Tree isomorphism

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Motivation

In some applications the chemical structures are often trees with millions of vertices:

- gene splicing,
- protein analysis,
- molecular biology.

Difference between $O(n)$, $O(n \log n)$, and $O(n^2)$ isomorphism algorithms is not just theoretical importance.

Graph isomorphism

Definition

Isomorphism of graphs $G_1(V_1, E_1)$ and $G_2(V_2, E_2)$ is a bijection between the vertex sets $\varphi : V_1 \to V_2$ such that

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- It is still an open question (!) whether graph isomorphism is $\mathcal{NP}$ complete.
- Polynomial time isomorphism algorithms for various graph subclasses such as trees are known.

Rooted trees

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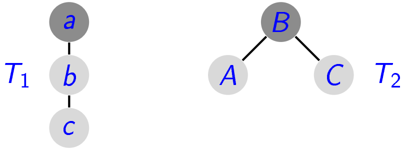
Example

T_1 and T_2 are isomorphic as *graphs* . . .



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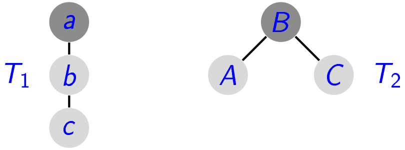
Example

T_1 and T_2 are isomorphic as *graphs* but not as *rooted trees*!



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       return $\mathcal{A}(T_1, c_1, T_2, c_2)$

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   2. each tree has exactly two centers (c_1, c_1' and c_2, c_2' respectively)
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    3. trees has different count of centers
       return False

□

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Algorithm

1: *Choose a random root* r.
2: *Find a vertex* v_1 *— the farthest form* r.
3: *Find a vertex* v_2 *— the farthest form* v_1.
4: *Diameter is a length of path from* v_1 *to* v_2.
5: *Center is a median element(s) of path from* v_1 *to* v_2.

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It is $O(n)$ algorithm.

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So if we find complete isomorphism invariant we can obtain algorithm from it.

Note
Starting from the next slide *tree* means *rooted tree*!

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Observation

The level number of a vertex is a tree isomorphism invariant.

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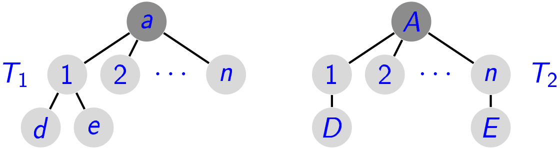

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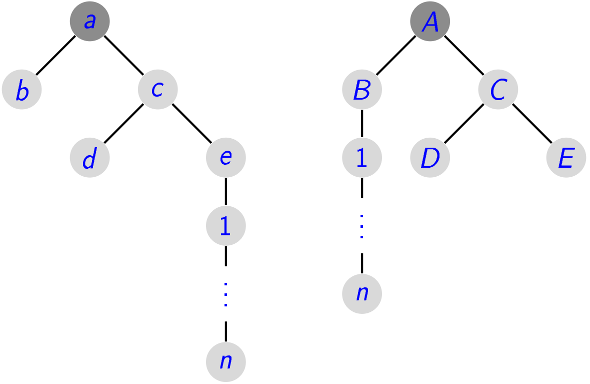

T_2

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If two trees have the same degree spectrum at each level, then they must automatically have the same numbers of levels, the same numbers of vertices at each level, and the same global degree spectrum!

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Observation

The number of leaf descendants of a vertex and the level number of a vertex are both tree isomorphism invariants.

