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## A DISTANCE BETWEEN ISOMORPHISM CLASSES OF TREES

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In [1] a certain distance between isomorphism classes of graphs was introduced. Here we shall study an analog of this distance for trees.

Consider the set  $\mathcal{T}_n$  of all isomorphism classes of trees with  $n$  vertices, where  $n \geq 3$ . For any two elements  $\mathfrak{T}_1, \mathfrak{T}_2$  of  $\mathcal{T}_n$  we introduce the number  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2)$  as the least integer with the property that there exists a tree with  $n + \delta_T(\mathfrak{T}_1, \mathfrak{T}_2)$  vertices which contains a subtree  $T_1 \in \mathfrak{T}_1$  and subtree  $T_2 \in \mathfrak{T}_2$ . For the sake of simplicity we shall also use the notation  $\delta_T(T_1, T_2)$  for two trees  $T_1$  and  $T_2$ ; this will mean  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2)$  for the classes  $\mathfrak{T}_1, \mathfrak{T}_2$  such that  $T_1 \in \mathfrak{T}_1, T_2 \in \mathfrak{T}_2$ .

**Theorem 1.** *The functional  $\delta_T$  is a metric on the set  $\mathcal{T}_n$ .*

*Proof.* Evidently  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2) \geq 0$  for any two elements  $\mathfrak{T}_1, \mathfrak{T}_2$  of  $\mathcal{T}_n$  and  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2) = 0$  if and only if  $\mathfrak{T}_1 = \mathfrak{T}_2$ . Also evidently  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2) = \delta_T(\mathfrak{T}_2, \mathfrak{T}_1)$ . Now let  $\mathfrak{T}_1, \mathfrak{T}_2, \mathfrak{T}_3$  be three elements of  $\mathcal{T}_n$ . There exists a tree  $T_{12}$  with  $n + \delta_T(\mathfrak{T}_1, \mathfrak{T}_2)$  vertices which contains a subtree  $T_1 \in \mathfrak{T}_1$  and a subtree  $T_2 \in \mathfrak{T}_2$  and there exists a tree  $T_{23}$  with  $n + \delta_T(\mathfrak{T}_2, \mathfrak{T}_3)$  vertices which contains a subtree  $T'_2 \in \mathfrak{T}_2$  and a subtree  $T_3 \in \mathfrak{T}_3$ . The trees  $T_2, T'_2$  are isomorphic; take an isomorphic mapping of  $T_2$  onto  $T'_2$  and identify each vertex of  $T_2$  with its image in this mapping. We may suppose that  $T_{12}$  and  $T_{23}$  are vertex-disjoint. The graph  $T$  obtained in the described way from the trees  $T_{12}$  and  $T_{23}$  is evidently a tree. It has  $n + \delta_T(\mathfrak{T}_1, \mathfrak{T}_2) + \delta_T(\mathfrak{T}_2, \mathfrak{T}_3)$  vertices and contains a subtree  $T_1 \in \mathfrak{T}_1$  and a subtree  $T_2 \in \mathfrak{T}_2$ . Hence

$$\delta_T(\mathfrak{T}_1, \mathfrak{T}_3) \leq \delta_T(\mathfrak{T}_1, \mathfrak{T}_2) + \delta_T(\mathfrak{T}_2, \mathfrak{T}_3)$$

and the triangle inequality holds.

**Theorem 2.** *Let  $\mathfrak{T}_1 \in \mathcal{T}_n, \mathfrak{T}_2 \in \mathcal{T}_n, T_1 \in \mathfrak{T}_1, T_2 \in \mathfrak{T}_2$ . Let  $k$  be a non-negative integer,  $k < n$ . Then the following two assertions are equivalent:*

- (i) *There exists a tree  $T$  with  $n + k$  vertices which contains a subtree isomorphic to  $T_1$  and a subtree isomorphic to  $T_2$ .*
- (ii) *There exists a tree  $T_0$  with  $n - k$  vertices such that both  $T_1$  and  $T_2$  contain subtrees isomorphic to  $T_0$ .*

Proof. (i)  $\Rightarrow$  (ii). Let (i) hold. Let  $T'_1, T'_2$  be subtrees of  $T$  isomorphic to  $T_1, T_2$ , respectively. As  $k < n$ , the trees  $T'_1, T'_2$  have a non-empty intersection and this intersection is a subtree  $T'_0$  of  $T$  which has at least  $n - k$  vertices. Choose a subtree  $T_0$  of  $T'_0$  with exactly  $n - k$  vertices. If we take an isomorphic mapping of  $T'_1$  onto  $T_1$  and an isomorphic mapping of  $T'_2$  onto  $T_2$ , then the images of  $T_0$  in these mappings are subtrees of  $T_1$  and  $T_2$  which are isomorphic to one another.

