ON THE NUMBER OF NONISOMORPHIC SUBTREES OF A TREE

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ABSTRACT. We show that a tree of order n has at most $O(5^{n/4})$ nonisomorphic subtrees, and that this bound is best possible. We also prove an analogous result for the number of nonisomorphic rooted subtrees of a rooted tree.

1. Introduction

Subtrees of a tree have been studied extensively: Jamison [3, 4] investigated the average number of vertices in a subtree, Székely and Wang studied the number of subtrees of trees [5, 6]. Chung, Graham and Coppersmith [2] found the smallest order (asymptotically) of a tree that contains all n-vertex trees as subtrees. A number of extremal results are known: in particular, it is known that a tree of order n has at least $\binom{n+1}{2}$ subtrees (with equality for the path) and at most $2^{n-1} + 1$ subtrees (with equality for the star).

Things change considerably, however, if one considers the number of distinct nonisomorphic subtrees. Bubeck and Linial [1] recently analyzed the distribution of subtrees of fixed order by isomorphism type. In this paper we consider the extremal problem of determining the smallest and largest number of nonisomorphic subtrees of a tree. Both the path and the star have only very few nonisomorphic subtrees (equal to the number of vertices, to be precise), and this is in fact the minimum:

Proposition 1. Every tree of order n has at least n distinct nonisomorphic subtrees.

Proof. This is easily established by noticing that every tree of order n has subtrees of every order k between 1 and n (obtained by repeatedly removing leaves from the original tree), which are trivially nonisomorphic.

The maximum is much more difficult to obtain; we will show that it is of the order $\Theta(5^{n/4})$. In a certain sense, this is a dual question to the aforementioned problem of Chung, Graham and Coppersmith: while they were looking for the minimum number of vertices needed to contain all small trees, we would like to know how many different trees can fit into a tree with a given number of vertices.

For our purposes, it turns out to be useful to also consider a closely related problem: for a rooted tree, we count the number of nonisomorphic subtrees that contain the root, where

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non-isomorphism is understood in the rooted sense, i.e., two subtrees containing the root are considered isomorphic if there is an isomorphism between them that maps the root to itself. Again, the maximum number is $\Theta(5^{n/4})$, as we will prove in the following. Let us first introduce some notation.

For a tree T, we let |T| be the number of vertices and $\operatorname{ns}(T)$ be the number of nonisomorphic subtrees of T. Likewise, for a rooted tree T, we let $\operatorname{nr}(T)$ be the number of nonisomorphic subtrees containing the root, in the sense explained in the previous paragraph. Moreover, we write

$$S_n = \max_{|T|=n} \operatorname{ns}(T)$$
 and $R_n = \max_{|T|=n} \operatorname{nr}(T)$

for the respective maxima among trees with n vertices. The following table gives explicit values for small n, obtained by means of a comprehensive computer search:

n	1	2	3	4	5	6	7	8	9	10
S_n	1	2	3	4	6	8	11	16	23	33
R_n	1	2	3	5	7	11	16	24	34	54

Table 1. S_n and R_n for small values of n.

While it appears difficult to determine S_n and R_n explicitly for general n, we will be able to bound them from above and to provide a construction that matches the bound up to a constant factor.

2. The asymptotic order of S_n and R_n

Our approach will consist of the following steps:

- Provide a construction that yields trees with "many" nonisomorphic subtrees,
- Bound S_n in terms of R_n ,
- Prove an upper bound on R_n .

The three statements of Proposition 3 below correspond to those three steps. In order to prove the upper bound on R_n , we will require the following simple lemma.

Lemma 2.

1. Let T be a rooted tree, and suppose that T is the union of two rooted trees R_1 and R_2 (nontrivial, i.e. of order at least 2) that only share the root. Then we have the inequality

$$\operatorname{nr}(T) \le \operatorname{nr}(R_1) \operatorname{nr}(R_2) - 1. \tag{1}$$

2. Let T_1, T_2, \ldots, T_d be the root branches (in other words, the components that remain when the root is removed) of a rooted tree T, endowed with their natural roots. Then the inequality

$$\operatorname{nr}(T) \le \prod_{j=1}^{d} (\operatorname{nr}(T_j) + 1) \tag{2}$$

holds.

Proof.

1. Note that each subtree S of T that contains the subtree decomposes naturally into a subtree S_1 of R_1 and a subtree of S_2 of R_2 , each containing the respective root. Two pairs of subtrees (S_1, S_2) and (S'_1, S'_2) of subtrees such that S_1 is isomorphic to S'_1 and S_2 is isomorphic to S'_2 induce isomorphic subtrees of T. Therefore, we clearly have

$$\operatorname{nr}(T) \leq \operatorname{nr}(R_1) \operatorname{nr}(R_2).$$

To show that even strict inequality must hold for nontrivial trees R_1 and R_2 (which implies the desired statement), note that the two-vertex subtree is counted twice in this argument: once as a subtree of R_1 , once as a subtree of R_2 (of course, this might also apply to other subtrees). Thus we obtain (1).