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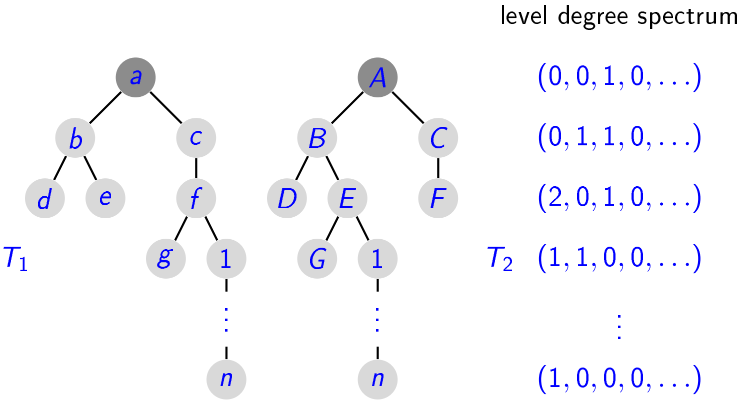

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Algorithm by Aho, Hopcroft and Ullman

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Let's discuss AHU algorithm. We start from $O(|V|^2)$ version and then I tell how to make it faster ($O(|V|)$).

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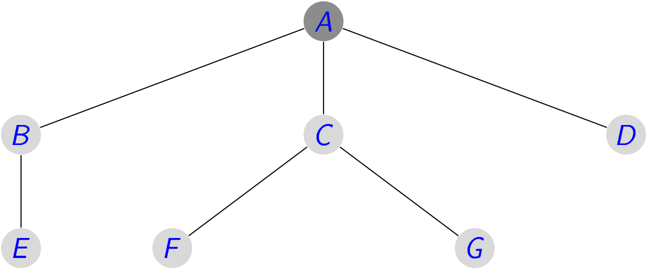

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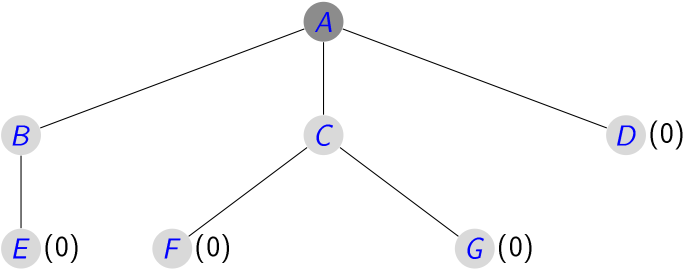

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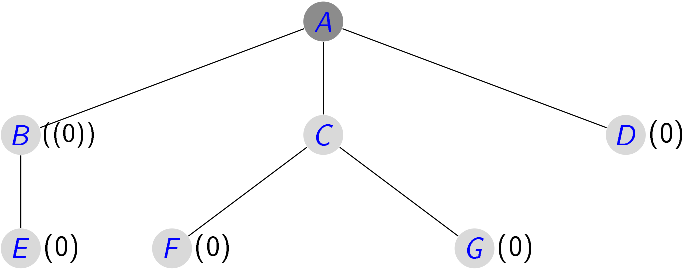

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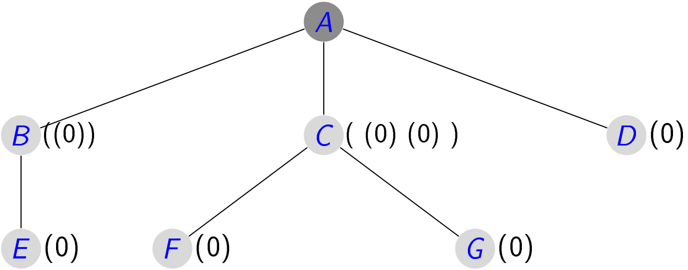

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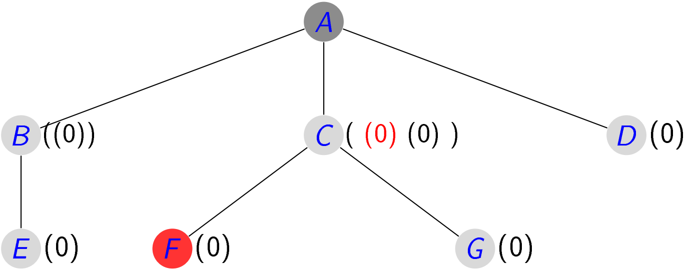

