Lecture 3: Trees and Isomorphism

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**Based on the slides of ADS-21/22 by Dr. George Mertzios*

Reminder from last lecture

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- Hamiltonian cycle (after William Hamilton (1805-65): if we can travel along the edges of a given graph so that we start and finish at the same vertex and visit each vertex exactly once.
- Usually no ‘easy’/‘efficient’ way to know if a graph of general topology has a Hamiltonian cycle besides enumerating cycles one by one.

Contents for today's lecture

- Trees and their properties;
- Applications of trees;
- Exercises involving trees;
- Isomorphism
- Examples of proof techniques;
- Properties of rooted trees.

Trees

We now turn to a special graph class that has many applications in many areas.

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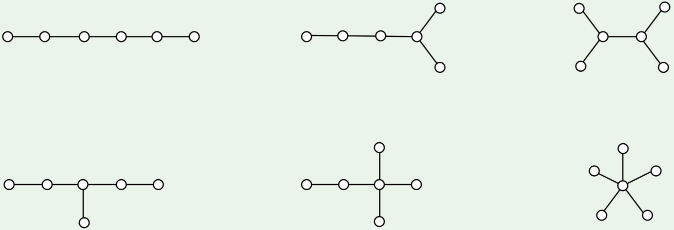
Examples

The different trees on 6 vertices are shown below.



We can also consider this as a forest on 36 vertices.

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Finding minimum-weight spanning trees in edge-weighted graphs is an important task in practice: we will learn fast algorithms for it in a few lectures.

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Can a tree have exactly one leaf?

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- Consider a longest path P and an end vertex v of P.
- All neighbours of v are on P. (why?)
- If $\deg(v) \geq 2$, then there is a cycle.
- The same also holds for the other end vertex u of P

$\Rightarrow \deg(u) = \deg(v) = 1$

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- Take a tree T on n vertices, for some $n \geq 3$.
- T contains a leaf v. Consider the graph $T-v$, it has one vertex less and one edge less than T.
- $T-v$ is still connected and (still) acyclic.
- $T-v$ is a tree with $n-1$ vertices, by induction hypothesis it has $n-2$ edges.
- T has one edge more, so $n-1$ edges.

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- T is a subgraph of G, and it has the same number of edges as G.
- Hence, T and G are the same.
- In particular, G is a tree.

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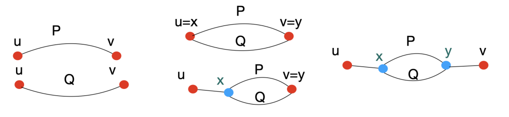

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- Then the segments of P and Q between x and y together form a cycle.
- This contradicts that T is a tree. Hence there is a unique (u, v)-path in T.

$\square$

Exercises

We have shown that, for a graph G on n vertices, the following conditions are equivalent:

1. G is tree;
2. G is connected and has $n-1$ edges.

Exercise 2: Show that these conditions are also equivalent to each of the following:

3. G is acyclic and has $n-1$ edges;
4. any two distinct vertices of G are connected by a unique path;
5. for any distinct $u, v \in V$, if $uv \notin E(G)$ then the graph $G + uv$ contains a unique cycle.

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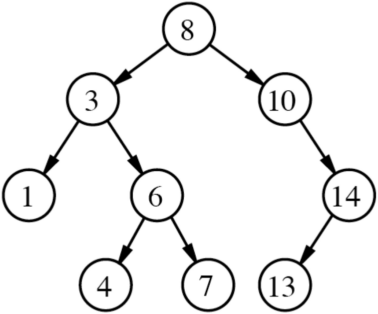
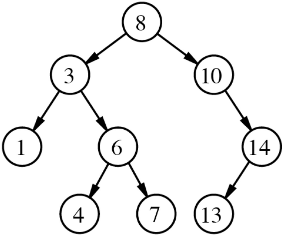


Rooted trees, children and parents



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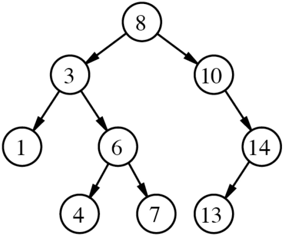

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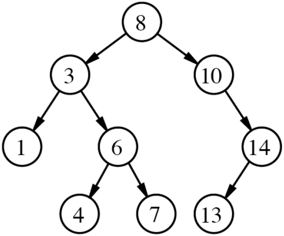

