Tree isomorphism

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Joint Advanced Student School 2008

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

$$\forall u, v \in V_1 \quad (u, v) \in E_1 \Leftrightarrow (\varphi(u), \varphi(v)) \in E_2.$$

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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.

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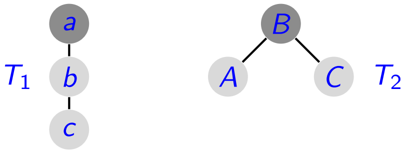
Example

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



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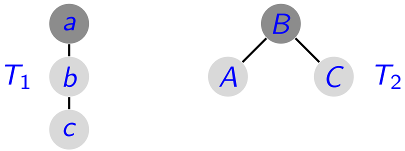
Example

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



Lemma

If there is $O(n)$ algorithm for rooted trees isomorphism, then there is $O(n)$ algorithm for ordinary trees isomorphism.

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

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    3. trees has different number of centers
       return False

□

Diameter and center

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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: *Centers are median elements of path from v_1 to v_2.*

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It is $O(n)$ algorithm.

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

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Observation

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

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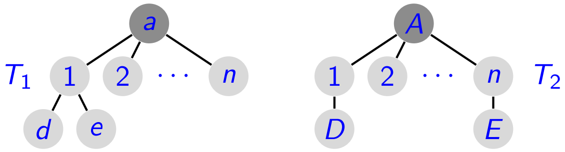

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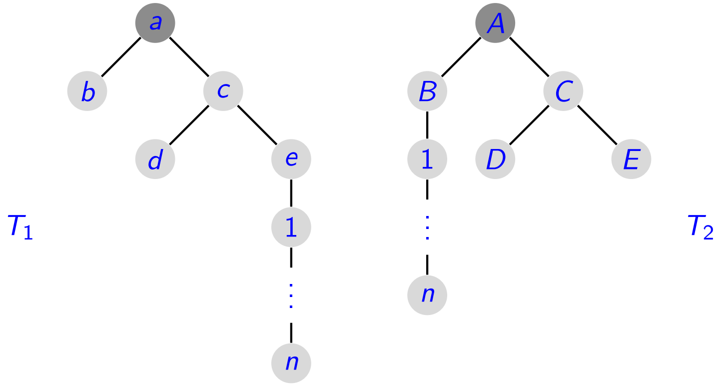

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If two trees have the same degree spectrum at each level, then they must automatically have the same number of levels, the same number of vertices at each level, and the same global degree spectrum!

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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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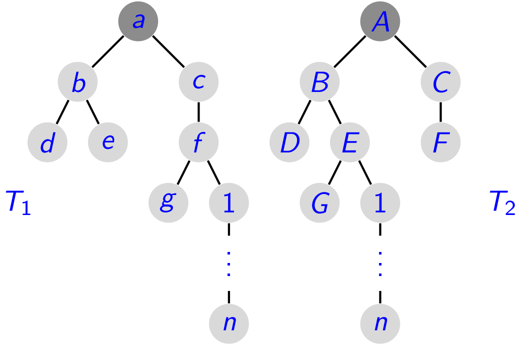

level degree spectrum

$(0, 0, 1, 0, \ldots)$

$(0, 1, 1, 0, \ldots)$

$(2, 0, 1, 0, \ldots)$

$(1, 1, 0, 0, \ldots)$

$\vdots$

$(1, 0, 0, 0, \ldots)$

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Algorithm by Aho, Hopcroft and Ullman

- Determine tree isomorphism in time $O(|V|)$.
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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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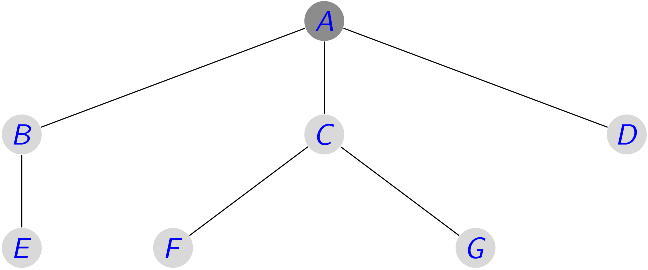

