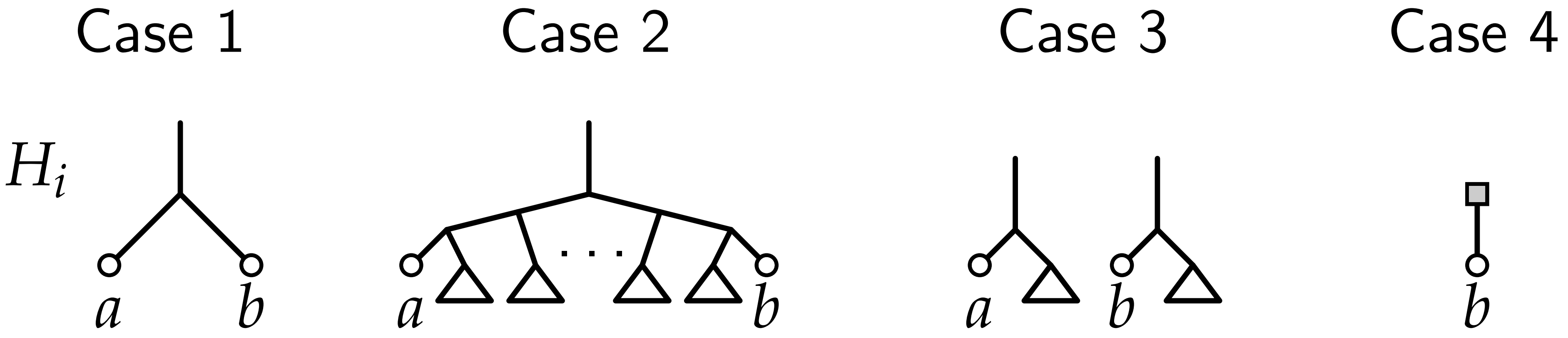
Case 2

Case 3

Approximation algorithm

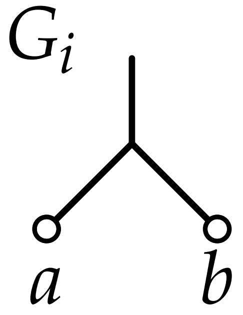
```
APPROXDSPR$(T, T')$
    $i \leftarrow 1$
    $G_i \leftarrow T$
    $H_i \leftarrow T'$
    while $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ do
        find the case that applies to $a$ and $b$ in $H_i$
    return $|H_i| - 1$
```

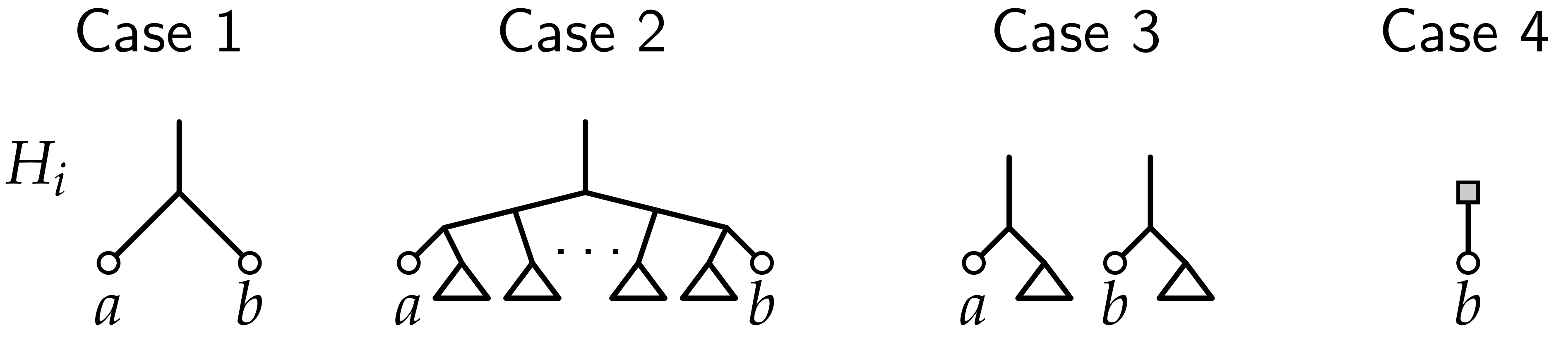




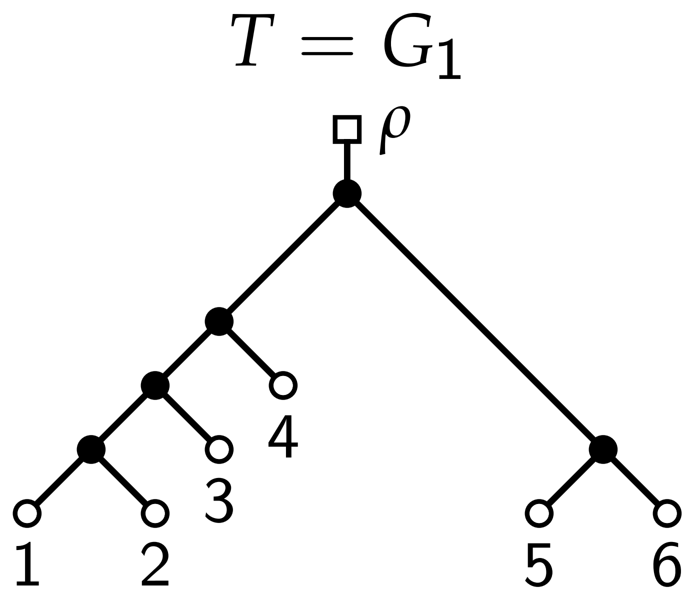
Approximation algorithm

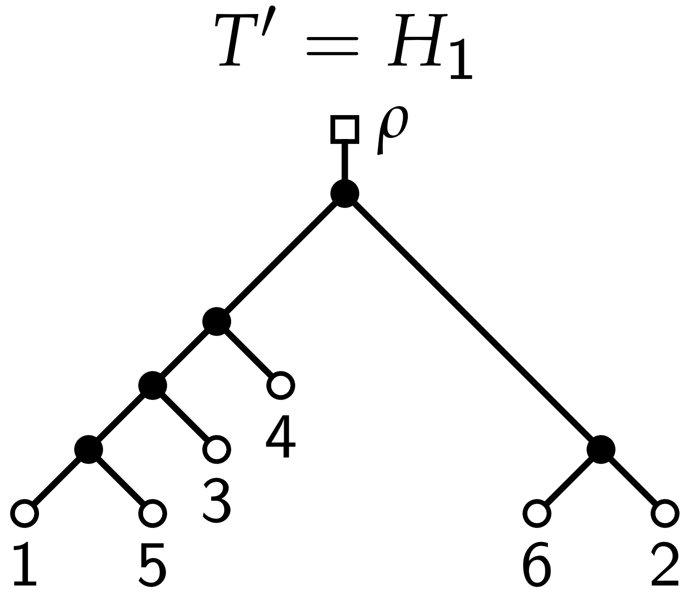
```
$\textsc{approx}\mathrm{DSPR}(T, T')$
  $i \leftarrow 1$
  $G_i \leftarrow T$
  $H_i \leftarrow T'$
  while $\exists$ pair of sibling leaves $a$ and $b$ in $G_i$ do
      find the case that applies to $a$ and $b$ in $H_i$
      apply the corresponding transaction
      to obtain $G_{i+1}$ from $G_i$ and $H_{i+1}$ from $H_i$
      $i++$
  return $|H_i| - 1$
```