2. The argument is analogous to the first part: every subtree of T induces a subtree that contains the root or the empty set in each T_i . The inequality (2) follows immediately (and it is generally strict because subtrees are counted repeatedly).

Proposition 3. The following inequalities hold for all $n \geq 1$:

- 1. $S_n \ge 2 \cdot 5^{n/4-2}$, 2. $S_n \le R_n + 3 \cdot 2^{n/2-1}$, 3. $R_n \le 5^{n/4}$.

Proof.

1. For n < 8, the stated inequality is essentially trivial, since it provides a lower bound of 1 (n < 7) or 2 (n = 7). For $n \ge 8$, we obtain the lower bound on S_n by an explicit construction (see Figure 1). Its core is formed by a path of $m = \lfloor \frac{n}{4} \rfloor - 2$ vertices, to each of which we attach three vertices: one leaf and two others forming a path of length 2. Depending on the residue class of n modulo 4, we add between 8 and 11 additional vertices as indicated in the figure to obtain an n-vertex tree that we denote by C_n .

It is clear that $S_n \geq \operatorname{ns}(C_n)$, so let us estimate $\operatorname{ns}(C_n)$. For a simple lower bound, we only consider subtrees that contain the entire "backbone" consisting of v_1, v_2, \ldots, v_m and $x_1, x_2, x_3, y_1, y_2, y_3$, as well as the vertex z. Note that the paths from x_1 to y_3 and from z to y_3 are always the only diameters of these subtrees, so they are uniquely determined by the parts "dangling" from $x_3, v_1, v_2, \ldots, v_m, y_1$. Including z in all subtrees we are counting guarantees that there is no double-counting due to mirror symmetry.

The leaf or leaves attached to x_3 can be included in such a subtree or not, which gives us 2 possibilities for $n \equiv 0, 1 \mod 4$ and 3 possibilities for $n \equiv 2, 3 \mod 4$. Likewise, the leaf or leaves attached to y_1 can be included or not, giving us 1, 2 or 3 possible options, depending on the residue class again. Finally, for each of the vertices v_1, v_2, \ldots, v_m , we have 5 distinct ways of extending the subtree by adding a subset of

 $n \equiv 0 \bmod 4$:



 $n \equiv 1 \bmod 4$:



 $n \equiv 2 \bmod 4$:



 $n \equiv 3 \mod 4$:



FIGURE 1. A construction that yields a lower bound.

the three vertices attached to it. Altogether, this gives us

$$\operatorname{ns}(C_n) \ge \begin{cases} 2 \cdot 5^m & n \equiv 0 \mod 4, \\ 4 \cdot 5^m & n \equiv 1 \mod 4, \\ 6 \cdot 5^m & n \equiv 2 \mod 4, \\ 9 \cdot 5^m & n \equiv 3 \mod 4, \end{cases}$$

where $m = \lfloor \frac{n}{4} \rfloor - 2$. It is easy to verify that $\operatorname{ns}(C_n) \geq 2 \cdot 5^{n/4-2}$ in each of the four cases, which completes our proof.

2. For the inequality between R_n and S_n , consider a tree T of order n for which the maximum S_n is attained, i.e., $\operatorname{ns}(T) = S_n$. Let v be a centroid vertex of T, which is a vertex for which the sum of the distances to all other vertices is minimized. It is well known that none of the centroid branches (the connected components that remain when the centroid is removed) can contain more than n/2 vertices, since one could then decrease the sum of distances by moving one step towards the largest branch (see Zelinka's paper [7]). Let T_1, T_2, \ldots, T_k be the centroid branches, so that $|T_1| + |T_2| + \cdots + |T_k| = n - 1$. The total number of subtrees that do not contain the

centroid v is clearly at most

$$\sum_{i=1}^{k} 2^{|T_i|}.$$

Some of these subtrees may of course be isomorphic, but we are only interested in an upper bound. Note that this sum increases if we transfer vertices from any of the branches to a branch with the same or greater number of vertices. Therefore, it reaches its maximum when there are only two branches, each containing either (n-1)/2 vertices (if n is odd) or n/2 and n/2-1 vertices respectively (if n is even). It follows that at most $2^{n/2}+2^{n/2-1}=3\cdot 2^{n/2-1}$ of the subtrees of T do not contain the centroid v. The number of distinct nonisomorphic subtrees containing v is clearly at most R_n by definition, so this completes the proof.

3. For the proof of the third statement, we use induction on n to prove a minimally stronger inequality, which makes the inductive argument simpler. Specifically, we claim that for a rooted tree T of order n,

$$\operatorname{nr}(T) \le 5^{n/4} - 1,\tag{3}$$

unless T is one of ten exceptional trees (denoted E_1, \ldots, E_{10} for future reference) that are shown in Figure 2. Note, however, that all these trees still satisfy inequality (3) without the final -1, which is what we actually want to obtain.

