Constructing incompatibility graphs of trees in optimal output-sensitive time

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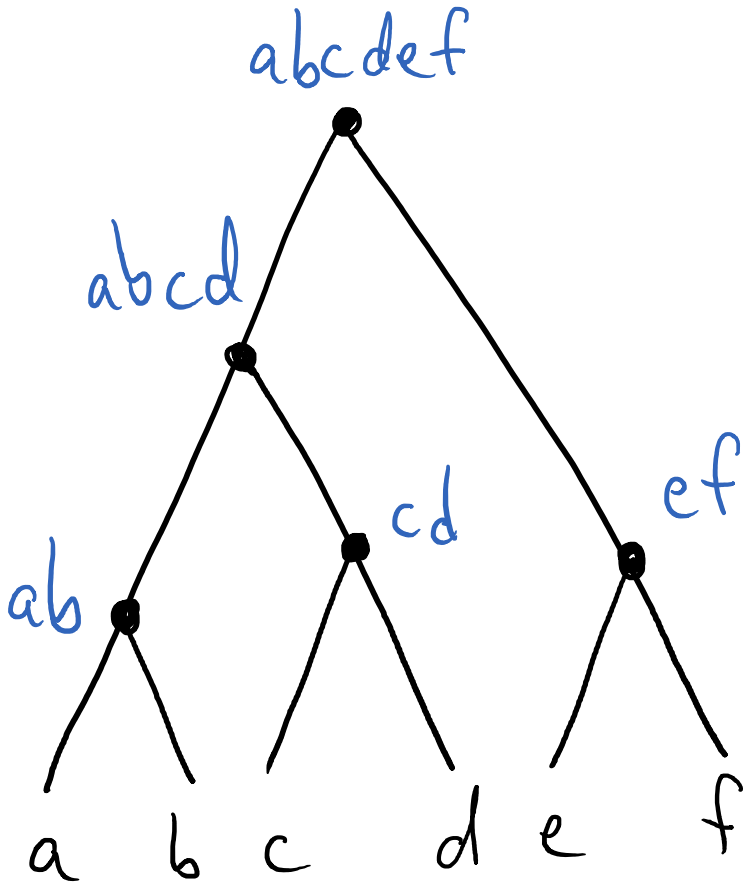
Clusters in trees

Given a (rooted) tree T and a node $v \in T$, $cluster_T(v)$ is the set of leaf taxa that descend from v.

$clusters(T) = \{cluster_T(v) : v \in V(T)\}$



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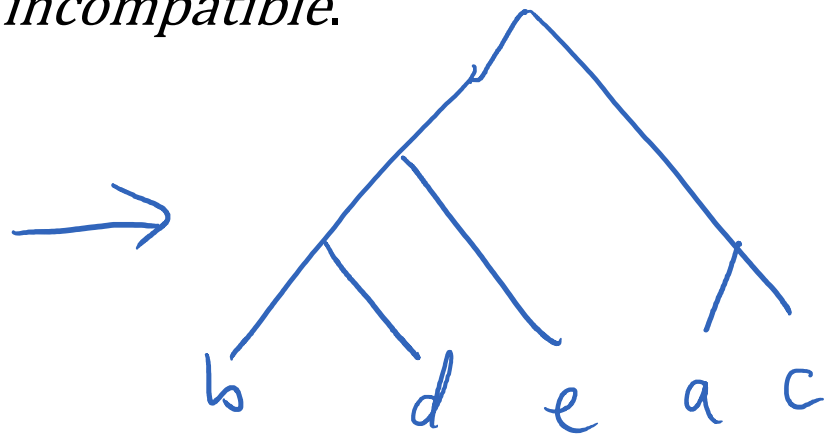

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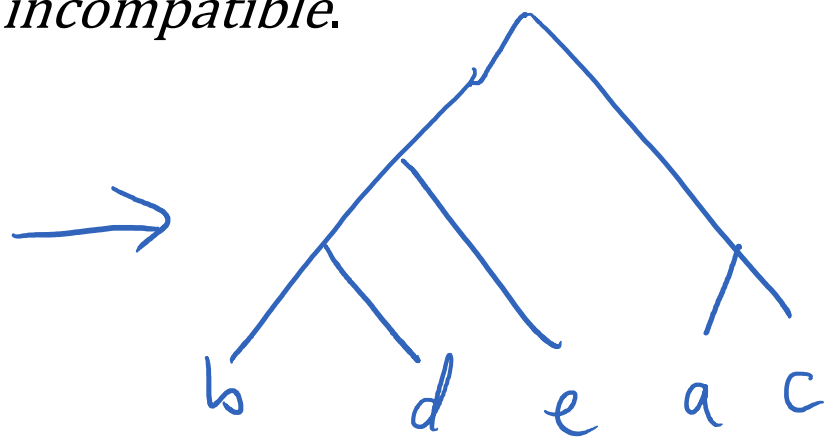

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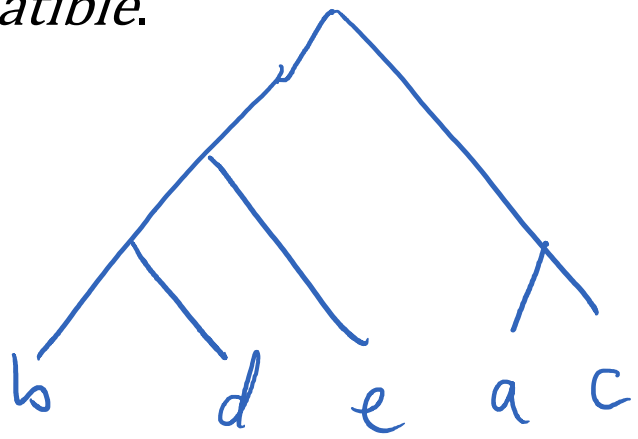

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Otherwise, A, B are *incompatible*.

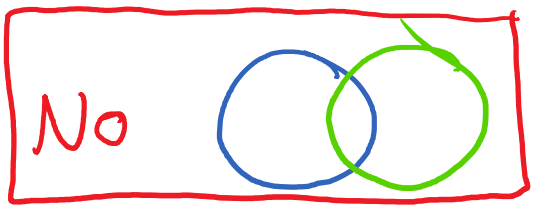
Classic problem: given a collection of sets of taxa $A = \{A_1, \ldots, A_k\}$, reconstruct a tree whose clusters are exactly A, if possible.

Theorem: feasible if and only if sets in A are pairwise-compatible.

Theorem: A, B are compatible if and only if one of the following holds: either

1. $A \subseteq B$;
2. $B \subseteq A$; or
3. $A \cap B = \emptyset$.

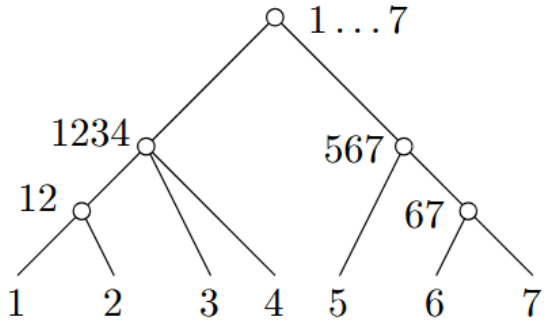
(i.e., there is no overlap)

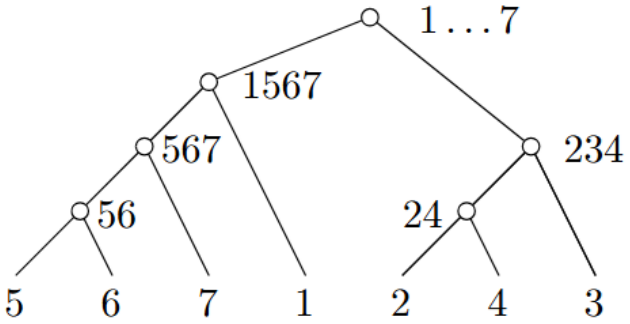


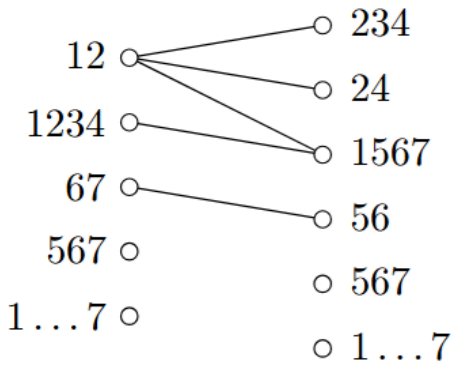
Incompatibility graphs

Let T_1, T_2 be two trees. Then $G(T_1, T_2)$ is the incompatibility graph of T_1, T_2. It has:

- one vertex for each cluster of T_1 and each cluster of T_2;
- an edge between clusters X and Y if and only if X, Y are incompatible.