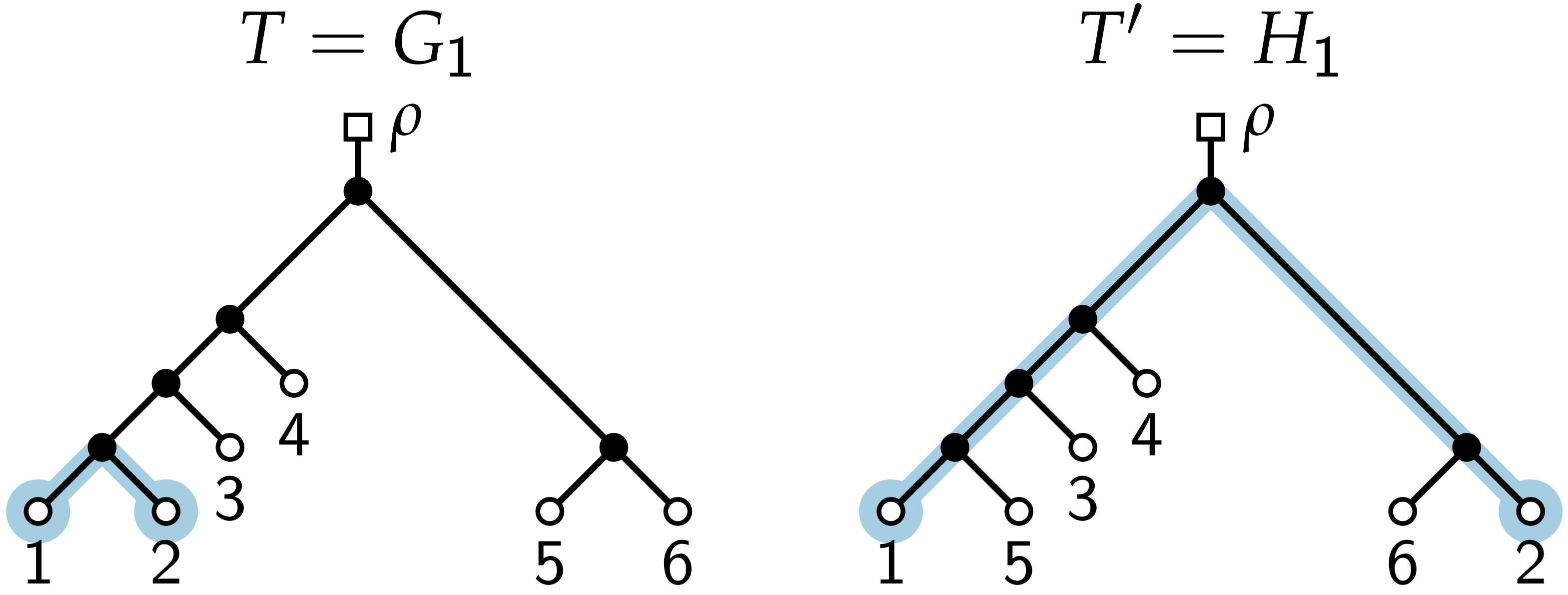


Approximation algorithm – example

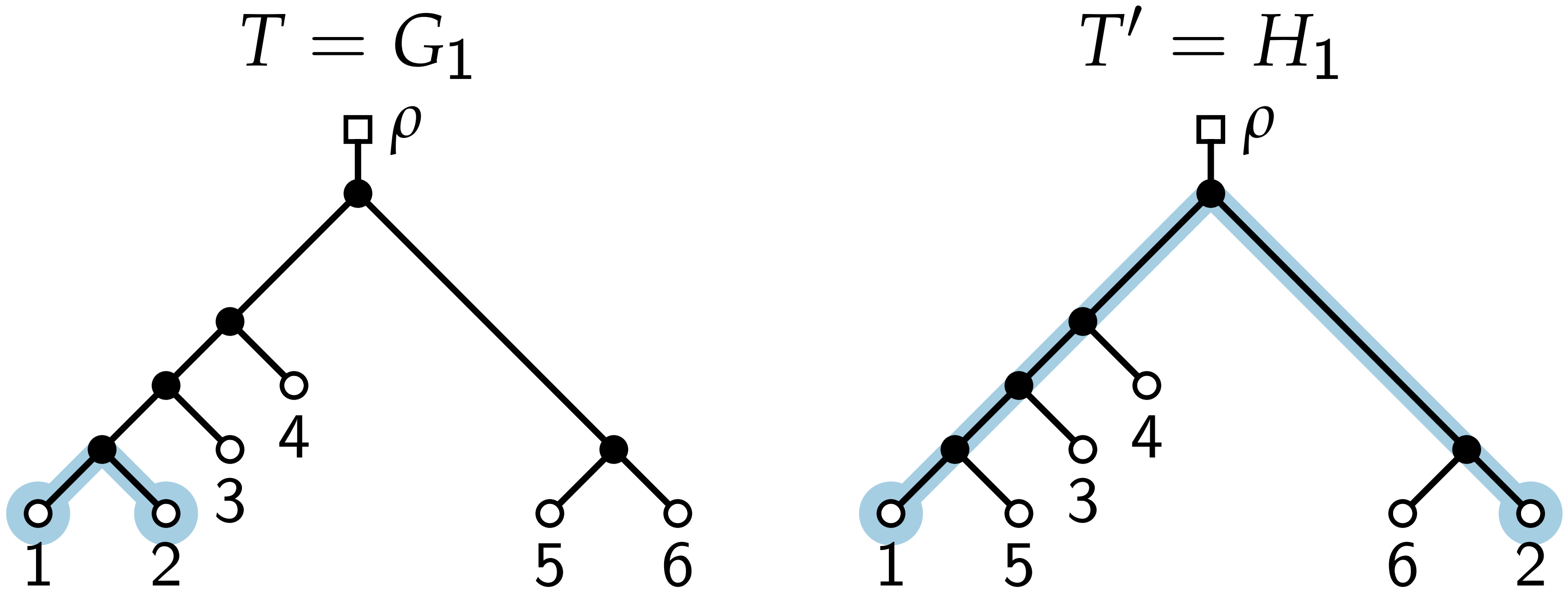




Approximation algorithm – example

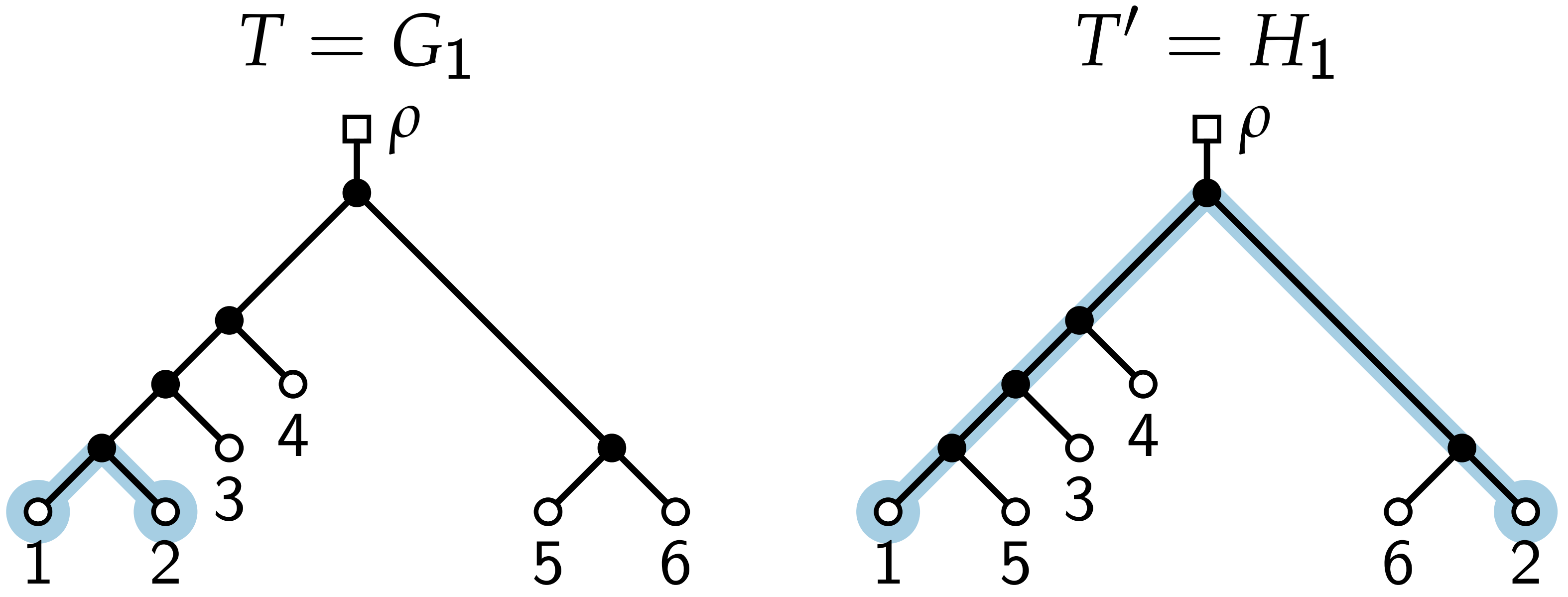


Approximation algorithm – example