(ii)  $\Rightarrow$  (i). Let (ii) hold. Without loss of generality suppose that  $T_1, T_2$  are vertex-disjoint. Let  $T'_0, T''_0$  be subtrees of  $T_1, T_2$ , respectively, which are both isomorphic to  $T_0$ . Take an isomorphic mapping of  $T'_0$  onto  $T''_0$  and identify each vertex of  $T'_0$  with its image in this mapping. The graph  $T$  obtained in this way is evidently a tree with  $n + k$  vertices and it contains  $T_1, T_2$  as subtrees.

Similarly as in [1] we may consider a graph  $\mathcal{G}_n$  whose vertex set is  $\mathcal{T}_n$  and in which two vertices  $\mathfrak{T}_1, \mathfrak{T}_2$  are adjacent if and only if  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2) = 1$ .

**Theorem 3.** *The distance of any two vertices  $\mathfrak{T}_1, \mathfrak{T}_2$  of  $\mathcal{G}_n$  is equal to  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2)$ .*

Proof. Let  $\mathfrak{T}_1, \mathfrak{T}_2$  be two vertices of  $\mathcal{G}_n$  and let  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2) = k$ . Then there exists a tree  $T$  with  $n + k$  vertices which contains a subtree  $T_1 \in \mathfrak{T}_1$  and a subtree  $T_2 \in \mathfrak{T}_2$ . In  $T$  exactly  $n - k$  vertices are common to  $T_1$  and  $T_2$  (see Theorem 2). Further, there are  $k$  vertices of  $T_1$  not belonging to  $T_2$  and  $k$  vertices of  $T_2$  not belonging to  $T_1$ . The vertices of  $T_1$  not belonging to  $T_2$  will be denoted by  $u_1, \dots, u_k$  in such a way that each  $u_i$  is adjacent either to a common vertex of  $T_1$  and  $T_2$ , or to a vertex  $u_j$  with  $j < i$ ; this can be easily done. The vertices of  $T_2$  not belonging to  $T_1$  will be denoted by  $v_1, \dots, v_k$  in such a way that each  $v_i$  is adjacent either to a common vertex of  $T_1$  and  $T_2$ , or to a vertex  $v_j$  with  $j > i$ . Then for each  $j = 1, \dots, k$ , the graph  $S_j$  obtained from  $T_2$  by deleting the vertices  $u_i$  for  $i \leq j$  and adding the vertices  $v_i$  for  $i \leq j$  together with the edges joining them with each other and with the common vertices of  $T_1$  and  $T_2$  in  $T$ , is a tree. Evidently  $S_k = T_1$ ,  $\delta_T(T_2, S_1) = 1$ ,  $\delta_T(S_i, S_{i+1}) = 1$  for  $i = 1, \dots, k - 1$ . The vertices  $T_2, S_1, \dots, S_k = T_1$  (here we speak about trees as vertices of  $\mathcal{G}_n$  instead of classes containing them; we do this for the sake of simplicity) form a path of the length  $k$  in  $\mathcal{G}_n$  and thus the distance of  $\mathfrak{T}_1$  and  $\mathfrak{T}_2$  in  $\mathcal{G}_n$  is at most  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2)$ . Now suppose that the distance between  $\mathfrak{T}_1$  and  $\mathfrak{T}_2$  in  $\mathcal{G}_n$  is  $l$ . There exists a path of the length  $l$  in  $\mathcal{G}_n$  consisting of the vertices  $T_1 = S'_0, S'_1, \dots, S'_k = T_2$ . We have  $\delta_T(S'_i, S'_{i+1}) = 1$  for  $i = 0, \dots, k - 1$ . Let  $S''_i$  be a tree with  $n + 1$  vertices which contains a subtree isomorphic to  $S'_i$  and a subtree isomorphic to  $S'_{i+1}$ . For each  $i = 0, \dots, k - 2$  we choose an isomorphism of the subtree of  $S''_i$  isomorphic to  $S'_{i+1}$  onto the subtree of  $S''_{i+1}$  isomorphic to  $S'_{i+1}$  and identify each vertex of the domain of this mapping with its image. Then we obtain a tree with  $n + l$  vertices which contains a subtree from  $\mathfrak{T}_1$  and a subtree from  $\mathfrak{T}_2$ . Thus the distance between  $\mathfrak{T}_1$  and  $\mathfrak{T}_2$  in  $\mathcal{G}_n$  is at least  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2)$ ; together with the previous result this yields that this distance is equal to  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2)$ .