Some motivations

Incompatibility graphs are notably used to:

- Reconstruct phylogenetic networks to combine trees with incompatible clusters. Each connected component of $G(T_1, T_2)$ corresponds to a blob of the network. [van Iersel et al, 2010]

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- Compute distances between trees. The BHV distance projects the trees in a continuous vector space, and asks for the shortest geodesic path between the projections.

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- others (e.g., obtain consensus trees)

Computing $G(T_1, T_2)$

$n =$ number of leaves of T_1 and of T_2.

Current implementations

- Represent clusters as bit vectors. Operations take time $O(n/w)$, where w is the machine word size.
- Then **for each pair** of clusters, check for compatibility in time $O(n/w)$.
- Total time: $O(n^2 \cdot n/w) = O(n^3/w)$.

Computing $G(T_1, T_2)$

$O(n^2)$ seems to be a lower bound on the complexity, because incompatibility graphs can have $\Theta(n^2)$ edges.

Need quadratic time just to write the output.

Yes but...

This work

Theorem

Let T_1, T_2 be two trees on n leaves, and let $d = |E\big(G(T_1, T_2)\big)|$.

Then there is an algorithm that, on input T_1, T_2, outputs $G(T_1, T_2)$ in optimal time $O(n + d)$.

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Note: d is not part of the input.

An algorithm whose time complexity depends on the size of the output is called *output-sensitive*.

Similar result exist to enumerate conflicting rooted triples [Weller, 2018].

The algorithm

lca-maps

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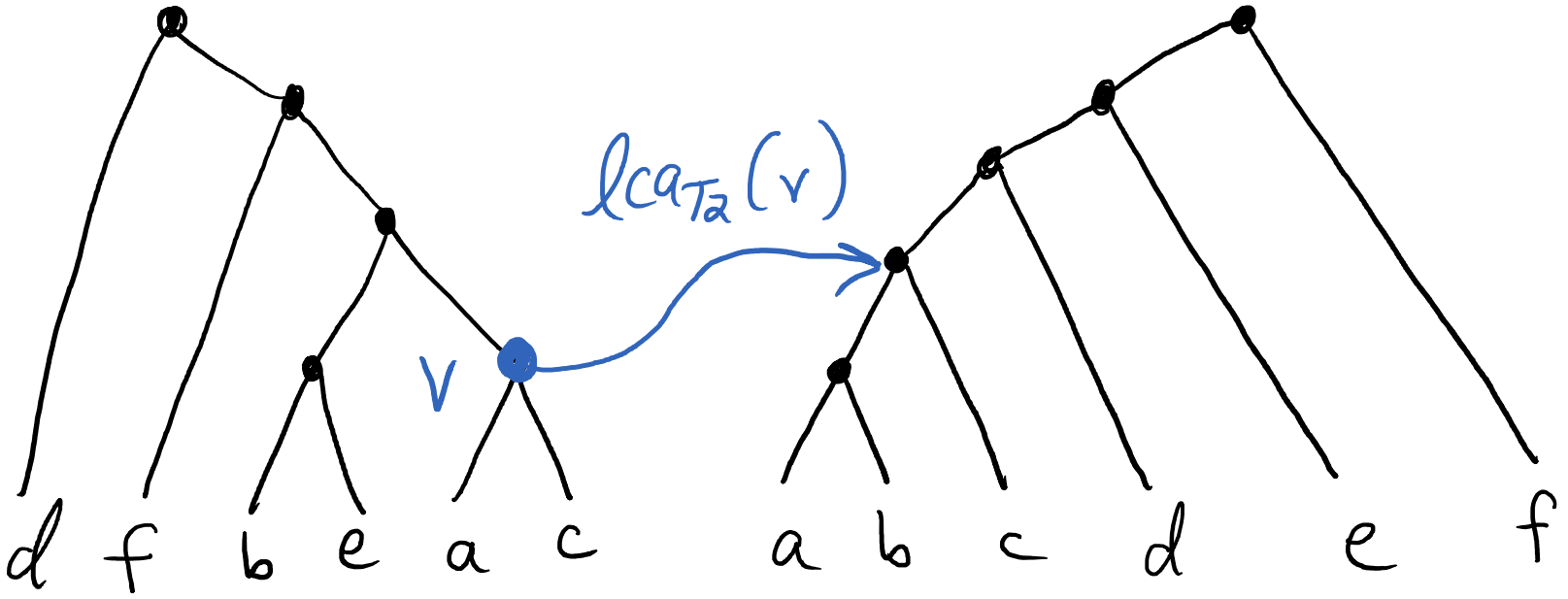

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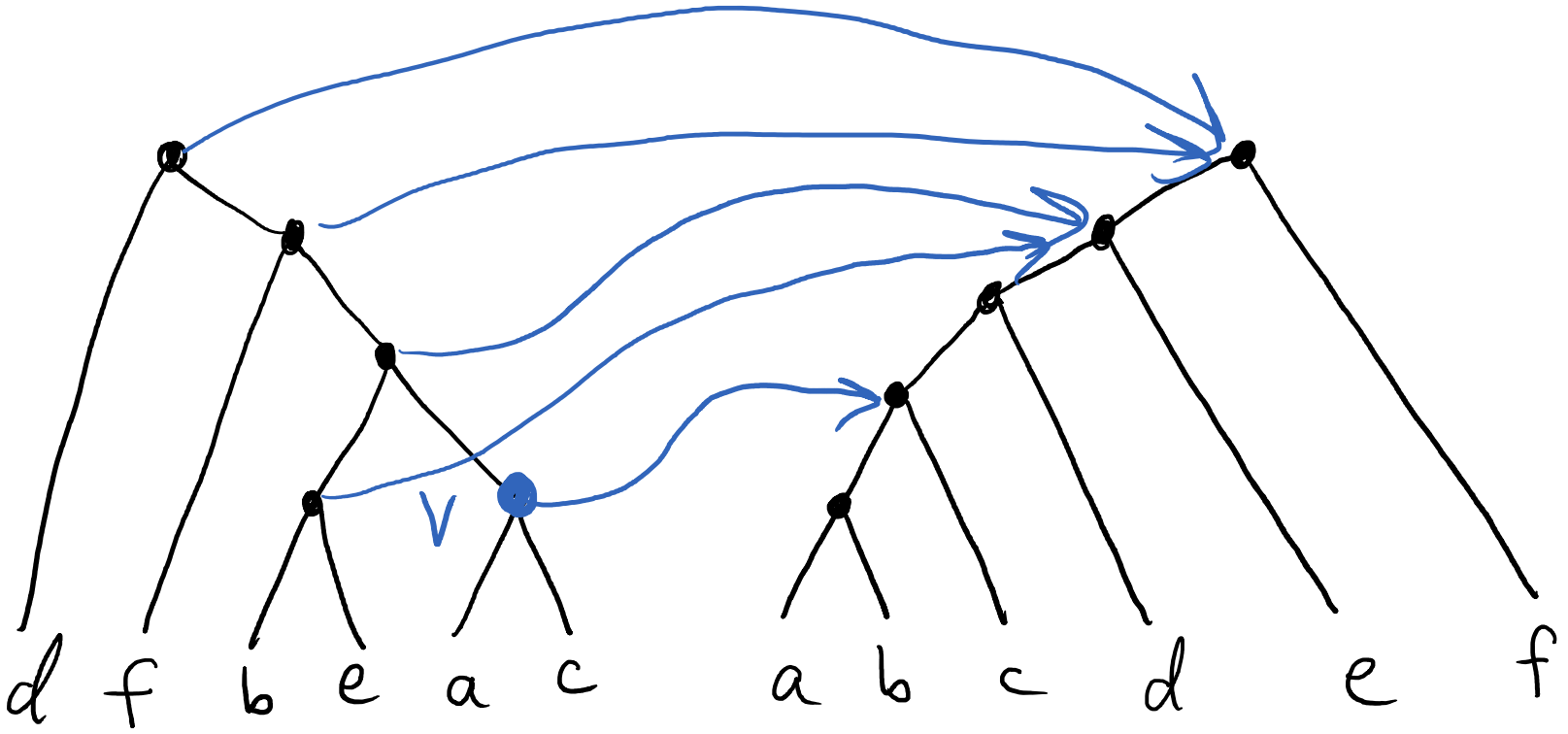