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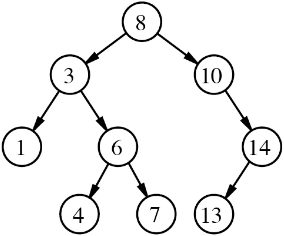

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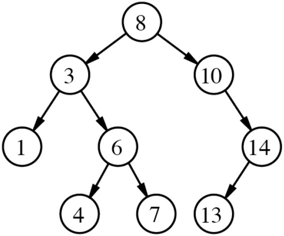

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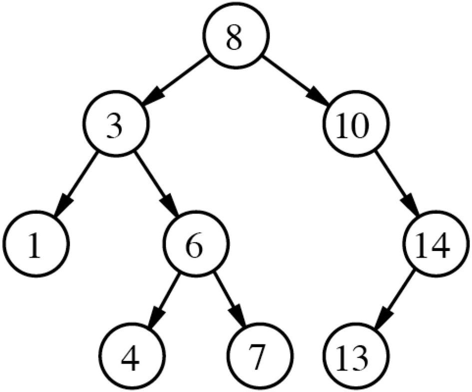
Some applications of trees

- Binary search trees (we have seen these earlier in ADS)



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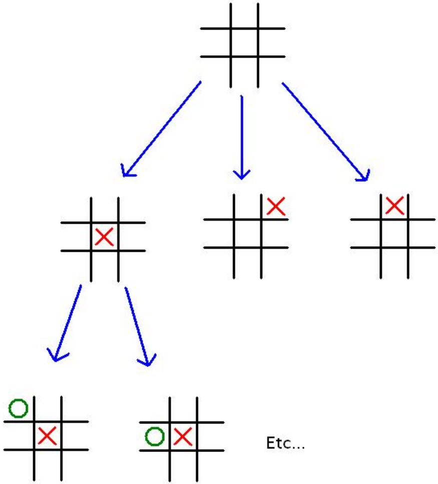

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- Phylogenetic trees (Bioinformatics)

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- Then $T' = T - u$ is a tree on $n - 1$ vertices. By the induction hypothesis, we have $\ell(T') \geq n_3(T') + 2$.

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What is the minimum number of leaves in a tree on at least 2 vertices?

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A tree with at least 2 vertices, n_3 of which have degree at least 3, has at least $n_3 + 2$ leaves.

Proof: Let T be a tree on $n \geq 2$ vertices. We use induction on n.

- Let $\ell(T)$ denote the number of leaves in T, and $n_3(T)$ denote the number of vertices of degree at least 3 in T.
- Induction Base : If $n = 2$, then $n_3 = 0$ and T has 2 leaves.
- Step: Now suppose that every tree on $< n$ vertices has at least $n_3 + 2$ leaves (induction hypothesis), and consider a tree T on $n \geq 3$ vertices.
- Since T is a tree on at least 3 vertices, T has a leaf u.
- Then $T' = T - u$ is a tree on $n - 1$ vertices. By the induction hypothesis, we have $\ell(T') \geq n_3(T') + 2$.
- The rest of the proof is on the next slide.

Proof continued

- We have: a leaf u in T, a tree $T' = T - u$, $\ell(T') \geq n_3(T') + 2$.
- Let v be the (unique) neighbour of u in T.
- T is connected and has at least 3 vertices, so v has at least 2 neighbors in T.

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This finishes the proof.

Note that induction on n_3 is also possible.

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- Choose any vertex v and put this vertex in the set V_1.
- For every vertex $u \neq v$, there is a unique path from v to u in T, consider the length of this path.
- If the length is odd, put u in V_2; otherwise put u in V_1.

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- If the length is odd, put u in V_2; otherwise put u in V_1.
- We have to show that this is a valid bipartition.
- V_1 and V_2 are disjoint and together make up $V(T)$. (Why?)
- Every edge has end vertices in both V_1 and V_2. (Why?)
- This completes the proof.

$\square$

Graph isomorphism

Definition

Two graphs $G = (V, E)$ and $G' = (V', E')$ are isomorphic if there exists a bijective function $f : V \to V'$ such that for every $u, v \in V$ we have: $uv \in E$ if and only if $f(u)f(v) \in E'$. Then we write: $G \cong G'$.