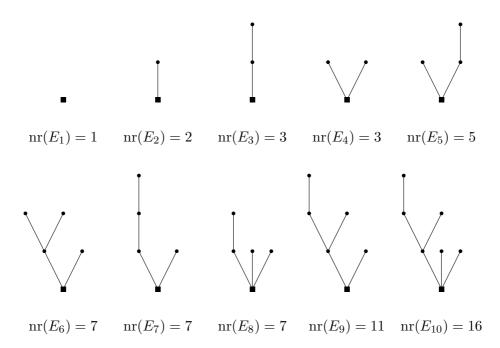


FIGURE 2. The ten exceptional rooted trees.

The statement can be verified directly for $n \leq 7$, so for the induction step, we consider a tree T of order $n \geq 8$, and we denote its root by r and its root branches by T_1, T_2, \ldots, T_d . Now consider the following cases:

Case 1: At least one of the branches (without loss of generality T_1) is not an exceptional tree. In this case, we can regard T as the union of the rooted trees $R_1 = \{r\} \cup T_1$ and $R_2 = T \setminus T_1$, both rooted at r. If the tree R_2 is nontrivial (in other words, if T has more than one branch), then we can apply (1) and the induction hypothesis to obtain

$$\operatorname{nr}(T) \le \operatorname{nr}(R_1) \operatorname{nr}(R_2) - 1 = (\operatorname{nr}(T_1) + 1) \operatorname{nr}(R_2) - 1$$
$$\le (5^{|T_1|/4} - 1 + 1) \cdot 5^{|R_2|/4} - 1$$
$$= 5^{(|T_1| + |R_2|)/4} - 1 = 5^{n/4} - 1.$$

which proves the desired inequality. If T_1 is the only branch, then we obtain from the induction hypothesis that

$$\operatorname{nr}(T) = 1 + \operatorname{nr}(T_1) \le 1 + 5^{(n-1)/4} - 1 = 5^{(n-1)/4} \le 5^{n/4} - 1.$$

- Case 2: We are left with the case that all branches are on the list of exceptional trees. Suppose that some set of branches (without loss of generality T_1, T_2, \ldots, T_k), together with the root of T, form a rooted tree R_1 such that $\operatorname{nr}(R_1) \leq 5^{(|R_1|-1)/4}$. In this case, we can apply the same argument as in the previous case: if R_1 is already all of T, we are done immediately; otherwise, set $R_2 = T \setminus R_1 \cup \{r\}$ and apply (1) in combination with the induction hypothesis as before. This means that we are done if any of the following cases applies:
 - At least four branches are single vertices (copies of E_1): in this case, $|R_1| = 5$ and $nr(R_1) = 5$.
 - At least three branches have order 2 (copies of E_2): in this case, $|R_1| = 7$ and $\operatorname{nr}(R_1) = 10$.
 - At least two branches are identical copies of one of the exceptional trees E_j , where $j \in \{3, 4, ..., 10\}$: in this case, $|R_1| = 2|E_j| + 1$ and $\operatorname{nr}(R_1) = (\operatorname{nr}(E_j) + 1)(\operatorname{nr}(E_j) + 2)/2$, since each subtree of R_1 that contains the root is obtained from an unordered pair of root-containing subtrees of E_j , or a single such subtree, or consists of the root only. For each j, the desired inequality is easily verified.
 - At least two of the branches belong to the set $\{E_6, E_7, E_8, E_9, E_{10}\}$ of "large" exceptional branches: in each of these cases, one verifies that the tree R_1 formed by the root and these two branches satisfies $\operatorname{nr}(R_1) \leq \frac{5(|R_1|-1)/4}{4}$

This leaves us with $4 \cdot 3 \cdot 2^3 \cdot 6 = 576$ remaining cases (determined by how often each exceptional tree occurs as a branch: up to three copies of E_1 , up to two copies of E_2 , either one or no copy for each of E_3, E_4, E_5 , and potentially one of E_6, E_7, \ldots, E_{10}), and these can be checked directly by a computer.

Our main result follows immediately:

Theorem 4. We have both $S_n = \Theta(5^{n/4})$ and $R_n = \Theta(5^{n/4})$.

Proof. Simply combine the inequalities of Proposition 3 (and note that $2^{1/2} < 5^{1/4}$).

Remark 1. Note the special role of the rooted tree E_5 in the construction of the trees C_n : these trees, which gave us the lower bound, mostly consist of copies of E_5 , attached to a long path. The reason why this construction is essentially optimal is the fact that $5^{1/4}$ is the maximum of $\operatorname{nr}(T)^{1/|T|}$ taken over all rooted trees T, and this maximum is only attained by E_5 .

Remark 2. Both the upper and lower bound on S_n and R_n are probably not even asymptotically sharp. The following question is therefore natural:

Does the limit $\lim_{n\to\infty} 5^{-n/4} S_n$ exist, and if so, what is its value?

It is conceivable that the limit does not exist in this form, but that it does exist if n is restricted to a specific residue class modulo 4 (compare the construction of the tree C_n , which depends on the residue class of n modulo 4).

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