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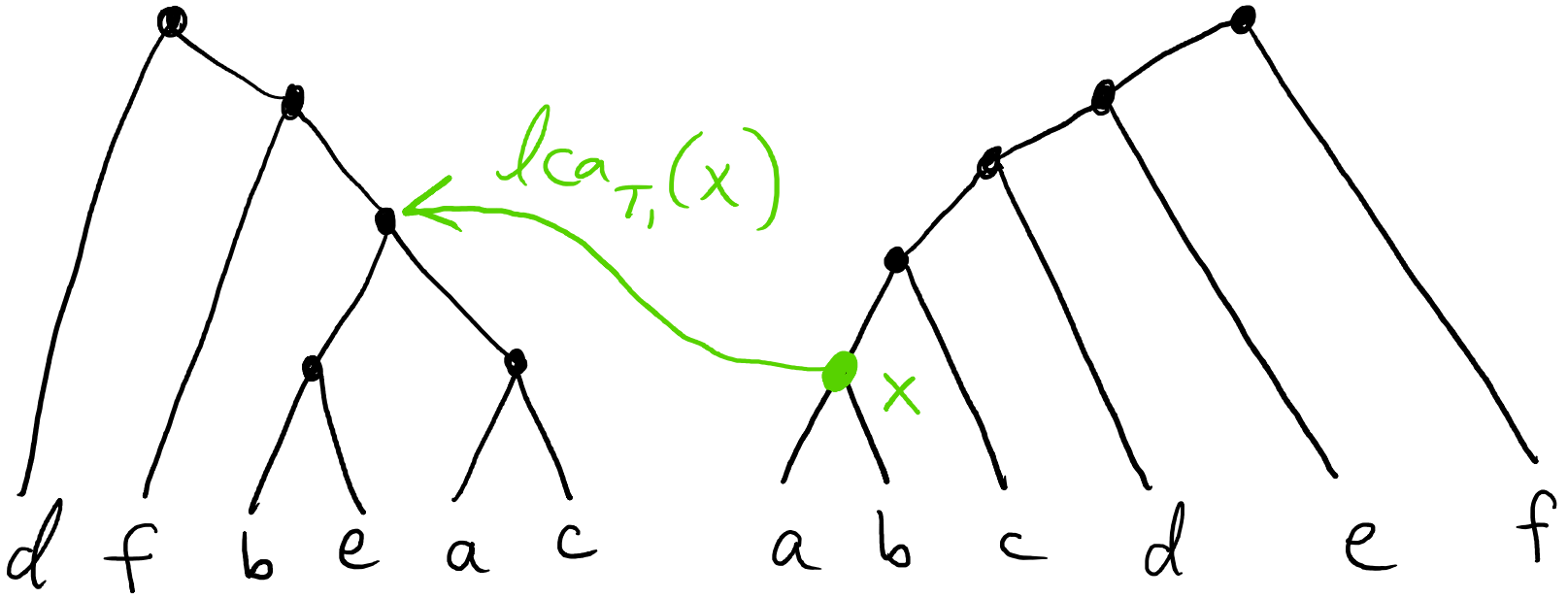

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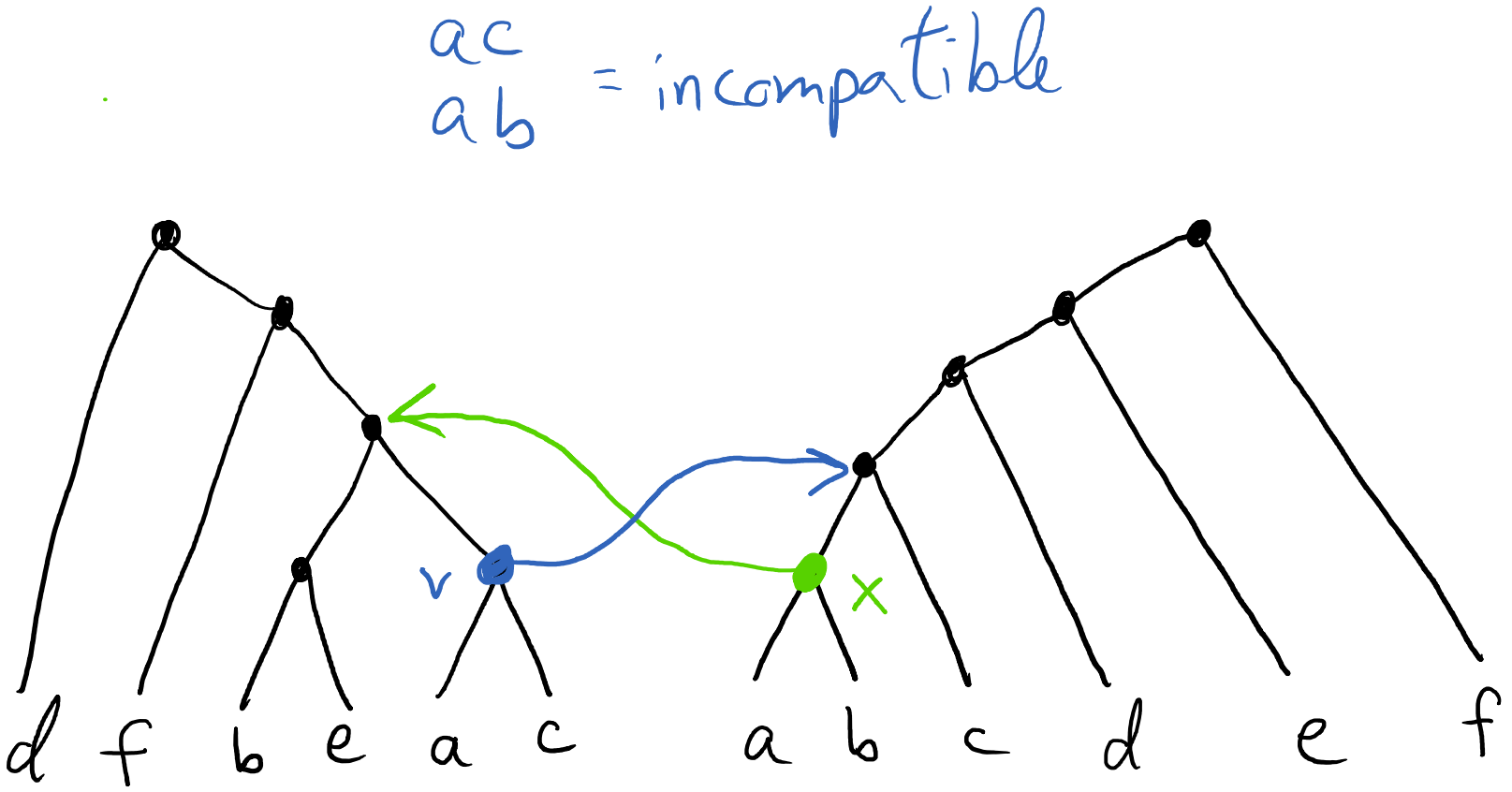

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Lemma

The clusters of nodes $v \in V(T_1)$ and $x \in V(T_2)$ are incompatible if and only if at least one of the two following conditions is true:

- $v \prec lca_{T_1}(x)$ and v has a child w such that $lca_{T_2}(w) \preccurlyeq x \prec lca_{T_2}(v)$; or
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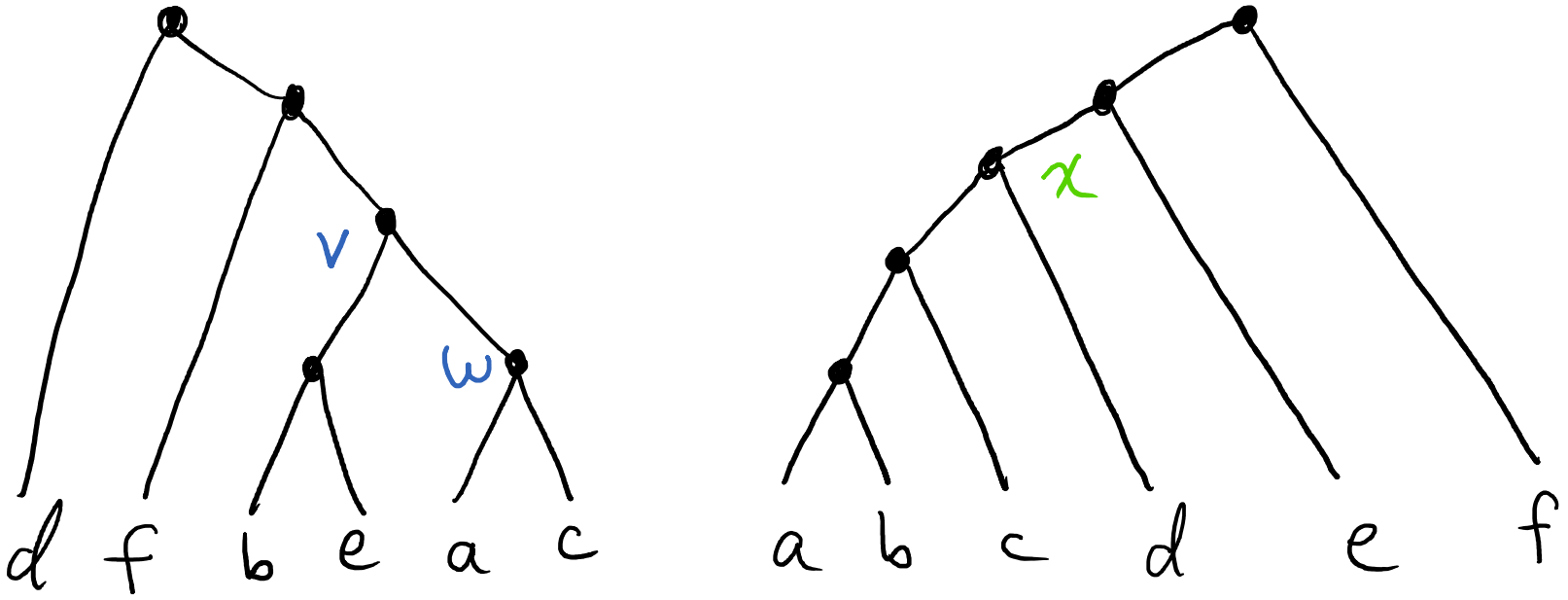

