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THE NUMBER OF MAXIMAL INDEPENDENT SETS IN A TREE*

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Abstract. We find the largest number of maximal independent sets of vertices that any tree of n vertices can have.

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1. Introduction. We determine, in § 2 below, the largest number of maximal independent sets of vertices that any tree of n vertices can have. In § 3 there is a linear time algorithm for the computation of the number of maximal independent sets of any given tree. The application that suggested these questions to us was the analysis of the complexity of an algorithm for computing the chromatic number of a graph. That application will be discussed in § 4.

2. The main theorem. Let T be a tree, let $V(T)$ be its vertex set and let $n = |V(T)|$ be its number of vertices. A set $S \subseteq V(T)$ is an *independent set* if no two vertices of S are joined by an edge of T. S is a *maximal independent set* (*m.i.s.*) if S is independent and every vertex of $V(T) - S$ is joined by an edge to at least one vertex of S. We write $\mu(T)$ for the number of m.i.s. of vertices of T ($\mu(\varnothing) = 1$).

THEOREM 1. *If we define*

$$f(n) = \begin{cases} 2^{n/2-1}+1 & \text{if } n \geqq 2 \text{ is even,} \\ 2^{(n-1)/2} & \text{if } n \text{ is odd,} \\ 1 & \text{if } n = 0, \end{cases} \tag{1}$$

then $f(n)$ is the largest number of maximal independent sets of vertices that any tree of n vertices can have.

Figure 1 shows that there are trees of n vertices that have $f(n)$ maximal independent sets (the reader may enjoy checking these counts since they are not quite trivial!). Hence it suffices to prove that no n-tree can have more than $f(n)$ such sets.

Let T be a tree of $n \geqq 3$ vertices, and let x be an endpoint of T. We *root* T at x and direct the edges of T away from x.

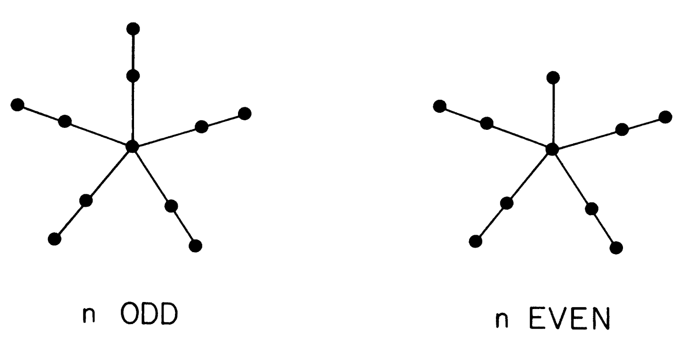

FIG. 1

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Let $\gamma=\gamma(x)$ be the child of x and let $\lambda_1, \cdots, \lambda_r$ be the children of γ. Let U_i be the subtree of T that is rooted at λ_i $(i=1, r)$.

We continue one layer further into T: in U_i, let $W_{i,j}$ $(j=1, s_i)$ be the subtrees that are rooted at the s_i children of λ_i, except that if λ_i is childless then we take $s_i=1$, and $W_{i,1}$ is then the empty tree $(i=1, r)$. The picture is now as shown in Fig. 2.

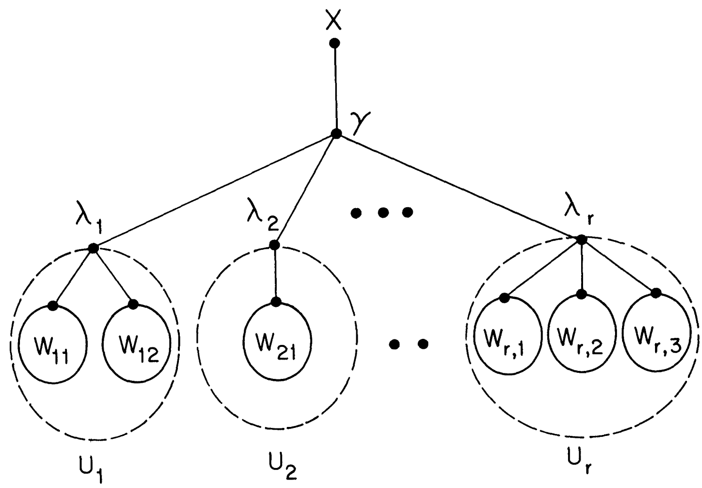

FIG. 2

LEMMA 1. *If T is a tree of $n \geqq 3$ vertices then*

$$\mu(T)=\prod_{i=1}^{r} \mu(U_i)+\prod_{i=1}^{r} \prod_{j=1}^{s_i} \mu(W_{i,j}). \tag{2}$$

Proof. Let $S \subseteq V(T)$ be a m.i.s. that contains x. Then $\gamma \notin S$. Let $S_i=S \cap V(U_i)$ $(i=1, r)$. Then S_i is maximal in U_i $(i=1, r)$, for if not then S can be augmented in T. Conversely, if $\forall i=1, r$: S_i is maximal in U_i, then $S=\{x\} \cup S_1 \cup \cdots \cup S_r$ is maximal in T.