- Should we cut of the leaves 1 or 2 or all in between them in H_1?

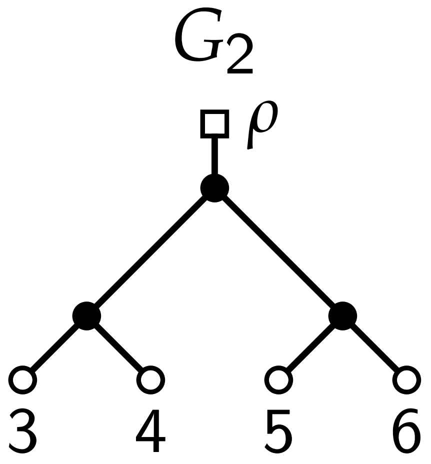
Approximation algorithm – example

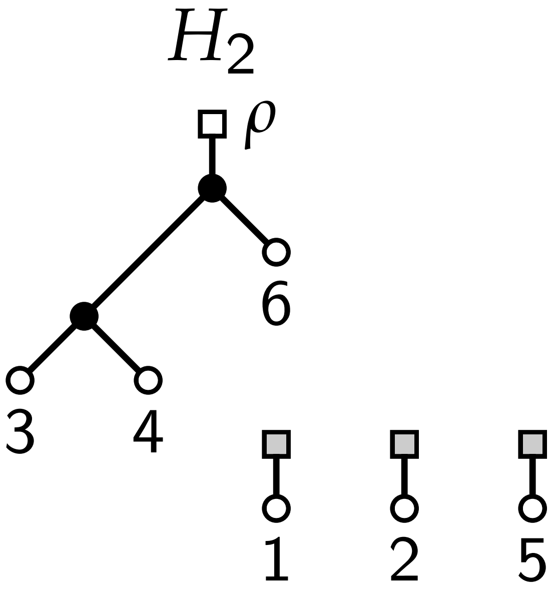


Case 2

- Should we cut of the leaves 1 or 2 or all in between them in H_1?
- Do parts of each!