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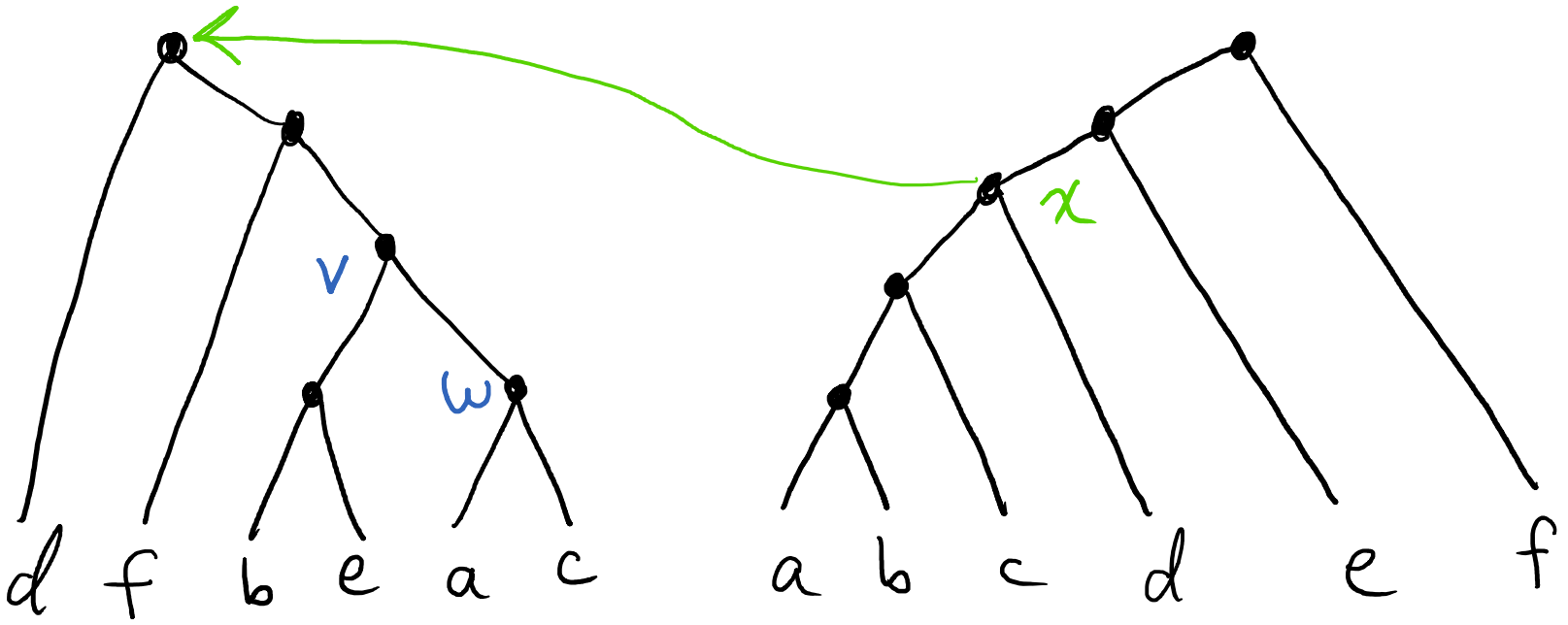

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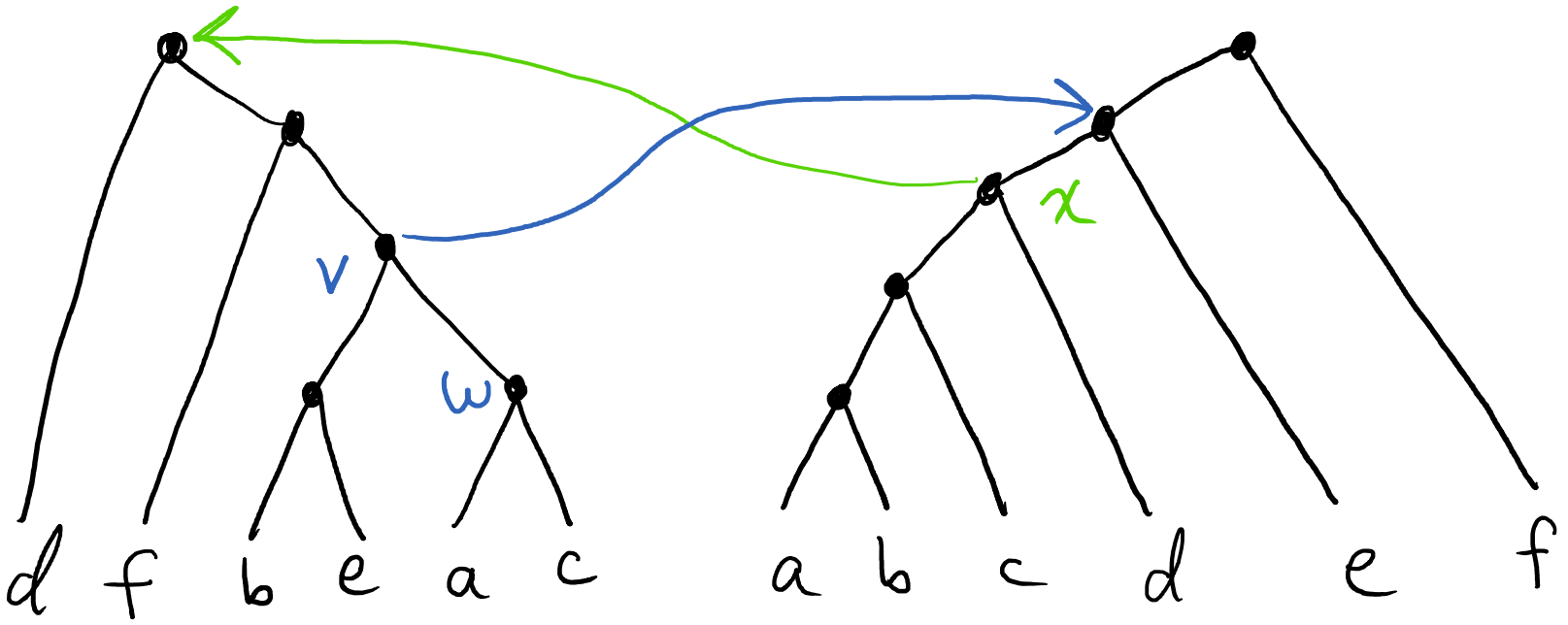

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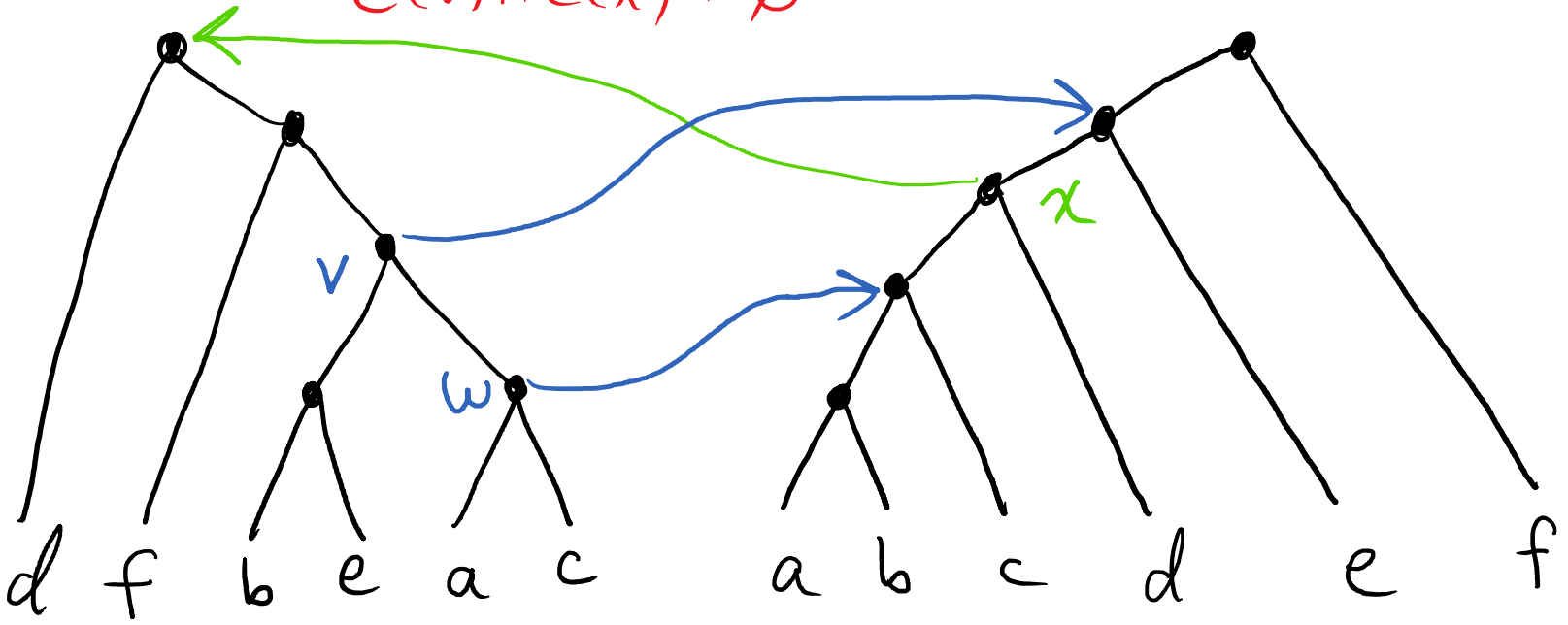

