Joint Advanced Student School

# Explanation for 'Tree isomorphism' talk

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# Abstract

In this talk we considered a problem of tree isomorphism. We made several attempts to find a complete invariant for rooted trees isomorphism and obtain efficient algorithm from it. In conclusion, we discuss main ideas algorithm from famous Aho, Hopcroft and Ullman book.


# 1 Motivation

In gene splicing, protein analysis, and molecular biology the problem the chemical structures are often trees with millions of vertices. So, the problem of checking whether two structures are equal corresponds to the problem of checking whether two trees are isomorphic. Thus, in such applications difference between $O(n)$, $O(n \log n)$, and $O(n^2)$ isomorphism algorithms is not just theoretical importance.

# 2 The idea

## 2.1 Graph isomorphism

Let's start with a definition of graph isomorphism.

**Definition 1.** ***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*

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

There are several common facts about graph isomorphism.

- No algorithm, other than brute force, is known for testing whether two arbitrary graphs are isomorphic.
- 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.

## 2.2 Rooted trees

We need a quick way to determine whether two ordinary trees are isomorphic. Consider a trick: let's convert trees to rooted trees and try to determine whether they are isomorphic as rooted trees. The idea of this trick is that it should be easier to determine rooted trees isomorphism comparatively to ordinary trees isomorphism because rooted trees give us a little bit more information.

**Definition 2.** ***Rooted tree*** *$(V, E, r)$ is a tree $(V, E)$ with selected root $r \in V$.*

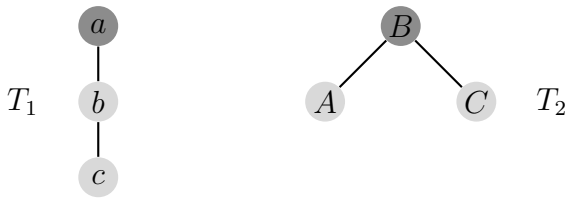
**Definition 3.** ***Isomorphism of rooted trees*** *$T_1(V_1, E_1, r_1)$ and $T_2(V_2, E_2, r_2)$ is a bijection between the vertex sets $\varphi : V_1 \to V_2$ such that*

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

*and $\varphi(r_1) = r_2$.*

Here you can see an example of two rooted trees, that are isomorphic as *graphs* (and as ordinary trees) but **not** as *rooted trees*.

**Example.**




**Lemma 1.** *If there is $O(n)$ algorithm for rooted trees isomorphism there is $O(n)$ algorithm for ordinary trees isomorphism.*

*Proof.* 1. Let $\mathcal{A}$ to be $O(n)$ algorithm for rooted trees.

2. Let $T_1$ and $T_2$ to be ordinary trees.

3. Lets find centers of this trees. There are three possibilities:

   (a) each tree has only one center ($c_1$ and $c_2$ respectively)
   **return** $\mathcal{A}(T_1, c_1, T_2, c_2)$

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

   (c) trees has different count of centers
   **return False**

□

To understand this lemma we should define center of tree and propose a way to find it.

## 2.3 Diameter and center

**Definition 4.** *The **diameter** of tree is the length of the longest path.*

**Definition 5.** *A **center** is a vertex $v$ such that the longest path from $v$ to a leaf is minimal over all vertices in the tree.*

Tree center(s) can be found using simple algorithm.

**Algorithm 1.** (Centers of tree)

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* $v_2$.

This is $O(n)$ algorithm. It is clear that we can't determine tree isomorphism faster than $O(n)$. So, if we find a $O(f(n))$ algorithm for rooted trees isomorphism we can also obtain $O(f(n))$ algorithm for ordinary trees.

## 2.4 The idea

**Definition 6.** ***Isomorphism invariant*** *is a function* $f(T)$ *such that* $f(T_1) = f(T_2)$ *for all pairs of isomorphic trees* $T_1$ *and* $T_2$.

**Definition 7.** ***Complete isomorphism invariant*** *is a function* $f(T)$ *such that two trees* $T_1$ *and* $T_2$ *are isomorphic if and only if* $f(T_1) = f(T_2)$.