Approximation algorithm – example

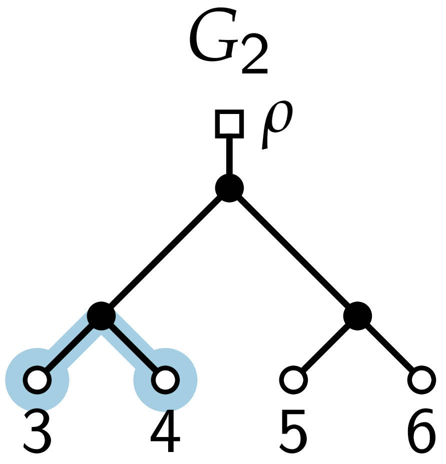


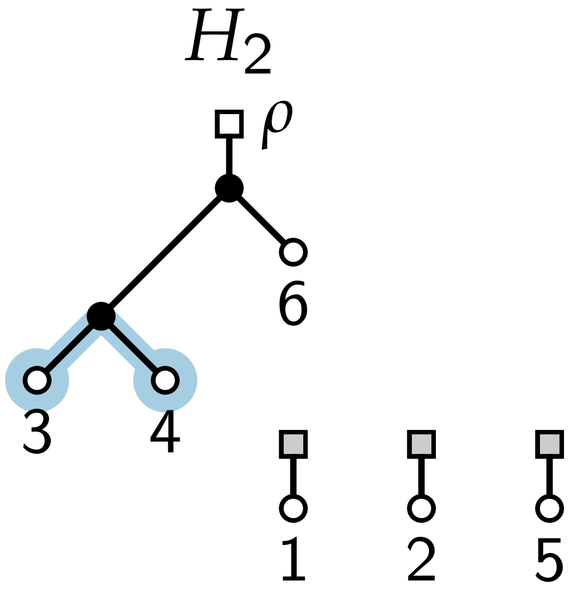


Case 2

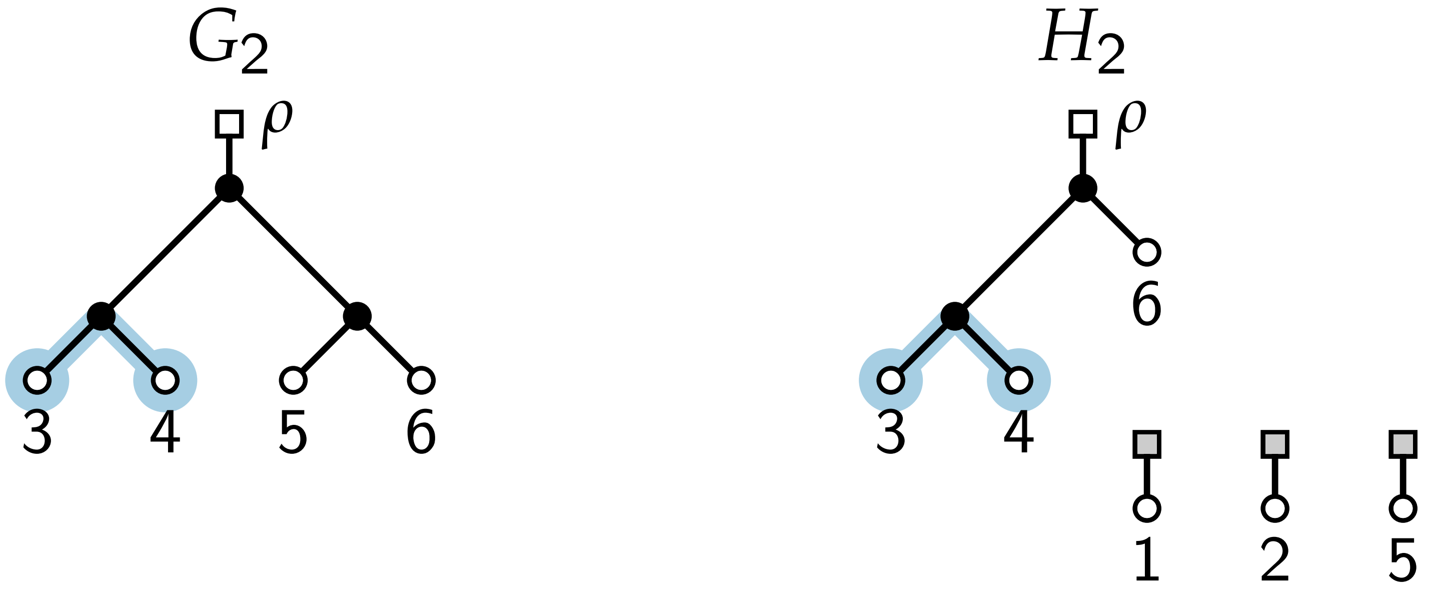
- Should we cut of the leaves 1 or 2 or all in between them in H_1?
- Do parts of each!

Approximation algorithm – example





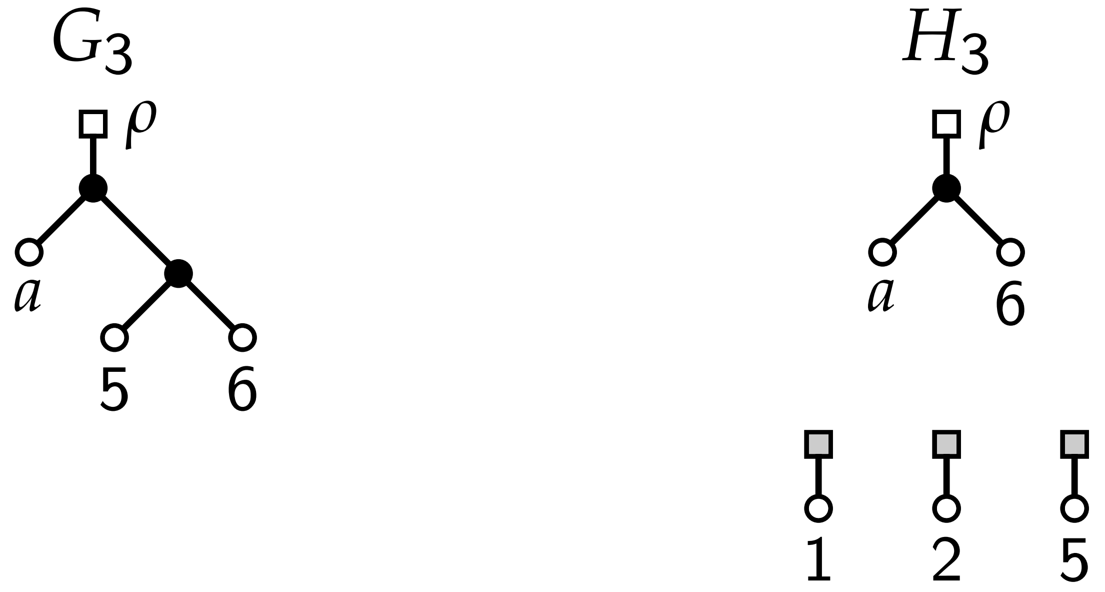
Approximation algorithm – example



Case 1

- If the same cherry occurs in H_i, we can simply reduce it.

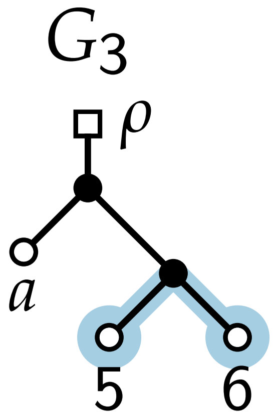
Approximation algorithm – example

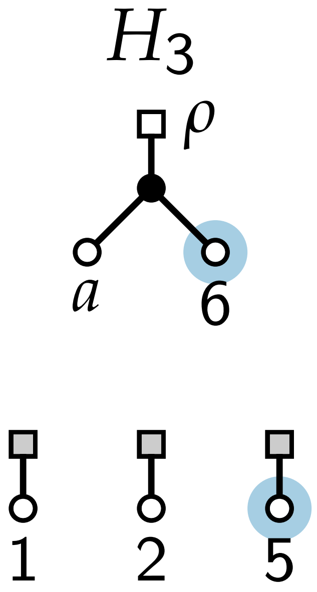


Case 1

- If the same cherry occurs in H_i, we can simply reduce it.