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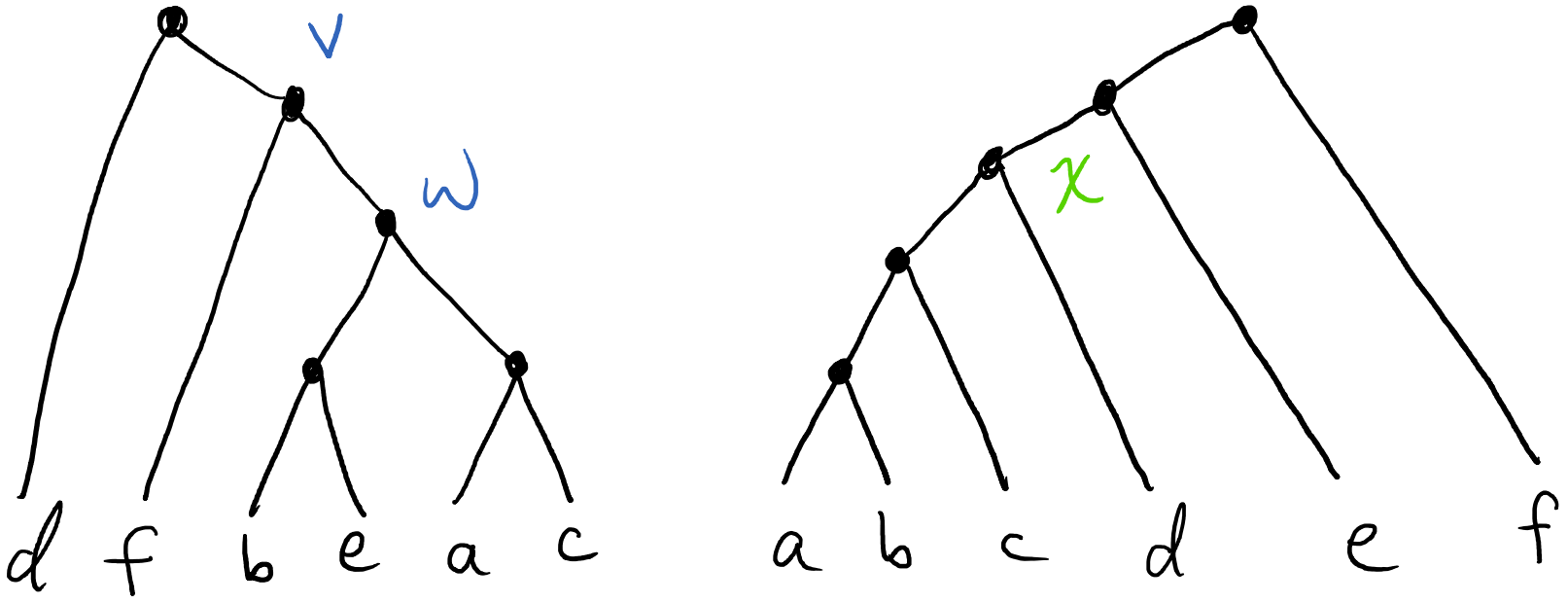

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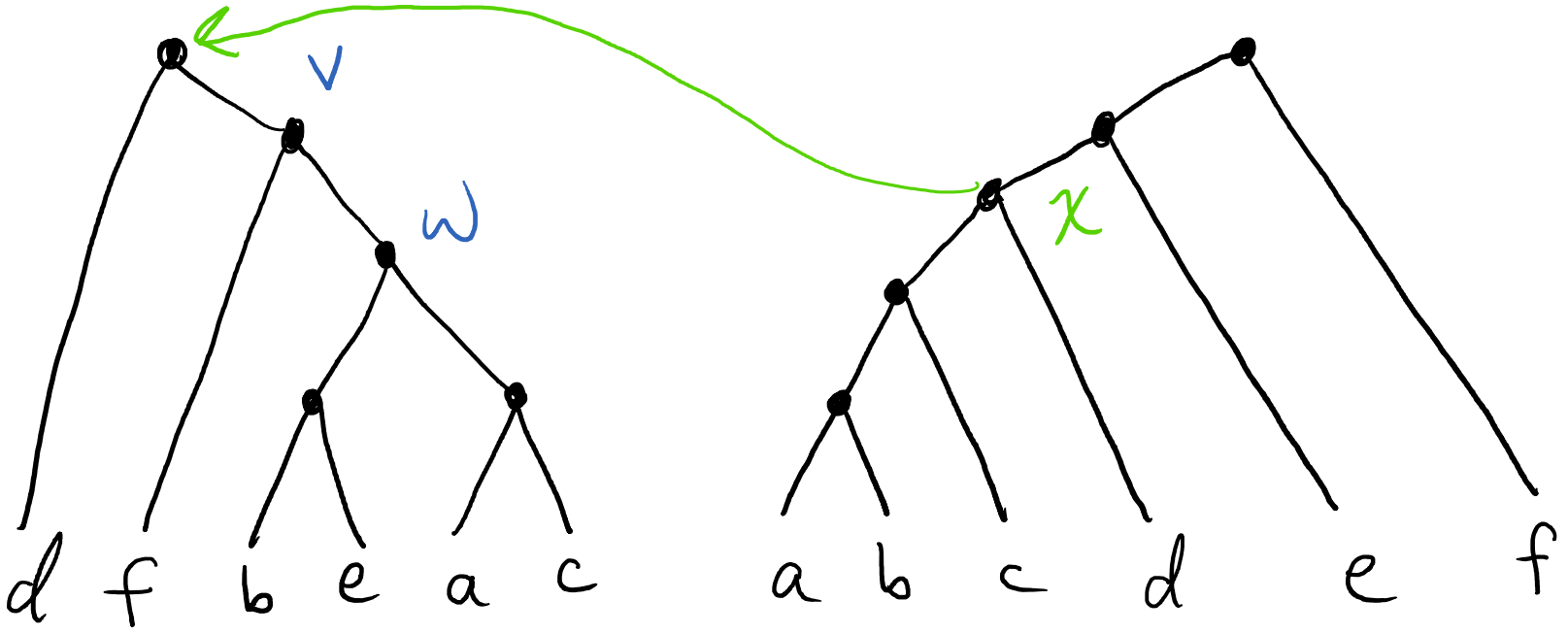