**Idea.** If we find complete isomorphism invariant we can obtain algorithm from it.

**WARNING!** Starting from this point *tree* means *rooted tree*!

# 3 Complete invariant candidates

Consider several candidates to be a complete isomorphism invariant.

## 3.1 Candidate 1

**Observation 1.** *The level number of a vertex is a tree isomorphism invariant.*

Using this observation...

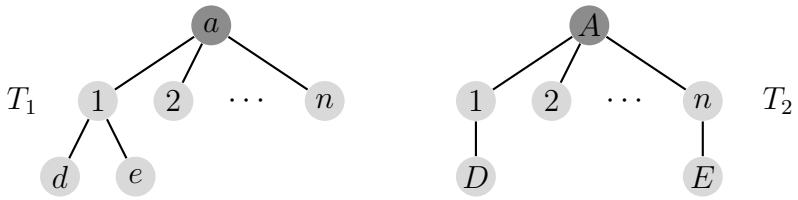
**Conjecture 1.** *Two trees are isomorphic if and only if they have the same number of levels and the same number of vertices on each level.*

Ok. It seems to be a good try. But...

**Observation 2.** *The number of the leaves is a tree isomorphism invariant.*

Using observation 2 we can build a contrary instance.

**Contrary instance.** Here you can see two trees that have the same number of vertices on each level, but different number of leaves (observation 2 is violated). It means, that conjecture 1 is wrong.




Each tree has the same number of vertices on each level:
1 vertex on level 0, $n$ vertices on level 1 and 2 vertices on level 2,
but $T_1$ and $T_2$ have different number of leaves ($n+1$ and $n$ respectively).

## 3.2 Candidate 2

What's wrong with candidate 1? We didn't take into account the *spectrum degree* of a tree.

**Definition 8.** ***Degree spectrum*** *of tree is the sequence of non-negative integers* $\{d_j\}$*, where* $d_j$ *is the number of vertices that have* $j$ *children.*

Let's fix it.

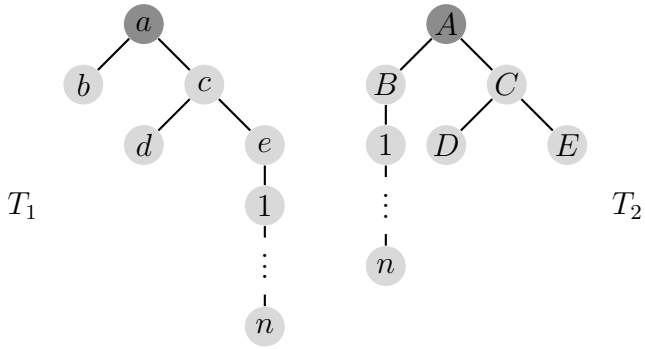
**Conjecture 2.** *Two trees are isomorphic if and only if they have the same degree spectrum.*

It seems to be better than first candidate, but...

**Observation 3.** *Since a tree isomorphism preserves longest paths from the root, the number of levels in a tree is a tree isomorphism invariant.*

Using observation 3 we can build a contrary instance.

**Contrary instance.** This two trees has the same degree spectrum but different number of levels (observation 3 is violated).




Each tree has degree spectrum $(3, n+2, 1, 0, \ldots)$ that means
3 vertices of degree 1, $n+2$ vertices of degree 2 and 1 vertex of degree 3.
But $T_1$ has $n+2$ levels and $T_2$ has only $n+1$ levels.

### 3.3 Candidate 3

What's wrong with candidate 2? We used some integral property for it. Consider an analogy: algorithm for determining whether two integer arrays are equal which just compares their sums. Obviously, it is a wrong algorithm.

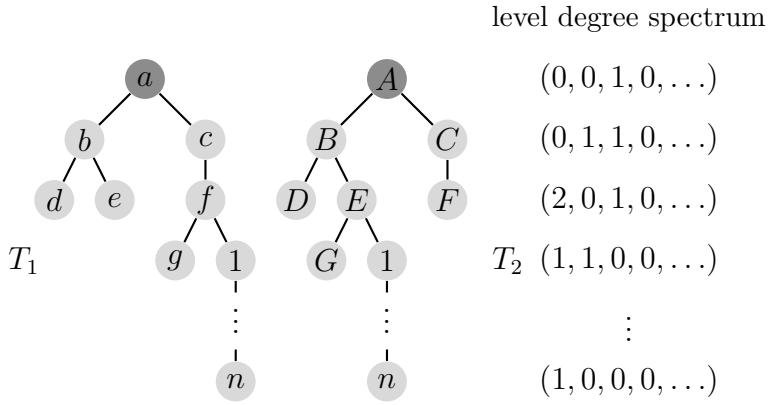
**Conjecture 3.** *Two trees are isomorphic if and only if they have the same degree spectrum at each level.*

This conjecture is very tricky. 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!