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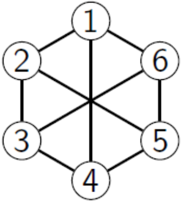

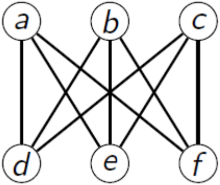

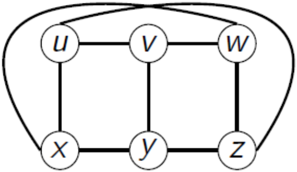

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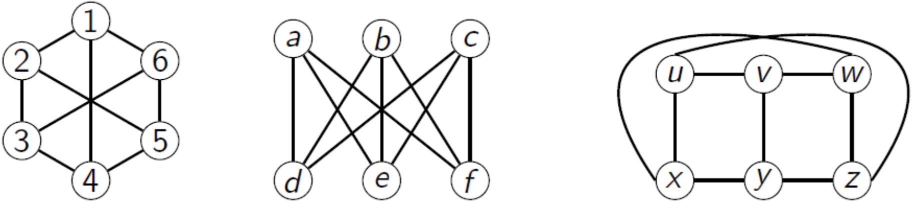

bijective function f for the first and second graph:
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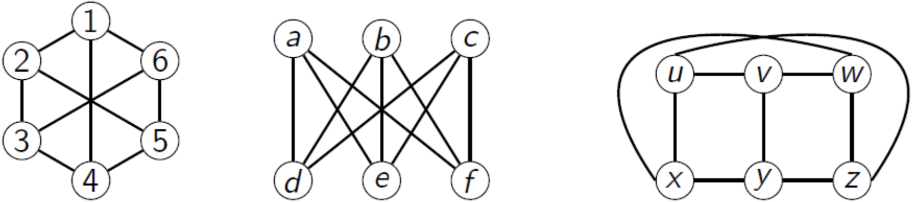

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bijective function f for the second and third graph:
$a \mapsto x,\ b \mapsto v,\ c \mapsto z,\ d \mapsto u,\ e \mapsto w,\ f \mapsto y$

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Can we quickly decide whether G and G' are isomorphic?

- one of the few most tantalising and tricky questions in Computer Science
- presumably not an "easy" problem (i.e. polynomial-time) and not a "hard" problem (i.e. NP-complete), but "somewhere in the middle"

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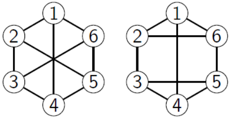

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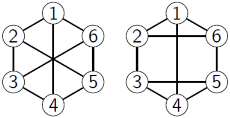

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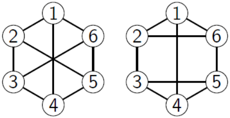

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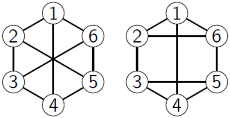

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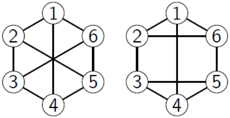

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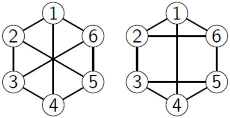

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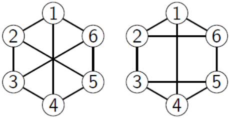

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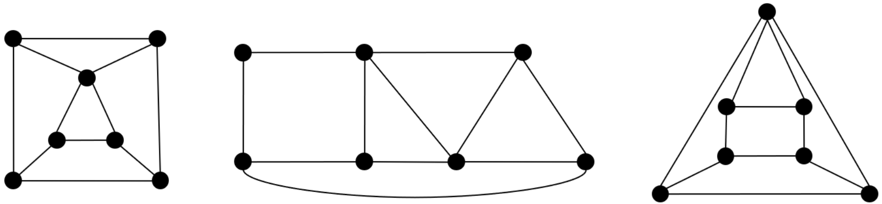
All these (and all other characteristics):

- can only be used to show non-isomorphism

Graph isomorphism

What about these graphs?



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Definition (Isomorphism of rooted trees)

Two rooted trees $T_1(V_1, E_1, r_1)$ and $T_2(V_2, E_2, r_2)$ are called isomorphic if there exists an isomorphism bijection $f : V_1 \mapsto V_2$ such that $f(r_1) = r_2$.

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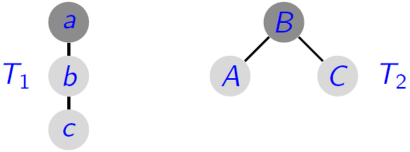
Example: T_1 and T_2 are isomorphic as graphs, but not as rooted trees !