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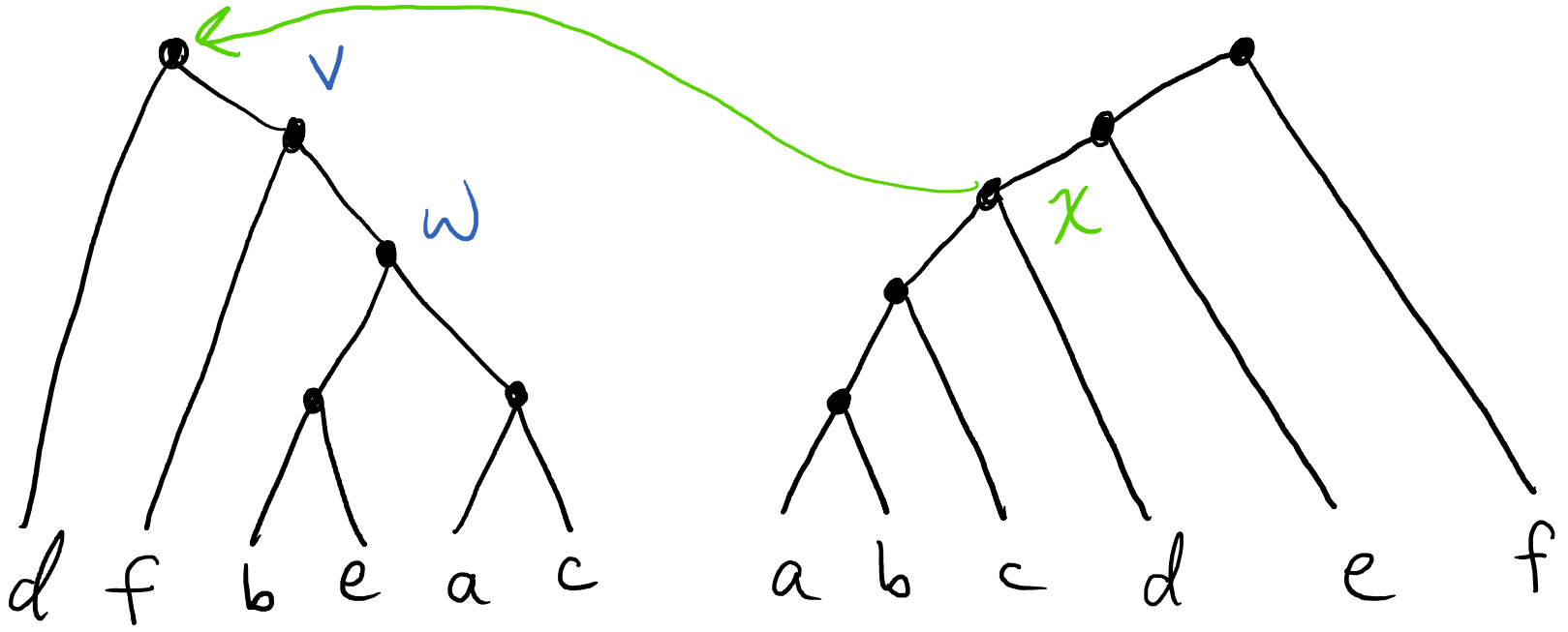

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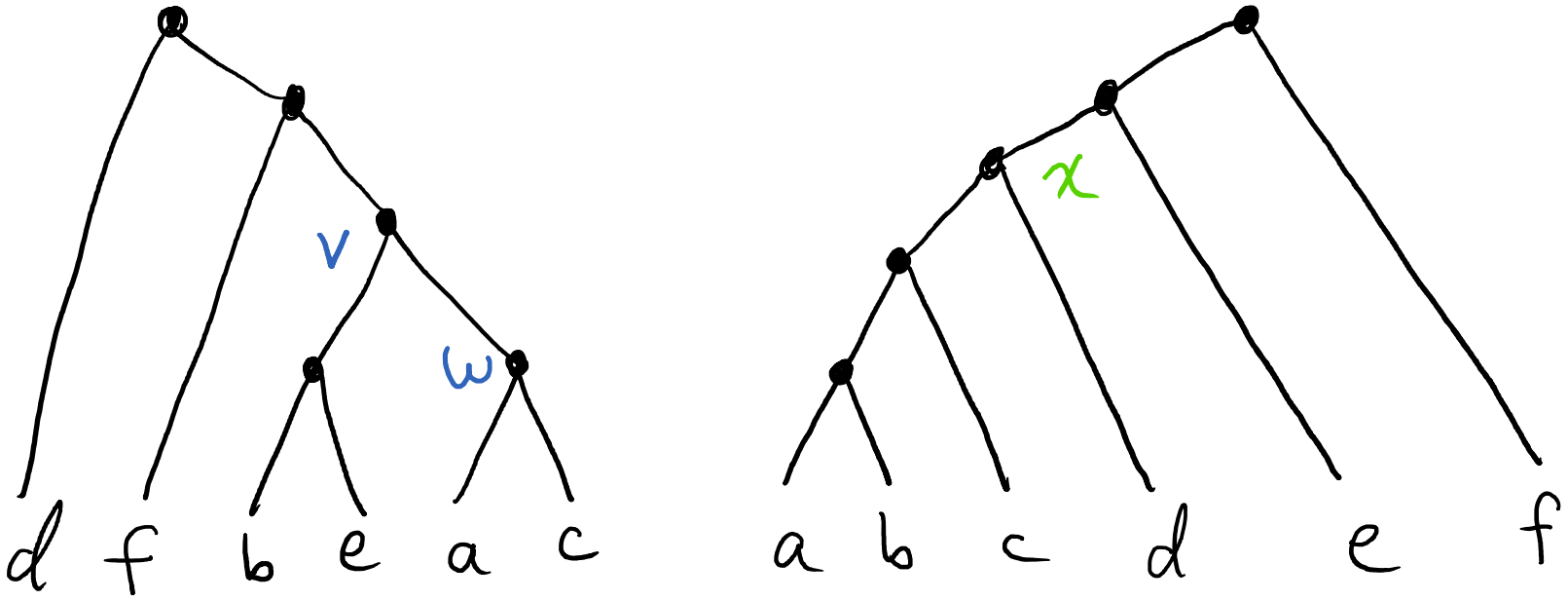

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3      Construct the lca-maps μ⃗ and ν⃖
4      Pre-process T' for O(1) diff_anc(x) queries
5      Let G be a graph with vertex set V(T) ∪ V(T') and no edge
6      Let Q be a global array of length |V(T')|, with values initialized to −1
7      for each v ∈ I(T) in a postorder traversal do
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17             Add {v, x} to E(G)
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19             x = parent_T'(x)
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for each $v \in V(T_1)$:

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        for each edge $\{w, x\}$:

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costs total $O(n)$

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for each $v \in V(T_1)$:

    for each child w of v:

        $x \leftarrow$ first ancestor of $lca_{T_2}(w)$ with $v \prec lca_{T_1}(x)$

        while $lca_{T_2}(w) \preccurlyeq x \prec lca_{T_2}(v)$

            add $\{v, w\}$ to $G(T_1, T_2)$

            $x \leftarrow x.parent$

Experiments

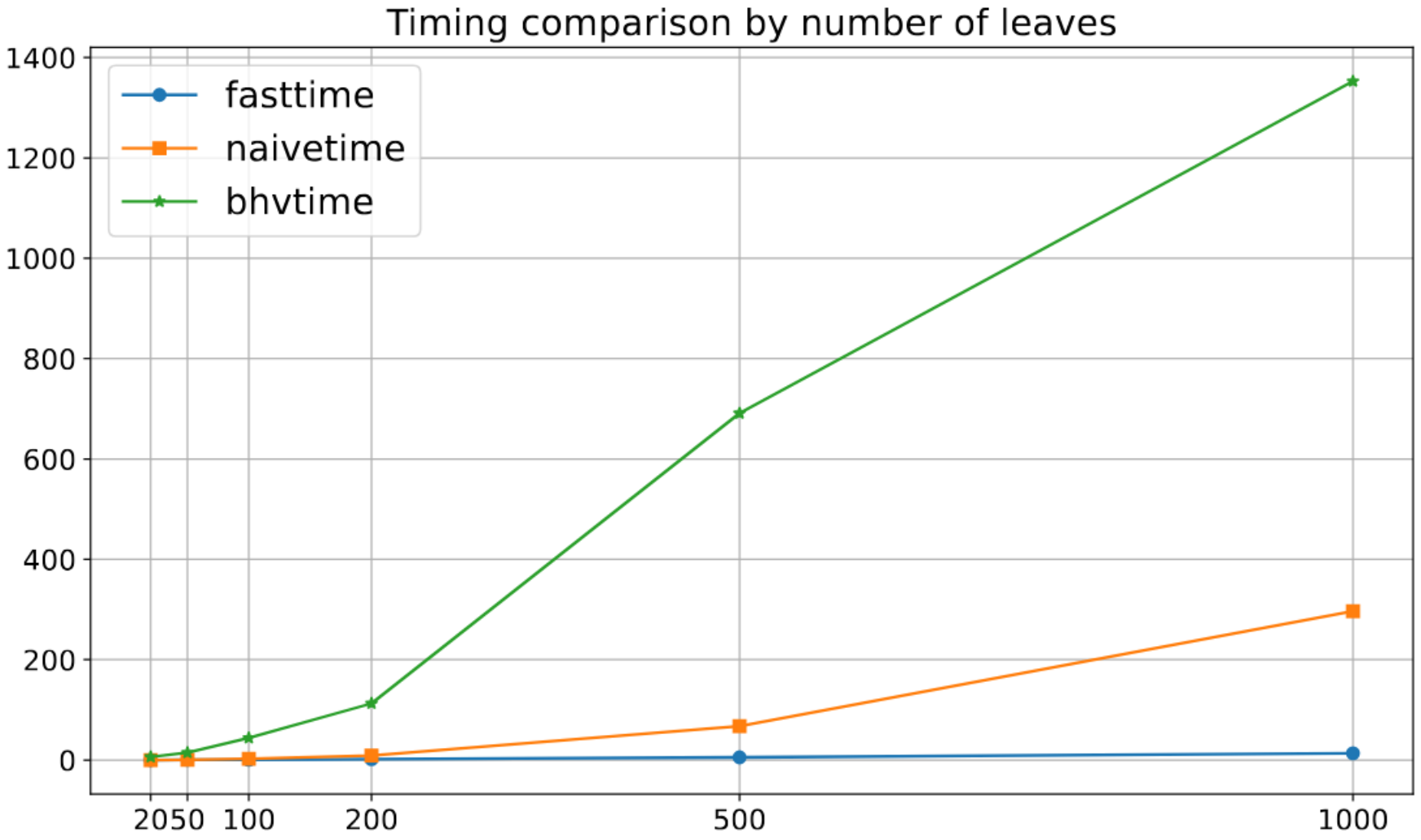
Two datasets

- Random trees (each chosen uniformly at random)
- SimPhy trees
  - Gene trees simulated with various levels of Incomplete Lineage Sorting (ILS)
  - More ILS = More dissimilar trees
- $n \in \{20, 50, 100, 200, 500, 1000\}$