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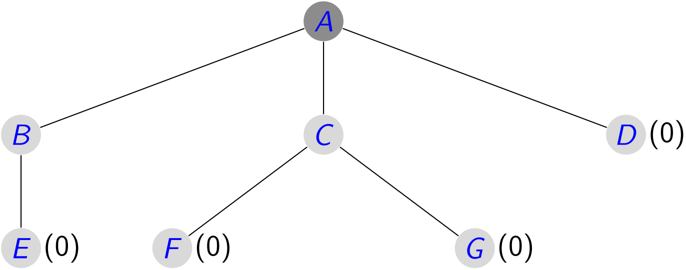

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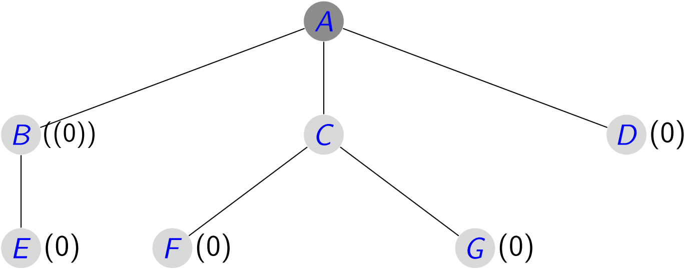

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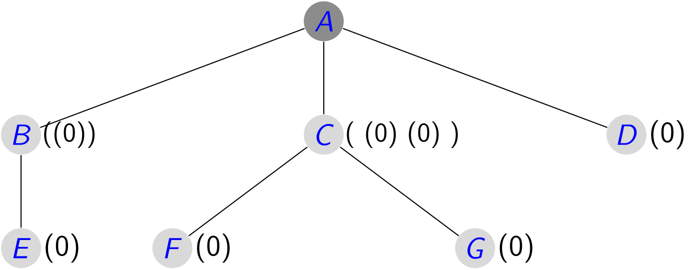

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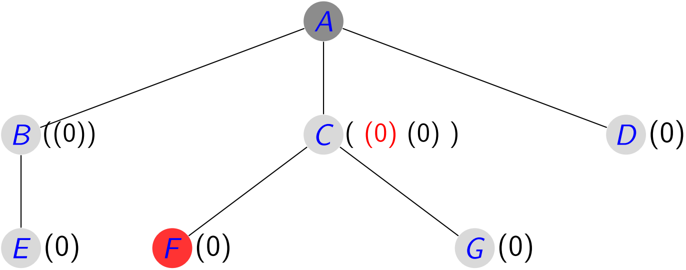

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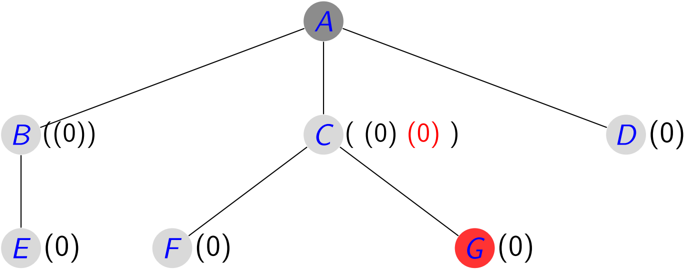

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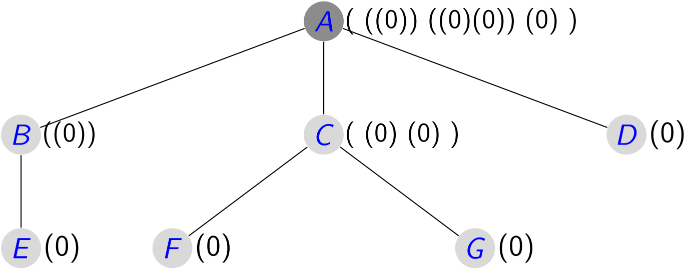

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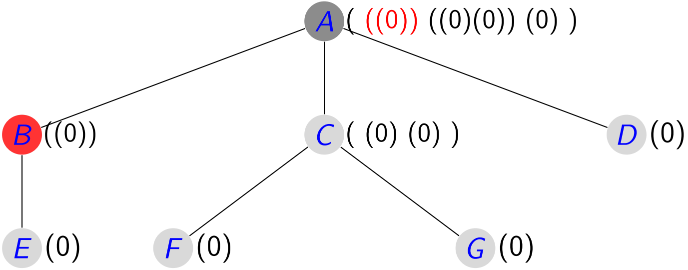