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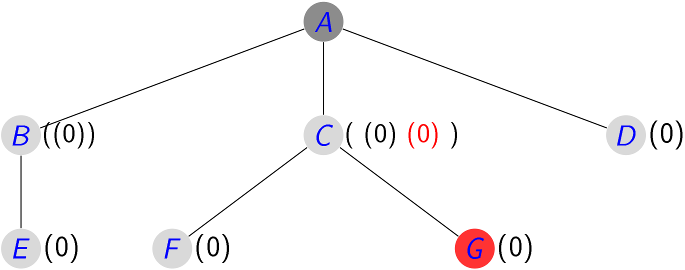

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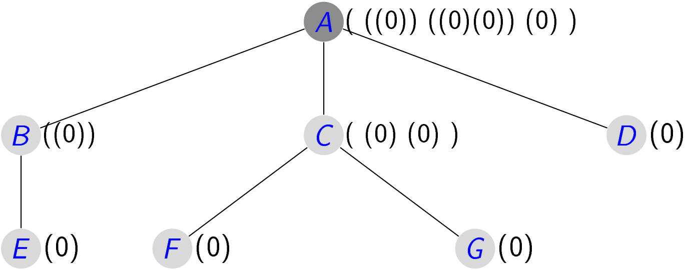

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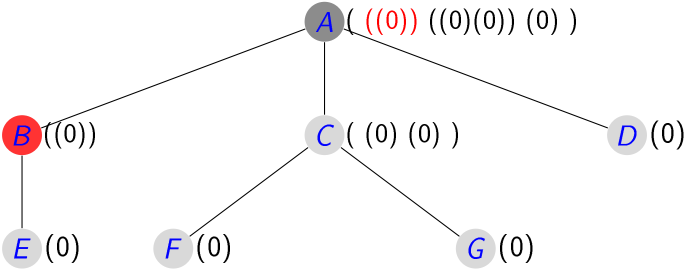

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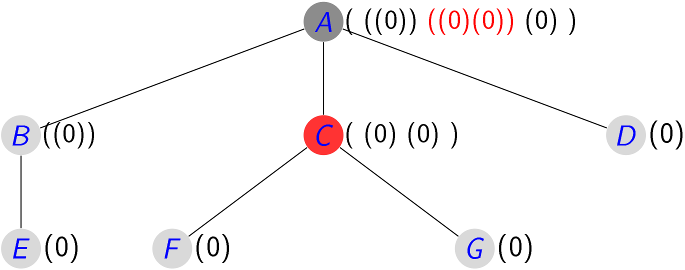

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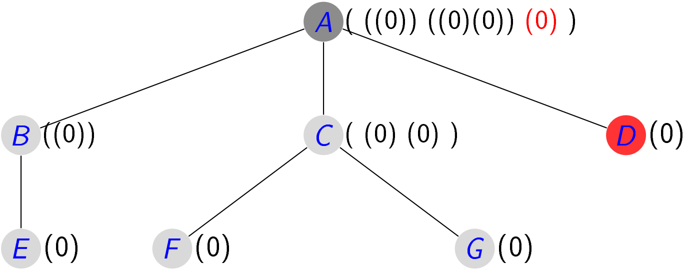

Understanding AHU algorithm (part 2)

There is algorithm Assign-Knuth-Tuples(v) that visits every vertex once or twice.

Assign-Knuth-Tuples(v)

```
if v is a leaf then
    Give v the tuple name (0)
else
    for all child w of v do
        Assign-Knuth-Tuples(w)
    end for
end if
Concatenate the names of all children of v to temp
Give v the tuple name temp
```

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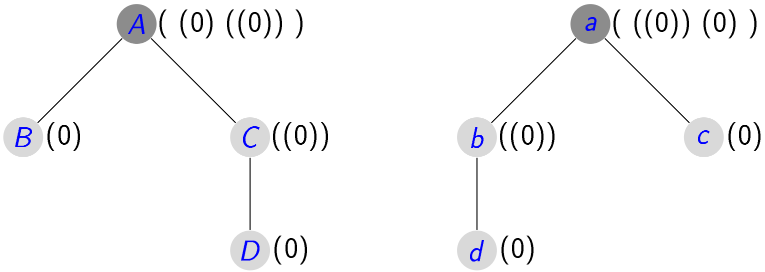