A snake is a tree consisting of one path. Its length is the length of this path.

**Theorem 4.** *The diameter of the graph  $\mathcal{G}_n$  is  $n - 3$ . There exists exactly one pair of vertices of  $\mathcal{G}_n$  whose distance is  $n - 3$ .*

*Proof.* As  $n \geq 3$ , each tree from  $\mathcal{G}_n$  contains a subtree which is a snake of the length 2; it has three vertices. If  $\mathfrak{T}_1 \in \mathcal{T}_n$ ,  $\mathfrak{T}_2 \in \mathcal{T}_n$ ,  $T_1 \in \mathfrak{T}_1$ ,  $T_2 \in \mathfrak{T}_2$ , then according to Theorem 2 there exists a tree with  $2n - 3$  vertices which contains a subtree isomorphic to  $T_1$  and a subtree isomorphic to  $T_2$ . Thus  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2) \leq n - 3$  for any two vertices  $\mathfrak{T}_1, \mathfrak{T}_2$  of  $\mathcal{G}_n$ . Now let  $S_1$  be the snake of the length  $n - 1$  and let  $S_2$  be a star with  $n - 1$  edges. Any subtree of  $S_1$  (or  $S_2$ ) with more than three vertices is a snake (or a star, respectively) with more than two edges. Therefore (ii) from Theorem 2 for  $k \leq n - 3$  does not hold, thus (i) does not hold, either, and the isomorphism classes containing  $S_1$  and  $S_2$  have the distance exactly  $n - 3$ . Any tree with  $n$  vertices which is neither a snake nor a star contains a snake with four vertices and a star with four vertices as subtrees; hence the distance of its isomorphism class from any other isomorphism class from  $\mathcal{T}_n$  is at most  $n - 4$ .

For every positive integer  $k \geq 3$  we shall define the tree  $T(k)$ . First we define the graph  $T_0(k)$ . The vertex set of  $T_0(k)$  consists of all vectors of the dimensions  $0, 1, \dots, \lfloor k/2 \rfloor - 1$  (the symbol  $\lfloor x \rfloor$  denotes the least integer greater than or equal to  $x$ ) whose coordinates are the numbers from the set  $\{1, \dots, k - 1\}$ . Two vectors  $\mathbf{u}, \mathbf{v}$  are adjacent if and only if one of them is obtained from the other by adding one coordinate. If  $k$  is odd, we take two disjoint copies of  $T_0(k)$  and join the vertices corresponding to the zero vector in both of them. If  $k$  is even, we take a new vertex  $a$  and  $k$  pairwise disjoint copies of  $T_0(k)$  and join  $a$  with the vertices corresponding to the zero vector in all of them. The tree thus obtained will be denoted by  $T(k)$ .

**Lemma 1.** *The tree  $T(k)$  has the maximal number of vertices among all trees with the diameter at most  $k$  and the maximal degree at most  $k$ .*

*Proof.* Let  $T$  be a tree with the diameter  $k$  and the maximal degree  $k$ . If  $k$  is even, then  $T$  has one centre  $c$  and the distance of each vertex of  $T$  from  $c$  is at most  $k/2$ . As the maximal degree of  $T$  is  $k$ , for each  $i = 1, \dots, k/2$  there are at most  $k(k - 1)^{i-1}$  vertices of  $T$  whose distance from  $c$  is  $i$ . Thus  $T$  has at most  $1 + k \sum_{i=0}^{k/2-1} (k - 1)^{i-1}$  vertices and this is the number of vertices of  $T(k)$ . The proof for  $k$  odd is analogous.