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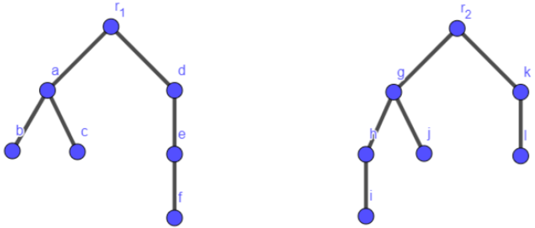

Graph isomorphism on rooted trees

An isomorphism algorithm for rooted trees (Algorithm 2):

Algorithm 1 LabelVertex(T, v)

```
if v is a leaf of T then
    label(v) ← "10"
else
    for every child w of v do
        ℓ(w) ← LabelVertex(T, w)
    Sort the labels of the children of v decreasingly: ℓ(w_1) ≥ ℓ(w_2) ≥ ... ≥ ℓ(w_k)
    label(v) ← "1" ℓ(w_1) ℓ(w_2) ... ℓ(w_k) "0"
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Algorithm 2 Labeled Tree Isomorphism$((T_1, r_1), (T_2, r_2))$

$label(r_1) \leftarrow$ LabelVertex(T_1, r_1)
$label(r_2) \leftarrow$ LabelVertex(T_2, r_2)
if $label(r_1) = label(r_2)$ **then**
    return YES
else
    return NO

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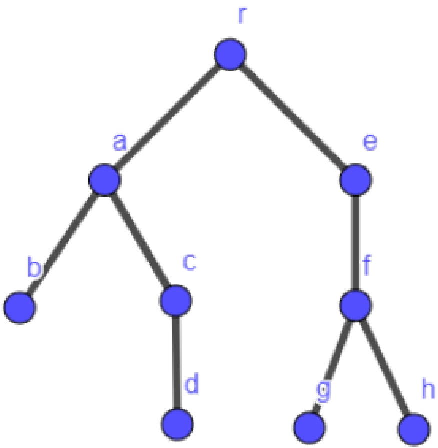

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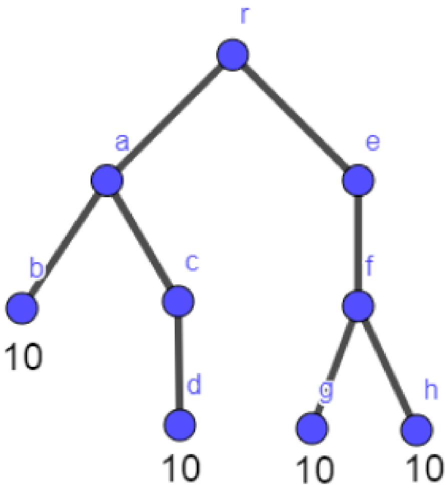

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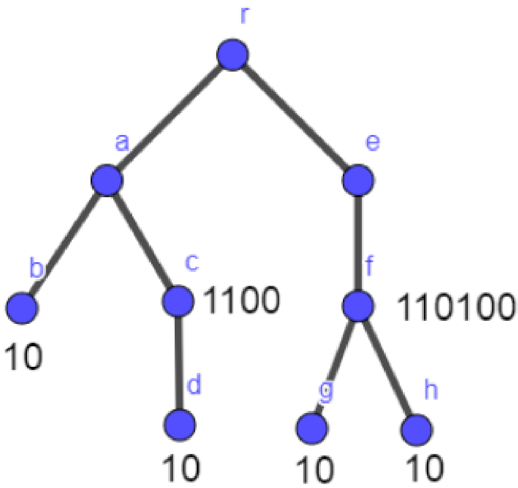

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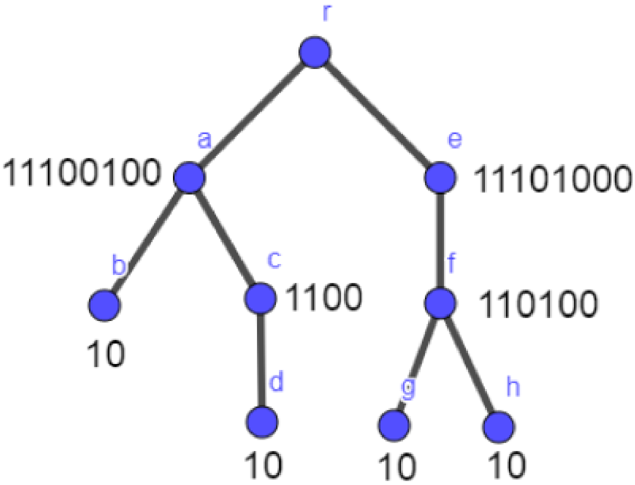

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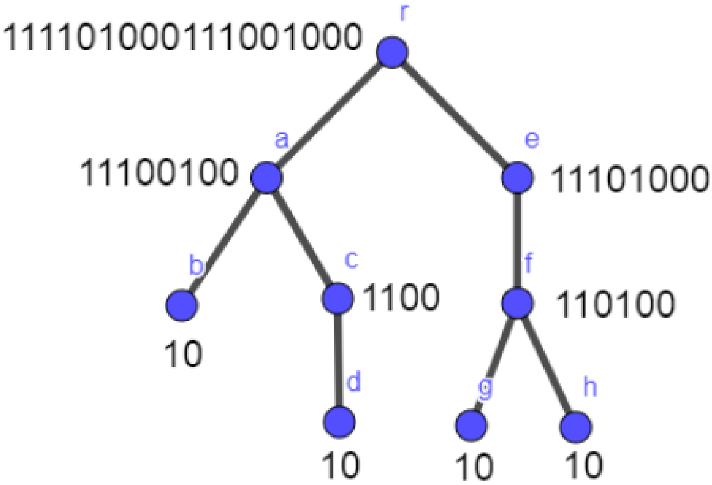

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Induction hypothesis: If two rooted trees (X_1, a_1) and (X_2, a_2) are isomorphic and have both k levels then the algorithm returns YES on input $((X_1, a_1), (X_2, a_2))$.

Induction step: Let (T_1, r_1) and (T_2, r_2) be two isomorphic rooted trees, each with $k + 1$ levels.

Let f be the bijection between T_1 and T_2 (from the definition). Then $r_2 = f(r_1)$ and, for every child a_1 of r_1 there exists a child a_2 of r_2 such that:

- the subtrees $(T_1(a_1), a_1)$ and $(T_2(a_2), a_2)$ are isomorphic, and
- $a_2 = f(a_1)$

Graph isomorphism on rooted trees

Proof (cont.):

Since every such pair of trees $(T_1(a_1), a_1)$ and $(T_2(a_2), a_2)$ is isomorphic, they have both k levels. Thus, by the induction hypothesis, Algorithm 1 returns the same labels for their roots, i.e. $label(a_1) = label(a_2)$.