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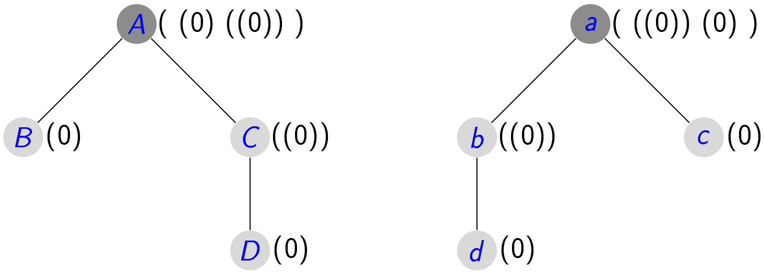

Let's convert parenthetical tuples to *canonical names*. We should drop all "0"-s and replace "(" and ")" with "1" and "0" respectively.

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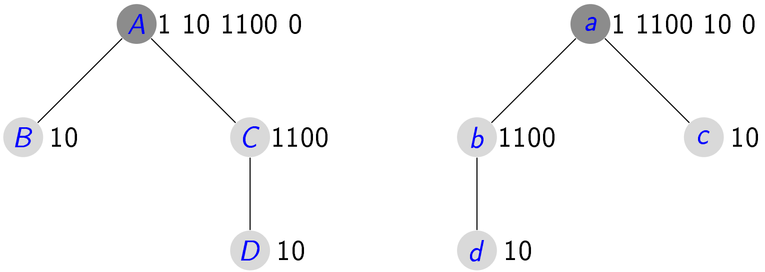

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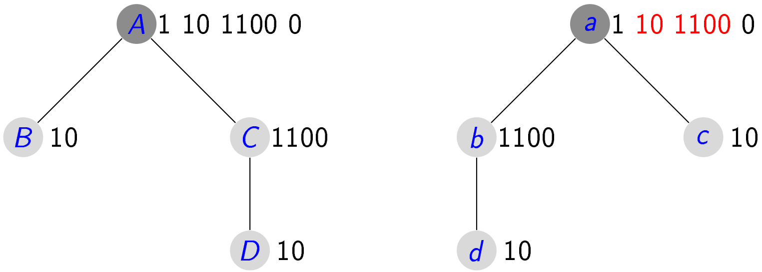

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Understanding AHU algorithm (part 4)

ASSIGN-CANONICAL-NAMES(*v*)

```
if v is a leaf then
    Give v the tuple name "10"
else
    for all child w of v do
        ASSIGN-CANONICAL-NAMES(v)
    end for
end if
Sort the names of the children of v
Concatenate the names of all children of v to temp
Give v the name 1temp0
```

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AHU-TREE-ISOMORPHISM($T_1(V_1, E_1, r_1),\ T_2(V_2, E_2, r_2)$)

```
ASSIGN-CANONICAL-NAMES(r1)
ASSIGN-CANONICAL-NAMES(r2)
if name(r1) = name(r2) then
    return True
else
    return False
end if
```

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For all levels i, *the canonical name of level* i *is a tree isomorphism invariant.*

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Two trees T_1 *and* T_2 *are isomorphic if and only if for all levels* i *canonical level names of* T_1 *and* T_2 *are identical.*

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The idea 2

Assign canonical names level and if canonical level names agree than replace canonical names with integers.