Approximation algorithm – example

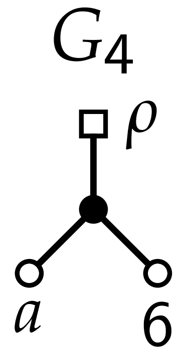


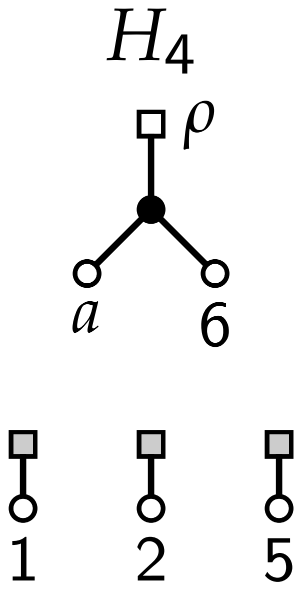


Case 4

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

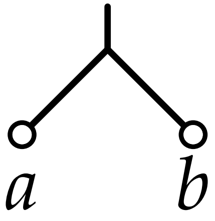
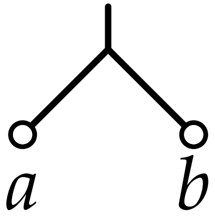
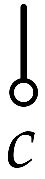
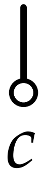
Approximation algorithm – example



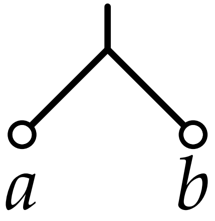
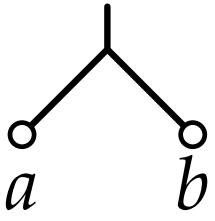
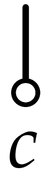
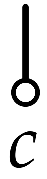


- Return 3.

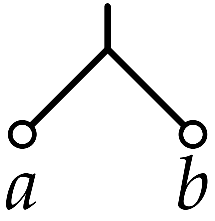
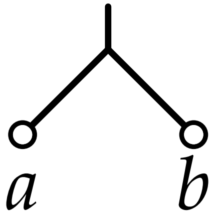
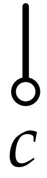
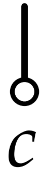
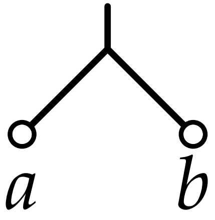
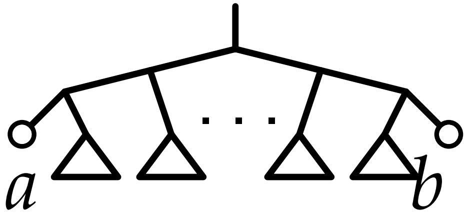
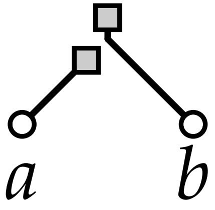
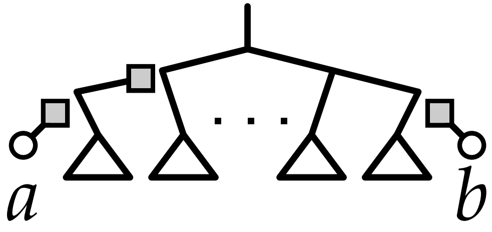
Approximation algorithm – analysis

Case	G_i	H_i		G_{i+1}	H_{i+1}	Cost
1						

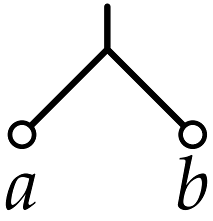
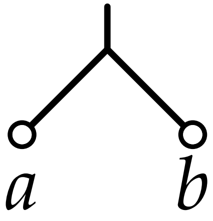
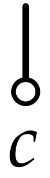
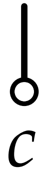
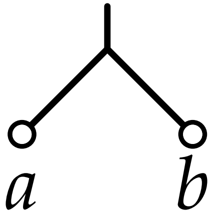
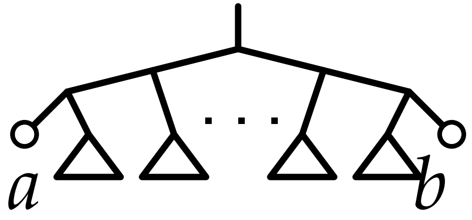
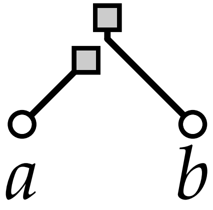
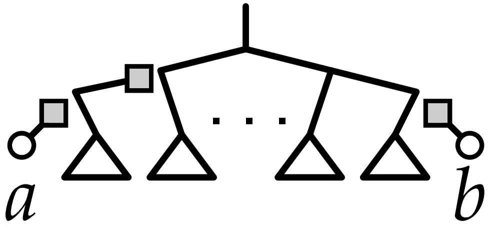
Approximation algorithm – analysis