By  $\tau(k)$  we denote the number of vertices of  $T(k)$  for each  $k \geq 3$ . Evidently

$$\tau(k) = 1 + k \sum_{i=0}^{k/2-1} (k - 1)^{i-1} \quad \text{for } k \text{ even,}$$

$$\tau(k) = 2 \sum_{i=0}^{k/2-1} (k - 1)^{i-1} \quad \text{for } k \text{ odd.}$$

Further, for  $n \geq 6$  we denote

$$\sigma(n) = \max \{k \in N \mid \tau(k) \leq n\},$$

where  $N$  denotes the set of all positive integers.

**Theorem 5.** *Let  $\varrho$  be the radius of  $\mathcal{G}_n$ . Then*

$$\varrho \leq n - \sigma(n) - 1.$$

*Proof.* Let  $k = \sigma(n)$  and construct the tree  $C$ . If  $\tau(k) = n$ , then  $C \cong T(k)$ . If  $\tau(k) < n$ , then the tree  $C$  is an arbitrary tree with  $n$  vertices containing  $T(k)$  as a subtree. Let  $T$  be an arbitrary tree with  $n$  vertices. If the diameter of  $T$  is greater than  $k$ , then both  $T$  and  $C$  contain a snake with  $k + 1$  vertices as a subtree. If  $\mathfrak{C}$  and  $\mathfrak{T}$  are isomorphism classes containing  $C$  and  $T$ , respectively, then  $\delta_T(\mathfrak{C}, \mathfrak{T}) \leq n - k - 1$ . If the diameter of  $T$  is less than  $k$ , then (as it has  $n \geq \tau(k)$  vertices) by Lemma 1 its maximal degree must be greater than  $k$ . Then both  $C$  and  $T$  contain a star with  $k + 1$  vertices as a subtree and again  $\delta_T(\mathfrak{C}, \mathfrak{T}) \leq n - k - 1$ . The distance of  $\mathfrak{C}$  from the isomorphism class containing a snake and from one containing a star is evidently exactly  $n - k - 1$ . Thus the radius of  $\mathcal{G}_n$  is at most  $n - k - 1 = n - \sigma(n) - 1$ .

**Conjecture 1.** *The radius of  $\mathcal{G}_n$  is equal to  $n - \sigma(n) - 1$ .*

In the sequel we shall study caterpillars. A caterpillar is a tree with the property that after deleting all of its terminal vertices (vertices of degree 1) a snake is obtained (a graph consisting of one vertex is also considered a snake). The snake just mentioned is called the *body of the caterpillar*.

**Theorem 6.** *Let  $\mathfrak{T}_1 \in \mathfrak{T}_n$ ,  $\mathfrak{T}_2 \in \mathfrak{T}_n$ ,  $T_1 \in \mathfrak{T}_1$ ,  $T_2 \in \mathfrak{T}_2$ . Let  $T_1, T_2$  be caterpillars and let  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2) = k$ . Then there exists a caterpillar  $T$  with  $n + k$  vertices which contains a subtree isomorphic to  $T_1$  and a subtree isomorphic to  $T_2$ .*

*Proof.* As  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2) = k$ , according to Theorem 2 there exists a tree  $T_0$  with  $n - k$  vertices such that both  $T_1$  and  $T_2$  contain subtrees isomorphic to  $T_0$ . We have  $n - k \geq 3$ , therefore  $T_0$  has at least two edges. As it is a subtree of a caterpillar, it is a caterpillar. Let  $B(T_1), B(T_2), B(T_0)$  be the bodies of the caterpillars  $T_1, T_2, T_0$ , respectively. Let  $T$  be the tree constructed as in the proof of Theorem 2. If  $T$  is not a caterpillar, then there exists an edge  $e_1$  of  $B(T_1)$  not belonging to  $B(T_2)$  and an edge  $e_2$  of  $B(T_2)$  not belonging to  $B(T_1)$ , such that they both are incident with a vertex  $v_0$  of  $B(T_0)$ . Let  $v_1$  (or  $v_2$ ) be the end vertex of  $e_1$  (or of  $e_2$ , respectively) distinct from  $v_0$ . By identifying the vertices  $v_1, v_2$  in  $T$  a tree with  $n + k - 1$  vertices is obtained which contains both  $T_1$  and  $T_2$  as subtrees; this is a contradiction with the assumption that  $\delta_T(\mathfrak{T}_1, \mathfrak{T}_2) = k$ . Thus  $T$  is a caterpillar, which was to be proved.