Graph isomorphism on rooted trees

Proof (cont.):

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Algorithm 1 now computes $label(r_1)$ by decreasingly sorting the labels of the children of r_1, say $\ell(w_1) \geq \ldots \geq \ell(w_k)$,
and then it sets $label(r_1) =$ "1" $\ell(w_1)\ell(w_2)\ldots\ell(w_p)$ "0".

Graph isomorphism on rooted trees

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Exactly the same happens for $label(r_2)$,
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Graph isomorphism on rooted trees

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Since all these labels are the same (by the induction hypothesis):
$label(r_1) = label(r_2)$, and thus Algorithm 2 returns YES. $\square$

Graph isomorphism on rooted trees

Proof (cont.):

Since every such pair of trees $(T_1(a_1), a_1)$ and $(T_2(a_2), a_2)$ is isomorphic, they have both k levels. Thus, by the induction hypothesis, Algorithm 1 returns the same labels for their roots, i.e. $label(a_1) = label(a_2)$.

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Does this theorem show that Algorithm 2 is a correct isomorphism algorithm for rooted trees?

Graph isomorphism on rooted trees

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Since every such pair of trees $(T_1(a_1), a_1)$ and $(T_2(a_2), a_2)$ is isomorphic, they have both k levels. Thus, by the induction hypothesis, Algorithm 1 returns the same labels for their roots, i.e. $label(a_1) = label(a_2)$.

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Since all these labels are the same (by the induction hypothesis):
$label(r_1) = label(r_2)$, and thus Algorithm 2 returns YES. □

Does this theorem show that Algorithm 2 is a correct isomorphism algorithm for rooted trees?

- we also need the reverse direction: if two trees are not isomorphic, then the algorithm returns NO
- this can be also proved (a bit more tricky)