**Observation 4.** *The number of leaf descendants of a vertex and the level number of a vertex are both tree isomorphism invariants.*

And again using observation 4 we can build a contrary instance.

**Contrary instance.** You can see two trees below that have the same degree spectrum at each level but on level two in $T_1$ there two vertices, $b$ and $c$, with 2 and $n+2$ descendants respectively and in $T_2$ there are two vertices, $B$ and $C$, with $n+3$ and 1 descendants respectively. So, observation 4 is violated.




# 4 AHU algorithm

We have failed tree times. Let's look for some existing algorithm and understand it.

### 4.1 Algorithm by Aho, Hopcroft and Ullman

This algorithm is from one famous book.

- Determine tree isomorphism in time $O(|V|)$.
- Uses *complete history of degree spectrum of the vertex descendants* as a complete invariant.

**The idea of AHU algorithm.** The AHU algorithm associates with each vertex a tuple that describes the complete history of its descendants.

**Hard question.** Why our previous invariants are not complete?

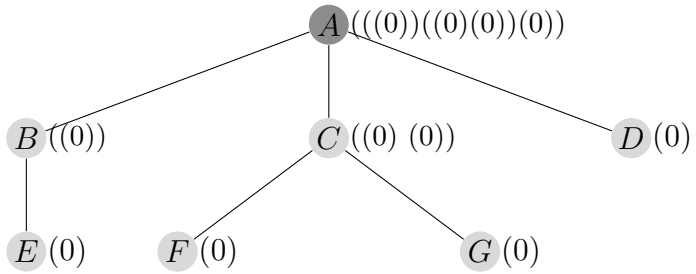
**Answer.** We discussed weakness for first two candidates. The third invariant was better than second but it also uses some integral properties.

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

## 4.2 Understanding AHU algorithms

**Knuth tuples.** Let's assign parenthetical tuples to all tree vertices.

**Knuth tuples example.** I don't want to define it formally. So, I just show an example.




You should have noticed that all leaves has (0) label
and each non-leafs label consist of children labels enclosed in parentheses.

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

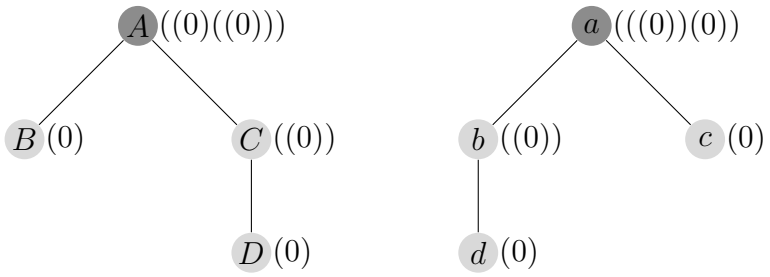
**Algorithm 2.** Assign-Knuth-Tuples($v$)

```
1: if v is a leaf then
2:     Give v the tuple name (0)
3: else
4:     for all child w of v do
5:         Assign-Knuth-Tuples(w)
6:     end for
7: end if
8: Concatenate the names of all children of v to temp
9: Give v the tuple name temp
```

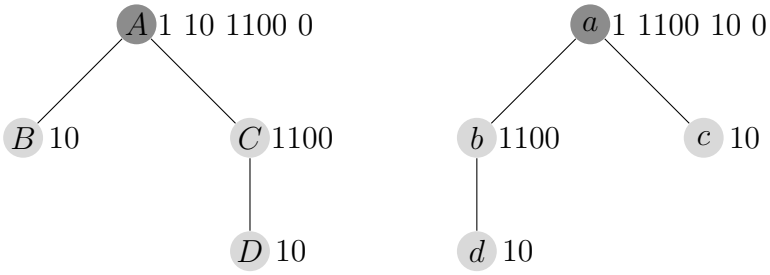
**Observation 5.** *There is no order on parenthetical tuples.*

Why we need an order? Let's look at example.