Case	G_i	H_i	→	G_{i+1}	H_{i+1}	Cost
1						no mistake

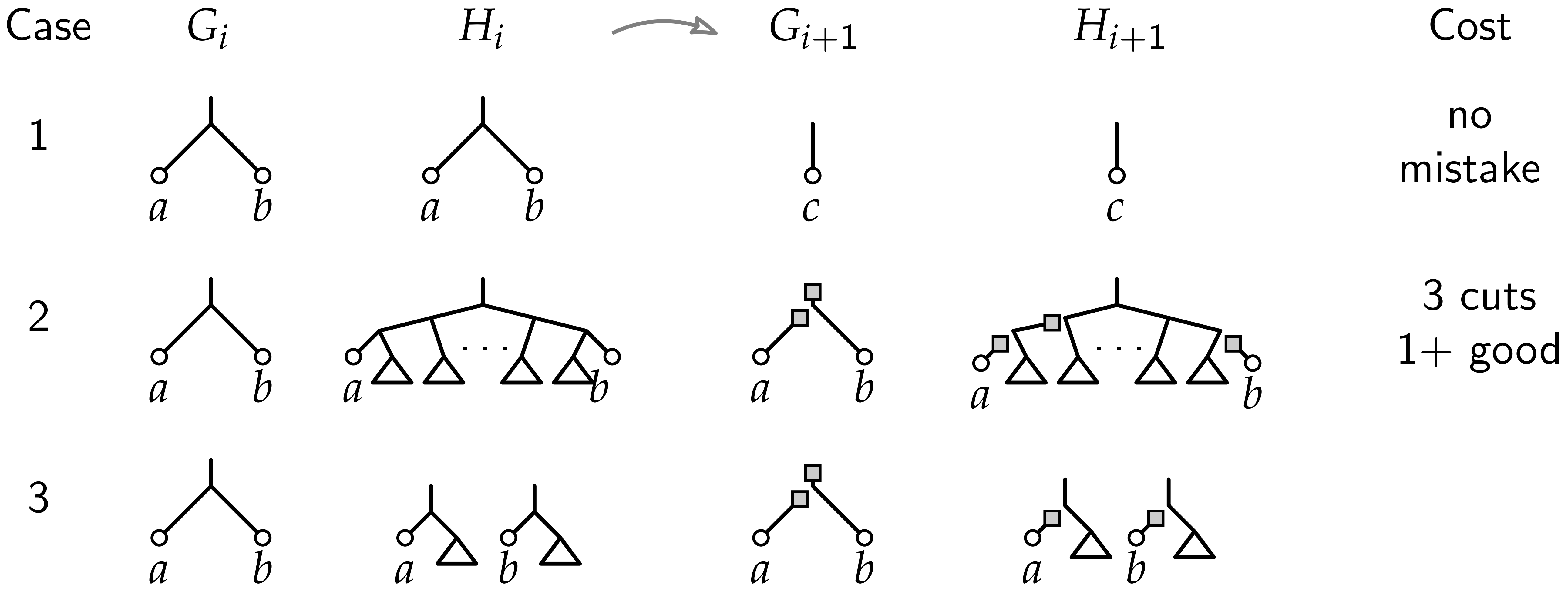
Approximation algorithm – analysis

Case	G_i	H_i	G_{i+1}	H_{i+1}	Cost
1					no mistake
2					

Approximation algorithm – analysis

Case	G_i	H_i	G_{i+1}	H_{i+1}	Cost
1					no mistake
2					3 cuts 1+ good

Approximation algorithm – analysis



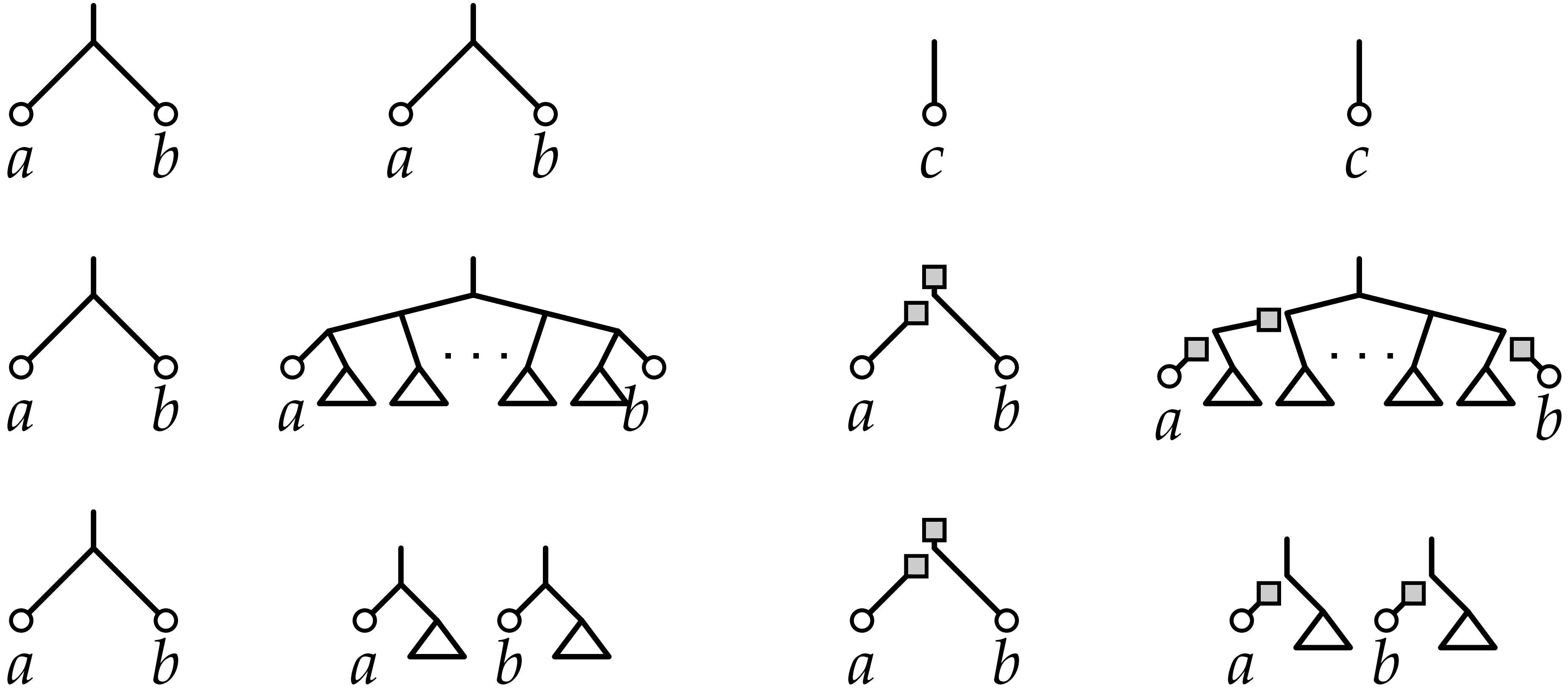
Case G_i H_i → G_{i+1} H_{i+1} Cost

1 no mistake

2 3 cuts 1+ good