Three implementations

- Naive: the $O(n^3/w)$ algorithm (my C++ code)
- BHV: the $O(n^3/w)$ algorithm from the BHV distance (Owen & Provan's Java code)
- Fast: the $O(n + d)$ algorithm

Running time on random trees



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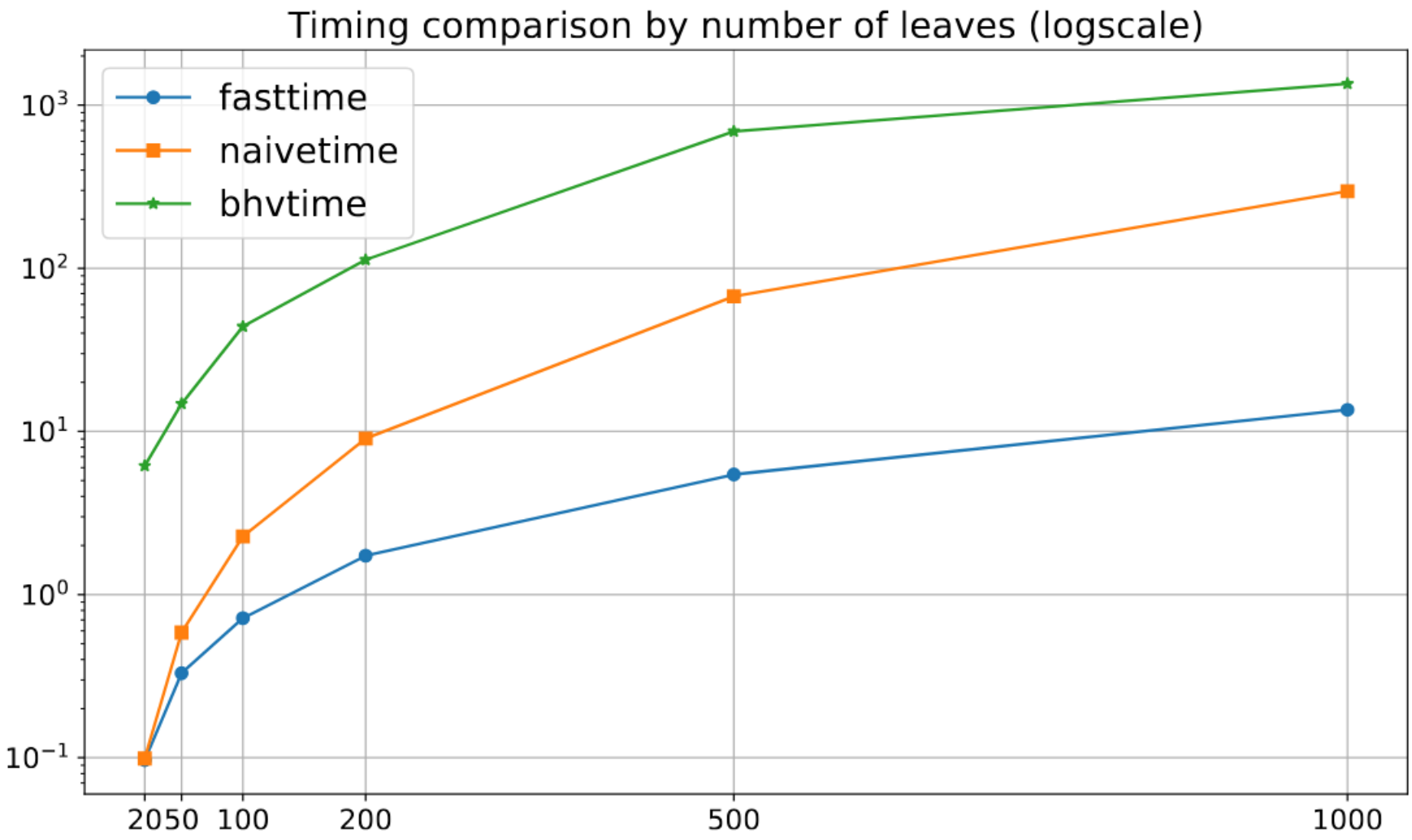
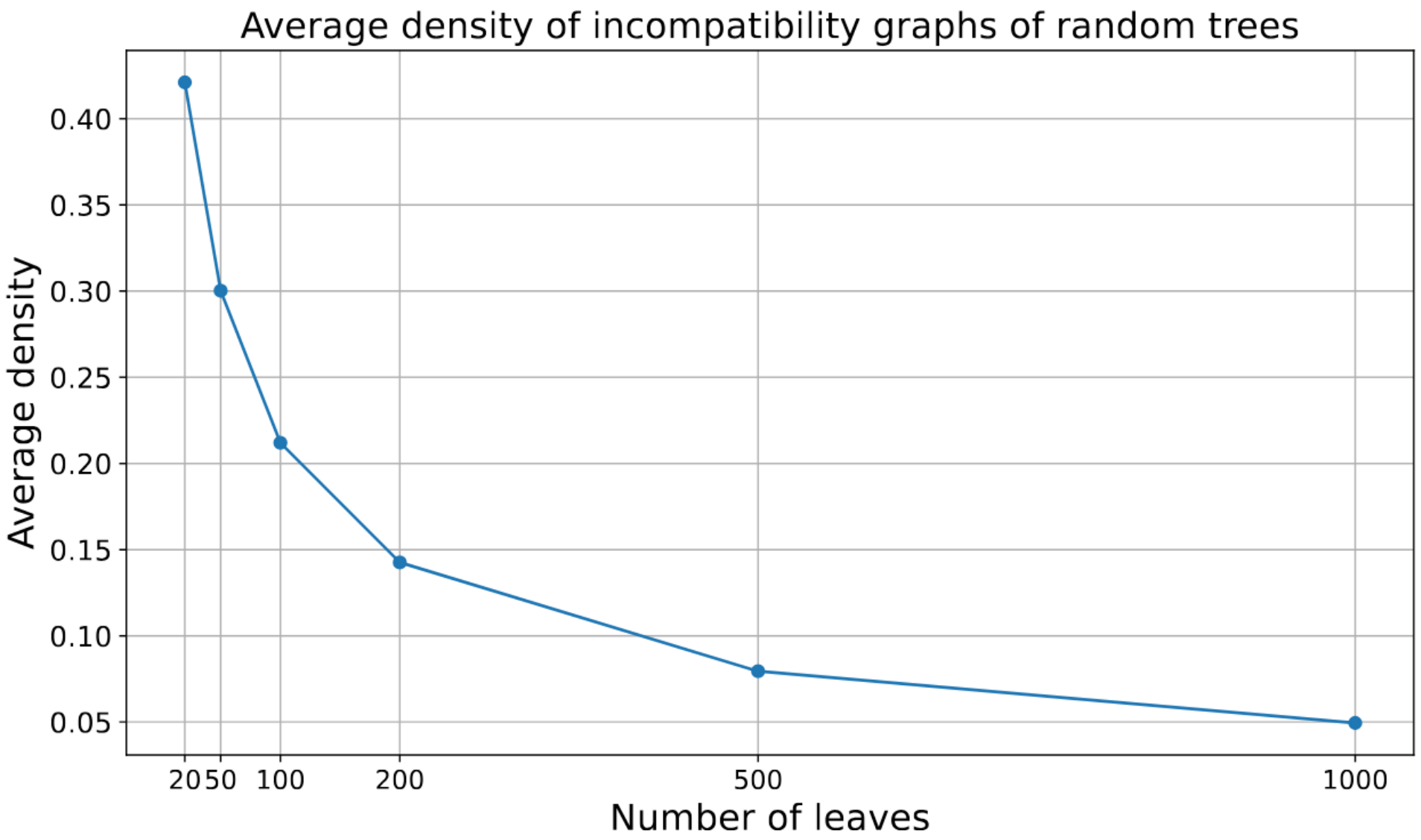


Density on random trees $\frac{|E(G(T_1,T_2))|}{|V(T_1)||V(T_2)|}$



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Density goes down as n grows.