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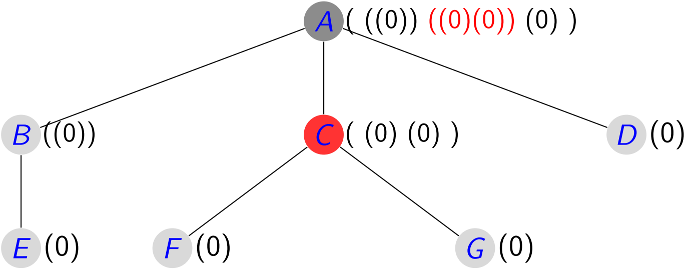

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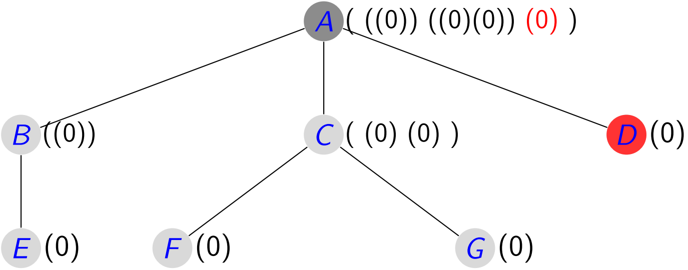

Understanding AHU algorithm (part 2)

There is algorithm ASSIGN-KNUTH-TUPLES 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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There is no order on parenthetical tuples.

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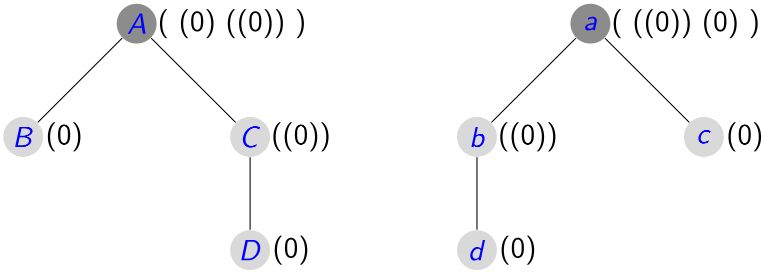

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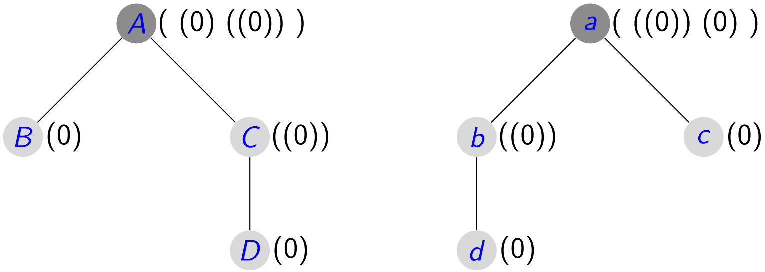

Let's convert parenthetical tuples to *canonical names*. We should drop all "0"-s and replace "(" and ")" with "1" and "0" respectively.

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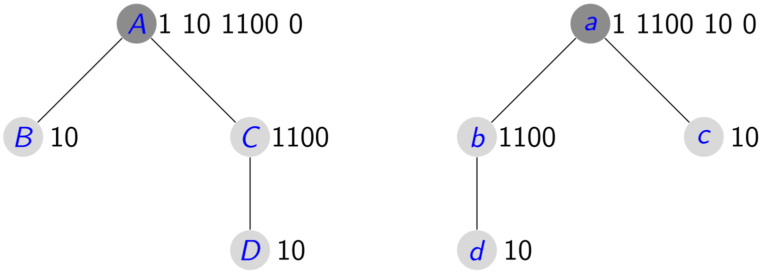

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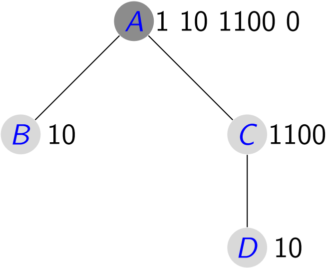

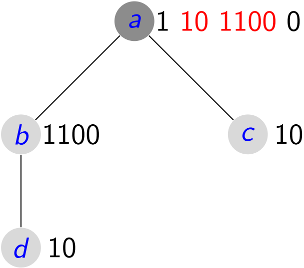

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Understanding AHU algorithm (part 4)