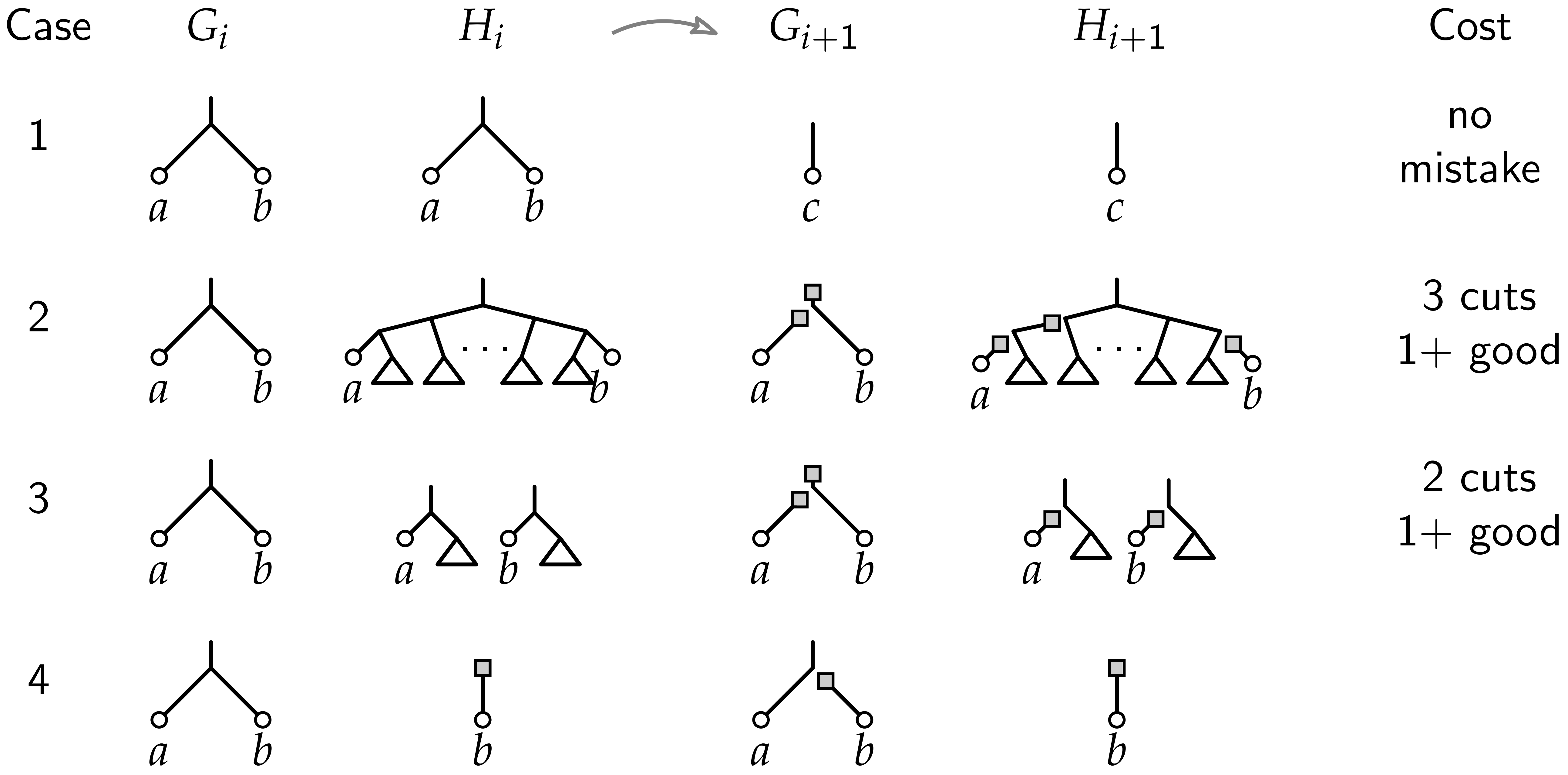
3

Approximation algorithm – analysis



Case	G_i	H_i	G_{i+1}	H_{i+1}	Cost
1					no mistake
2					3 cuts 1+ good
3					2 cuts 1+ good

Approximation algorithm – analysis



Case G_i H_i → G_{i+1} H_{i+1} Cost

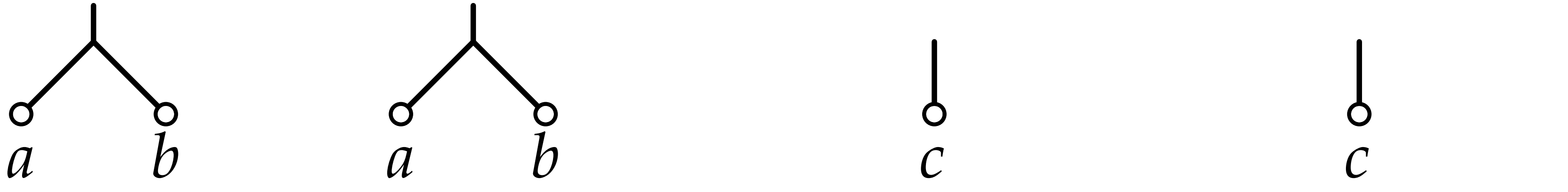
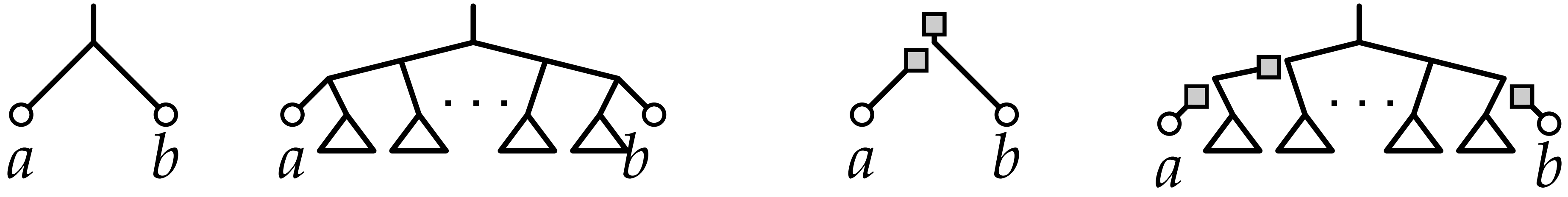
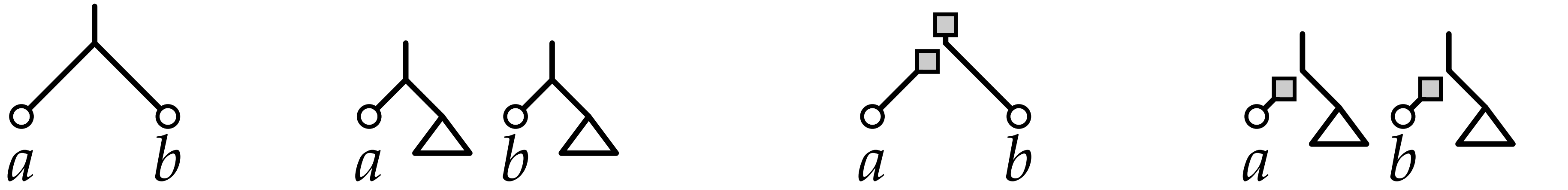
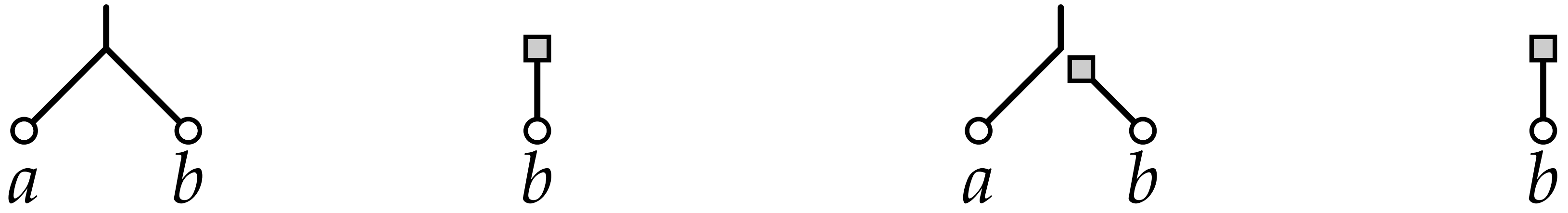
1 — no mistake