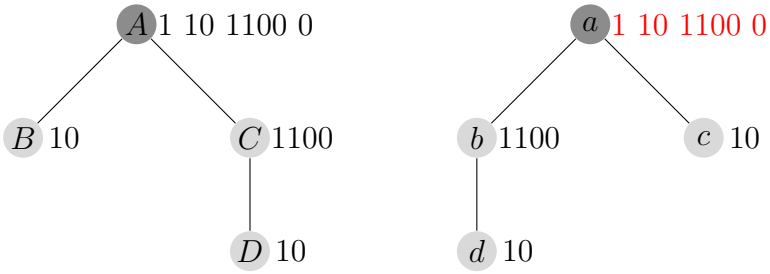
**Example.** There are two isomorphic trees with assigned Knuth tuples.




We know that trees are isomorphic but roots have different assigned tuples. Let's convert parenthetical tuples to *canonical names*. We should drop all "0"-s (zeros are not necessary) and replace "(" and ")" with "1" and "0" respectively.




Canonical name is just a numbers. So, we can sort it. Let's sort canonical names of children for each non-leaf node.




Gotcha! Roots has the same assigned canonical names.

There is an algorithm Assign-Canonical-Names($v$) that visits every vertex once or twice (it is a modification of Assign-Knuth-Tuples).

**Algorithm 3.** Assign-Canonical-Names($v$)

```
1: if v is a leaf then
2:     Give v the tuple name "10"
3: else
4:     for all child w of v do
5:         Assign-Canonical-Names(v)
6:     end for
7: end if
```

*8: Sort the names of the children of $v$*
*9: Concatenate the names of all children of $v$ to temp*
*10: Give $v$ the name* **1***temp***0**

**Conjecture 4.** *Two trees are isomorphic if and only if they have the same canonical name assigned to root.*

We should discuss some important questions.

**Invariant?** Is canonical name of a root is a *tree isomorphism invariant*?

**Answer.** Yes. Obviously, two isomorphic trees has the same label assigned to root.

**Complete invariant?** Is canonical name of a root is a *complete tree isomorphism invariant*?

**Answer.** Yes. We can show it easily by reconstructing tree from root canonical name. So, there is a bijection between tree and roots canonical names.

**Algorithm 4.** AHU-Tree-Isomorphism($T_1(V_1, E_1, r_1)$, $T_2(V_2, E_2, r_2)$)
*1:* Assign-Canonical-Names($r_1$)
*2:* Assign-Canonical-Names($r_2$)
*3:* ***if*** name($r_1$) = name($r_2$) ***then***
*4:* **return True**
*5:* ***else***
*6:* **return False**
*7:* ***end if***

## 4.3 AHU algorithm improvement

**Observation 6.** *To compute the root name of a tree of $n$ vertices in one long strand, takes time proportional to $1 + 2 + \cdots + n$, which is $\Omega(n^2)$.*

This observation shows that AHU-Tree-Isomorphism is $O(|V|^2)$. But there is a way we can improve it to be $O(|V|)$.

**Observation 7.** *For all levels $i$, the canonical name of level $i$ is a tree isomorphism invariant.*

**Observation 8.** *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.*

Using this two observations...

**The idea 1.** Assign canonical names level, sort by level, and check by level that the canonical level names agree.

**The idea 2.** Assign canonical names level and if canonical level names agree than replace canonical names with integers.

This ideas shows us how improve AHU-Tree-Isomorphism it to be $O(|V|)$. Using unique integers on each level instead of strings we can get rid of effect we discover in observation 6. On slides you can see animated example of AHU-Tree-Isomorphism algorithm work.

**But...** There is a hole in our discussion — we have forgot about sorting in Assign-Canonical-Names. So, in this case AHU-Tree-Isomorphism just $O(n \log n)$... But there is a way to sort canonical names in linear time — you can read about it in AHU's book.

# 5 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.