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, T_2)

$r_1 \leftarrow \mathrm{root}(T_1)$
$r_2 \leftarrow \mathrm{root}(T_2)$
ASSIGN-CANONICAL-NAMES(r_1)
ASSIGN-CANONICAL-NAMES(r_2)
if $\mathrm{name}(r_1) = \mathrm{name}(r_2)$ **then**
    return True
else
    return False
end if

AHU algorithm improvement

Observation

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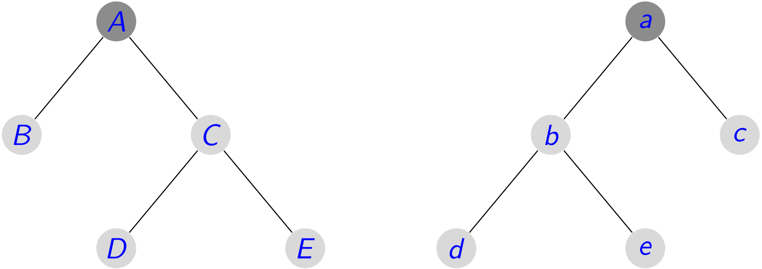
The idea 2

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

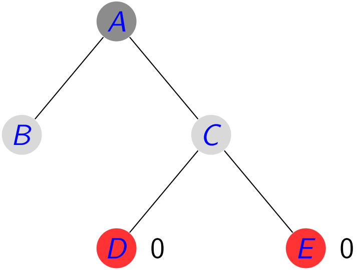
AHU algorithm example

Example



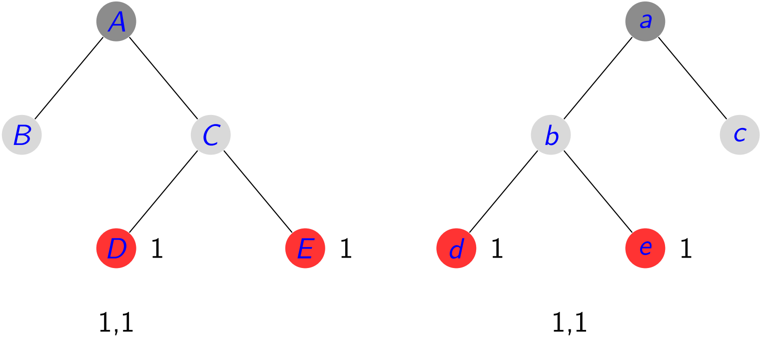
AHU algorithm example

Example



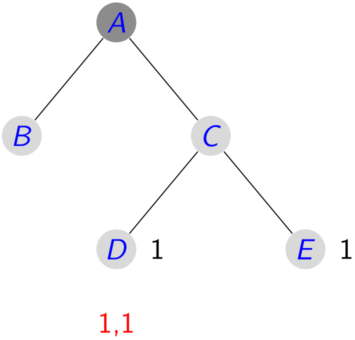
AHU algorithm example

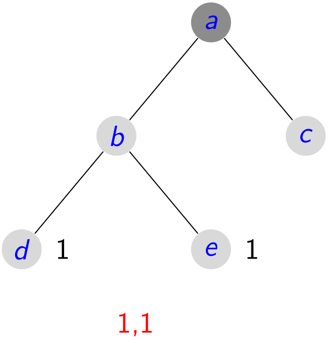
Example