2 — 3 cuts 1+ good

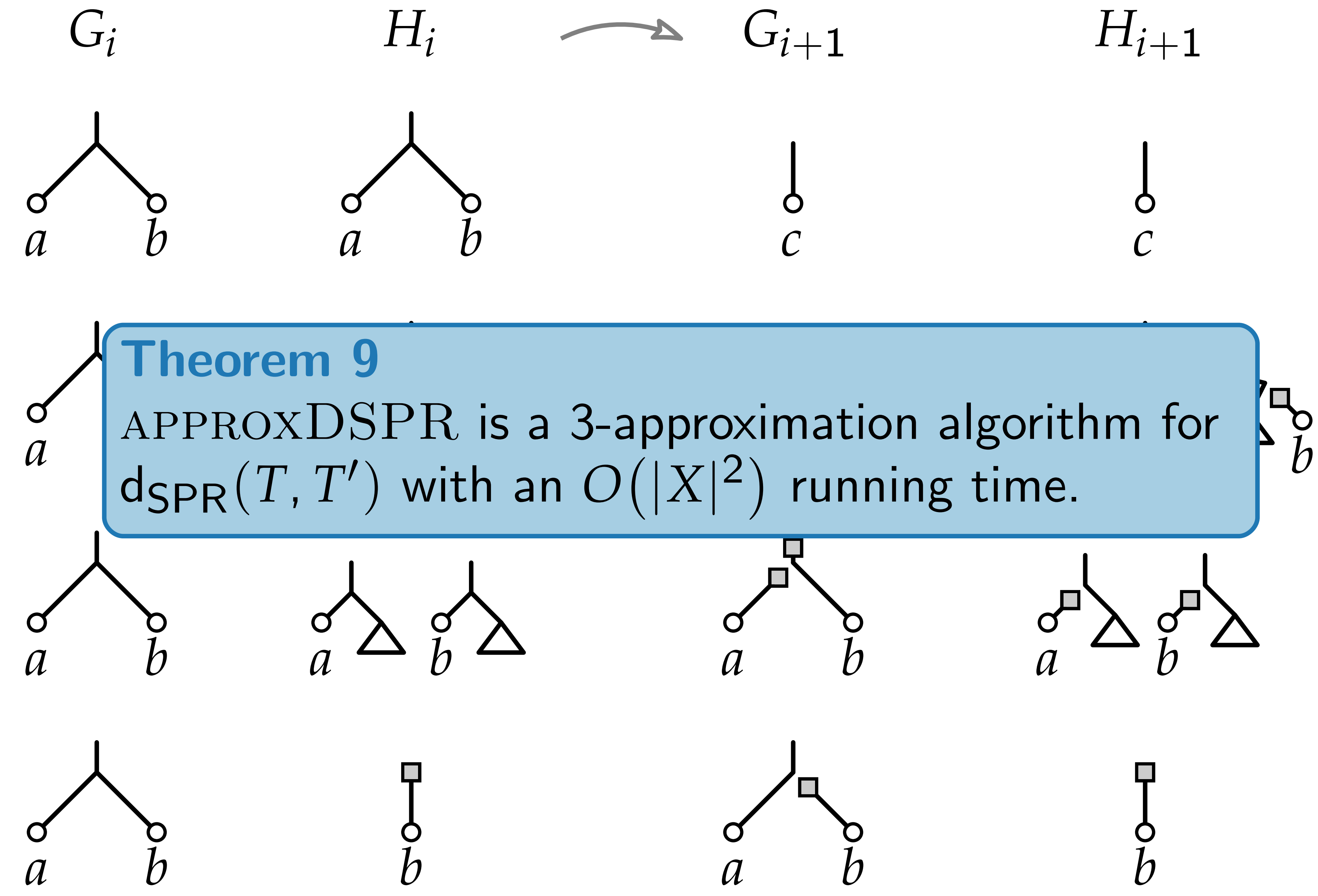
3 — 2 cuts 1+ good

4

Approximation algorithm – analysis

Case	G_i H_i → G_{i+1} H_{i+1}	Cost
1		no mistake
2		3 cuts 1+ good
3		2 cuts 1+ good
4		1 cut 1 good

Approximation algorithm – analysis



Case	G_i	H_i	G_{i+1}	H_{i+1}	Cost
1					no mistake
2					3 cuts 1+ good
3					2 cuts 1+ good
4					1 cut 1 good

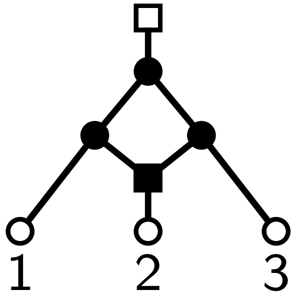
Theorem 9

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

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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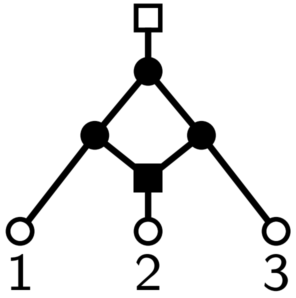

Maximum Agreement Forests.

- Reframing (characterising) a problem in a different way, can sometimes make your life a lot easier.
- MAF can be generalized to Maximum Agreement Graphs, but these don’t characterize the SPR-distance of networks anymore.

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 $15k - 9$.
- With further reduction rules can get size below $11k - 9$. [KL '18]
- Divide & conquer algorithm can (in practice) reduce further reduce problem sizes. [LS '11]

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Approximation algorithm.

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

Literature

Original papers:

- [BS ’05] “On the computational complexity of the rooted subtree prune and regraft distance” for SPR, MAF, characterisation, fpt, divide & conquer
- [RSW ’06] “The maximum agreement forest problem: Approximation algorithms and computational experiments”

Referenced papers:

- [HJWZ ’96] “On the complexity of comparing evolutionary trees” for NP-hardness proof
- [KL ’19] “New reduction rules for the tree bisection and reconnection distance”
- [CHW ’17] “A New 2-Approximation Algorithm for rSPR Distance”
- [LS11] “A cluster reduction for computing the subtree distance between phylogenies”