**Corollary.** *The set of all isomorphism classes of caterpillars with  $n$  vertices induces a subgraph  $\tilde{\mathcal{G}}_n$  of  $\mathcal{G}_n$  with the property that the distance in  $\tilde{\mathcal{G}}_n$  is the same as in  $\mathcal{G}_n$ . The diameter of  $\tilde{\mathcal{G}}_n$  is  $n - 3$ .*

Now for every positive integer  $k$  we construct a caterpillar  $\tilde{T}(k)$ . The body of  $\tilde{T}(k)$  is a snake of the length  $k - 2$ . The degree of any vertex of this body in  $\tilde{T}(k)$  is  $k$ . Evidently the number of vertices of  $\tilde{T}(k)$  is  $k^2 - 2k + 3$ .

**Lemma 2.** *The caterpillar  $\tilde{T}(k)$  has the maximal number of vertices among all caterpillars with the diameter at most  $k$  and the maximal degree at most  $k$ .*

*Proof.* Evidently the diameter of a caterpillar is the length of its body plus two. This implies the assertion.

**Theorem 7.** *Let  $\tilde{q}$  be the radius of  $\tilde{\mathcal{G}}_n$ . Then*

$$\tilde{q} \leq n - \tilde{\sigma}(n) - 1,$$

where

$$\tilde{\sigma}(n) = \max \{k \in N \mid k^2 - 2k + 3 \leq n\}.$$

*Proof* is analogous to that of Theorem 5.

**Conjecture 2.** *The radius of  $\mathcal{G}_n$  is equal to  $n - \tilde{\sigma}(n) - 1$ .*

In the end we shall compare the distance  $\delta_T$  with the distance introduced in [1] on the set of all isomorphism classes of undirected graphs with  $n$  vertices. The distance  $\delta(\mathcal{G}_1, \mathcal{G}_2)$  of two such classes was defined as the least number  $k$  such that there exists a graph with  $n + k$  vertices which contains an induced subgraph belonging to  $\mathcal{G}_1$  and an induced subgraph belonging to  $\mathcal{G}_2$ .

**Theorem 8.** *For two elements  $\mathcal{I}_1, \mathcal{I}_2$  of  $\mathcal{I}_n$  for  $n \geq 7$  the distances  $\delta_T(\mathcal{I}_1, \mathcal{I}_2)$ ,  $\delta(\mathcal{I}_1, \mathcal{I}_2)$  are different in general.*

*Proof.* Let  $\mathcal{S}_1$  (or  $\mathcal{S}_1$ ) be the isomorphism class containing a snake (or a star, respectively) with  $n$  vertices. We know that  $\delta_T(\mathcal{S}_1, \mathcal{S}_2) = n - 3$ . Now let  $S_1 \in \mathcal{S}_1$ ,  $S_2 \in \mathcal{S}_2$ . In  $S_1$  take an independent set with the maximal number of elements; it has  $\lceil n/2 \rceil$  vertices. Identify each vertex of this set with one terminal vertex of  $S_2$ . We obtain a graph with  $\lceil 3n/2 \rceil$  vertices which contains  $S_1$  and  $S_2$  as induced subgraphs. Thus

$$\delta(\mathcal{S}_1, \mathcal{S}_2) \leq \lceil 3n/2 \rceil - n = \lceil n/2 \rceil < n - 3 = \delta_T(\mathcal{S}_1, \mathcal{S}_2).$$

#### Reference

- [1] *Zelinka, B.:* On a certain distance between isomorphism classes of graphs. Časop. pěst. mat. 100 (1975), 371–373.

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