AHU algorithm example

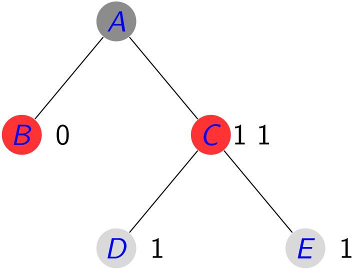
Example





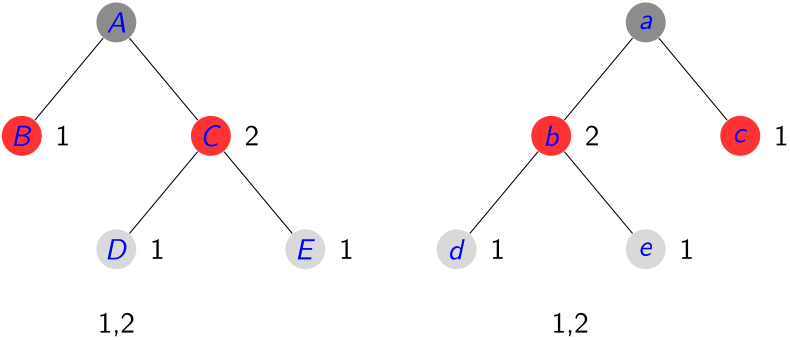
AHU algorithm example

Example



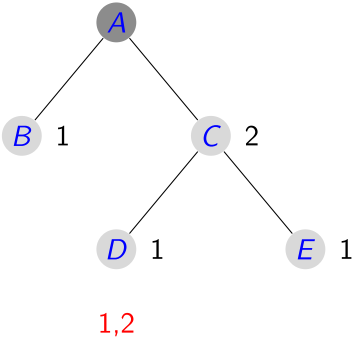
AHU algorithm example

Example



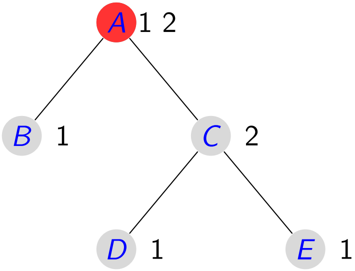
AHU algorithm example

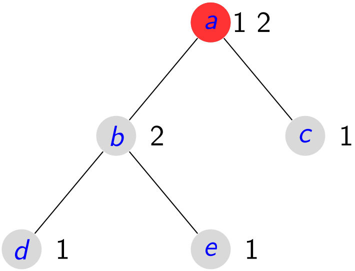
Example



AHU algorithm example

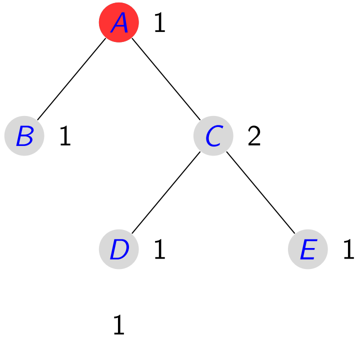
Example

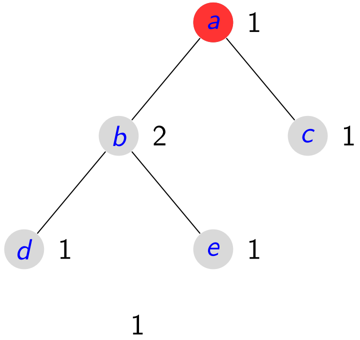




AHU algorithm example

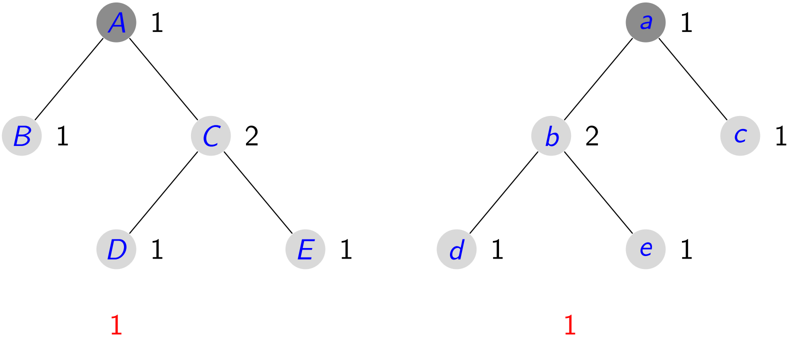
Example





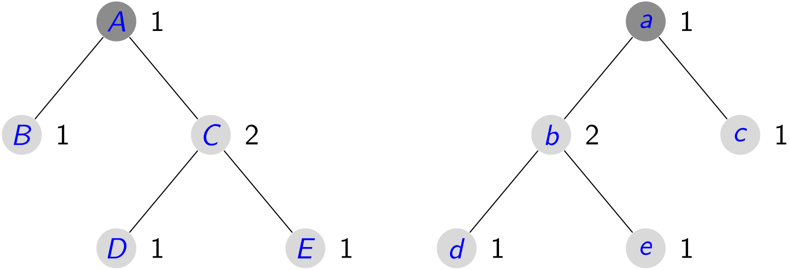
AHU algorithm example

Example



AHU algorithm example

Example



OK

Resume

Resume

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

Thank you for your attention!

Any questions?