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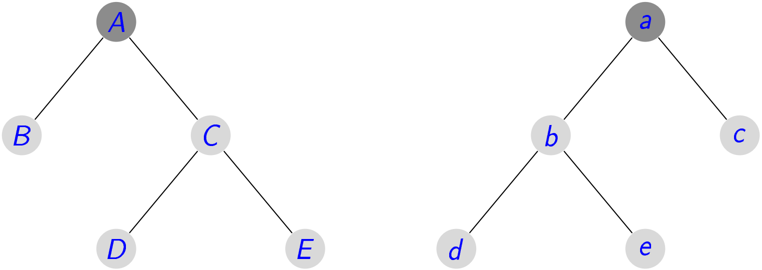
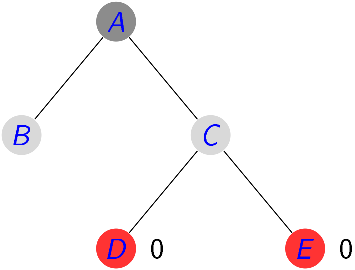


AHU algorithm example

Example



AHU algorithm example

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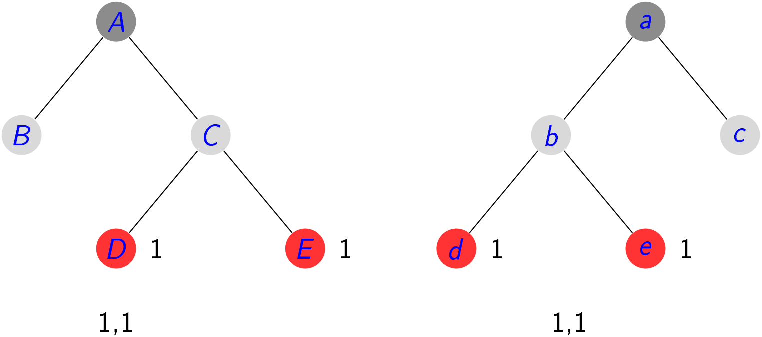

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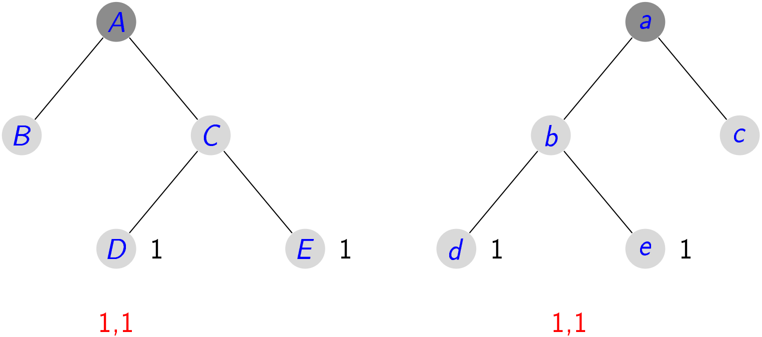

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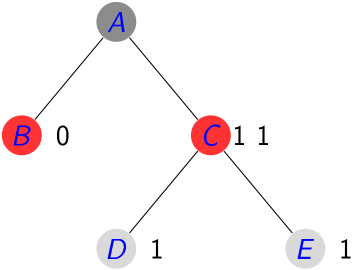

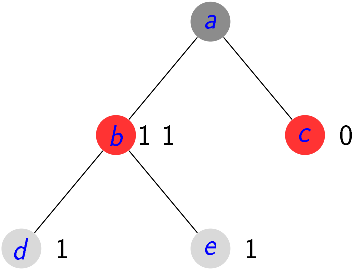

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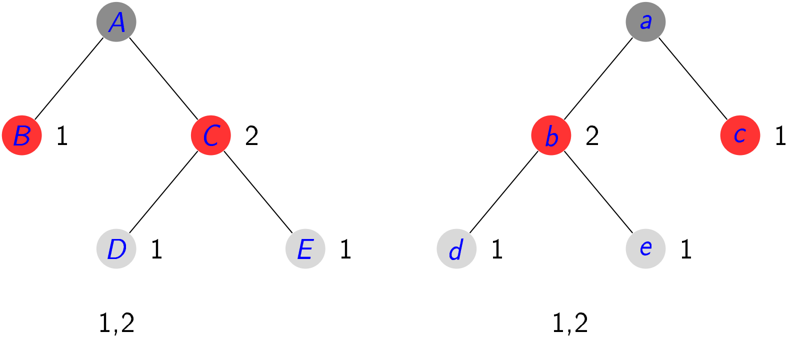