$d = |E(G(T_1, T_2))|$ is closer to n on large trees.

Large trees are those that need fast algorithms!

- Good to have "close" to linear.

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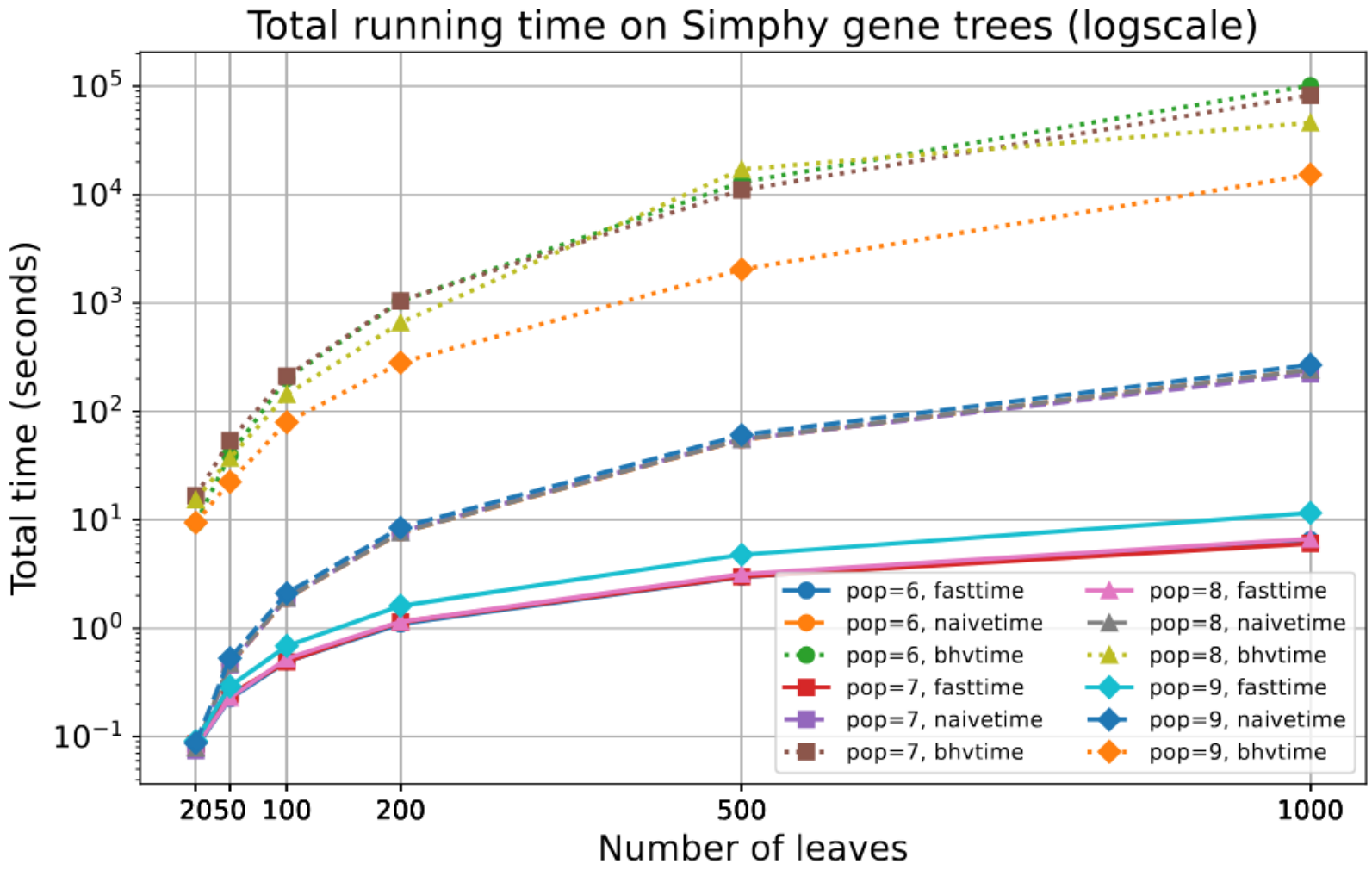
Why does density go down?

- Large trees have lots of tiny clusters, which are compatible with almost everything.

Running time on SimPhy trees



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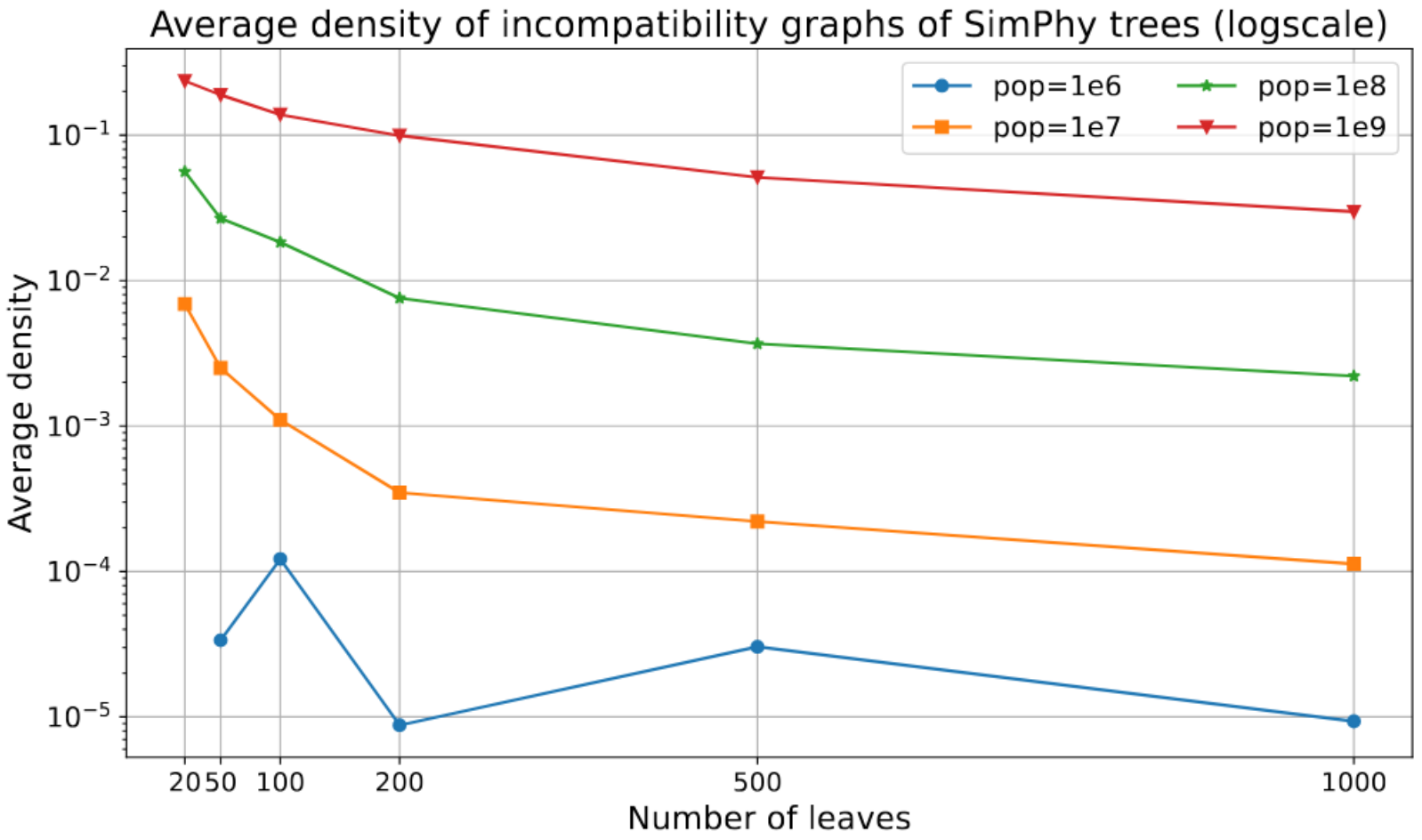

Density on SimPhy trees $\frac{|E(G(T_1,T_2))|}{|V(T_1)||V(T_2)|}$

Density goes down, but also depends on rate of ILS.

More ILS = Denser incompatibility graphs.

Because more ILS = more differences.

Future work

1. Complexity of computing $G(T_1, T_2, \ldots, T_k)$?
   - Conjecture: $O(k^2 n + d)$ is optimal.
2. Using $|E\big(G(T_1, T_2)\big)|$ as a dissimilarity measure.
   - Are there nice metric properties? Triangle inequality?
   - Diameter with respect to tree shape
3. Better understand $G(T_1, T_2)$ on random trees.
   - Expected number of edges?