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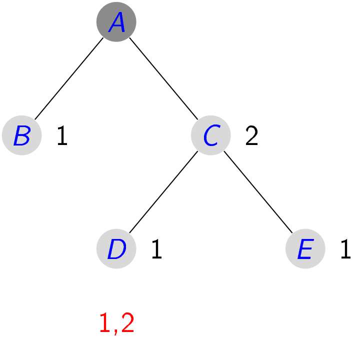

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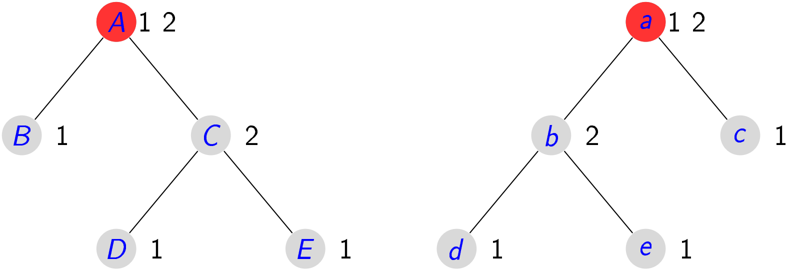

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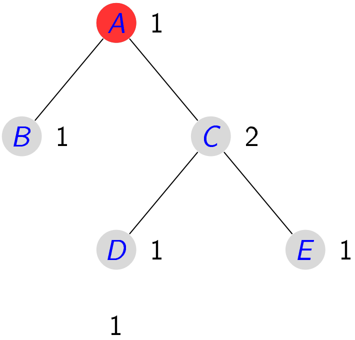

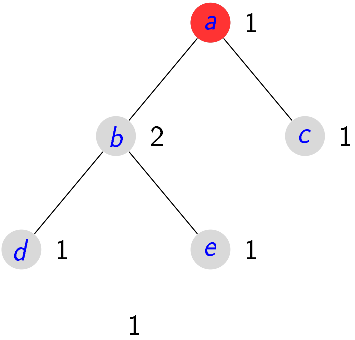

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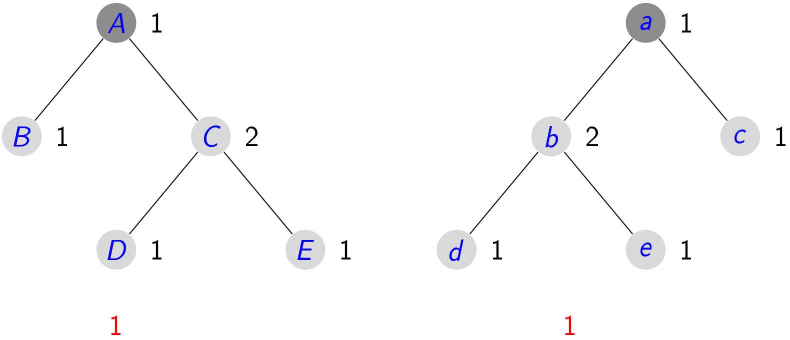

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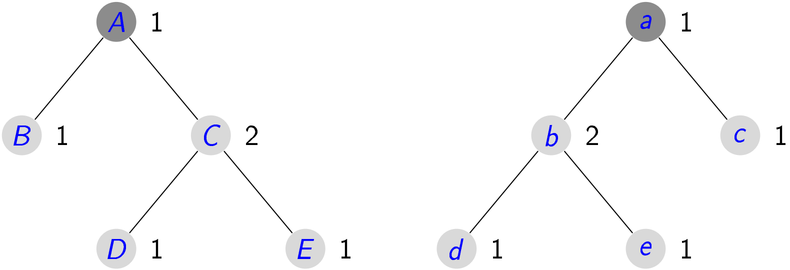

OK

Resume

- We have three unsuccessful tries to construct complete tree isomorphism invariant.
- We discussed $O(|V|^2)$ version of AHU algorithm.
- We discussed ways of improvement of AHU algorithm to make it work in $O(|V|)$ time.

Thank you for your attention!

Any questions?