Next consider a m.i.s. $S \subseteq V(T)$ such that $x \notin S$, and therefore $\gamma \in S$. Hence $\forall i=1, r$: $\{\lambda_i \notin S$, and $\forall j=1, s_i$: {if $S_{i,j}=S \cap V(W_{i,j})$ then $S_{i,j}$ is maximal in $W_{i,j}$ and conversely}}. □

Let

$$h(n)=\max_{|V(T)|=n} \mu(T). \tag{3}$$

We will now prove that $\forall n \geqq 0$: $h(n)=f(n)$. Clearly $h(n)=f(n)$ if $n \leqq 2$. Suppose that $n \geqq 3$, and that $\forall j=0, n-1$: $h(j)=f(j)$. Let T be a tree of n vertices, and let x, $U_i(T)$, $W_{i,j}(T)$ be as in Fig. 2. Write $u_i=|V(U_i(T))|$ $(i=1, r)$ and $w_{i,j}=|V(W_{i,j}(T))|$ $(j=1, s_i; i=1, r)$. Then by (2) and the induction hypothesis,

$$\mu(T) \leqq \prod_{i=1}^{r} f(u_i)+\prod_{i=1}^{r} \prod_{j=1}^{s_i} f(w_{i,j}). \tag{4}$$

We will carry out a maximization of (4) over all n-trees T in two stages, as follows. As the problem is presented in (4) we are to maximize the right-hand side over all partitions $\mathbf{u}$ of $n-2$ and all partitions $\mathbf{w}$ of the parts of $\mathbf{u}$ (each reduced by 1). In Stage 1 below we will identify, for given $\mathbf{u}$, the maximizing partition $\mathbf{w}$, and we will be left with maximization over just the partitions $\mathbf{u}$.

In Stage 2 we will show that the maximum depends only on two integers, the number r of parts of $\mathbf{u}$, and the number e of *even* parts of $\mathbf{u}$, but not otherwise on $\mathbf{u}$. We will then carry out the maximization over the admissible integer pairs (r, e), with the end result that the maximum of the right side of (4) will have been shown to be $f(n)$, as defined in (1).

Stage 1 (*in which the trees and the $w_{i,j}$'s are eliminated*).

Fix integers $m, r \geqq 1$, let $\Gamma(r, m)$ denote the set of all r-tuples of positive integers whose sum is m, and write $\Gamma(1, 0) = \{0\}$. If we take the maximum of (4) over all n-trees T, we get

$$h(n) \leqq \max_{r \geqq 1} \max_{\mathbf{u} \in \Gamma(r, n-2)} \left\{ \prod_{i=1}^{r} f(u_i) + \max \prod_{i=1}^{r} \prod_{j=1}^{s_i} f(w_{i,j}) \right\} \tag{5}$$

in which the innermost "max" is over the set of $\mathbf{w}$'s such that for $i = 1, r$:

$$(w_{i,1}, \cdots, w_{i,s}) \in \Gamma(s_i, u_i - 1).$$

Consider an integer r and partitions $\mathbf{u}$, $\mathbf{w}$ that occur on the right side of (5) and in which one or more of the $w_{i,j} \geqq 3$. We claim that this set of integers can be ignored when seeking the maximum in (5).

Indeed, replace $w_{1,1}$ by $\lfloor w_{1,1}/2 \rfloor$ 2's, plus, possibly a 1, leaving all other w's, u's and r untouched. Then the double product on the right will contain a factor

$$f(2)^{\lfloor w_{1,1}/2 \rfloor} = 2^{\lfloor w_{1,1}/2 \rfloor}$$

instead of the factor $f(w_{1,1})$. But from (1), $f(k) \leqq 2^{\lfloor k/2 \rfloor}$ for all $k \geqq 3$. Hence the right side of (5) cannot decrease by such a replacement.

Therefore, for fixed r and $\mathbf{u} \in \Gamma(r, n-2)$ we need consider only partitions of each $u_i - 1$ into 0's, 1's and 2's, say α 2's, β 1's and γ 0's ($\alpha \leqq (u_i - 1)/2$). However, such a partition of $u_i - 1$ contributes a factor of 2^α to the innermost product in (5), and this is maximal when $\alpha = \lfloor (u_i - 1)/2 \rfloor$. Hence for r fixed and $\mathbf{u} \in \Gamma(r, n-2)$, the double product in (5) cannot exceed

$$\prod_{i=1}^{r} 2^{\lfloor (u_i - 1)/2 \rfloor} = 2^{(n-2-r-e)/2}$$

where $e = e(\mathbf{u})$ is the number of even numbers among $u_1, \cdots, u_r$.

Stage 2 (*in which the u_i's are eliminated*).

As a result of stage 1 we have found that

$$h(n) \leqq \max_{r \geqq 1} \max_{\mathbf{u} \in \Gamma(r, n-2)} \left\{ \prod_{i=1}^{r} f(u_i) + 2^{(n-2-r-e(\mathbf{u}))/2} \right\}. \tag{6}$$

Thus we have now a maximization problem over integer partitions, instead of over trees.

Fix three integers r, e, t such that $r \geqq 1$, $0 \leqq e \leqq r$ and $t \geqq e$. Consider the subclass $J(r, e, t) \subseteq \Gamma(r, n-2)$ of those partitions of $n-2$ into r positive parts, exactly e of which are even, and in which the sum of the even parts is $2t$. More precisely, then, $J(r, e, t)$ is the class of all partitions of the form

(7)
(a) $n - 2 = 2l_1 + 2l_2 + \cdots + 2l_e + (2l_{e+1} + 1) + \cdots + (2l_r + 1)$,

(b) $l_i \geqq 1 \quad (i = 1, e), \qquad l_i \geqq 0 \quad (i = e+1, r)$,

(c) $l_i + \cdots + l_e = t$.

Among the partitions $\mathbf{u} \in J(r, e, t)$ the second term in the brace in (6) is constant, so we consider

$$\max_{J(r,e,t)} \prod_{i=1}^{r} f(u_i) = \max_{J(r,e,t)} \prod_{i=1}^{e} f(2l_i) \prod_{i=e+1}^{r} f(2l_i+1)$$

$$(8) \qquad = \max_{J(r,e,t)} \prod_{i=1}^{e} (2^{l_i-1}+1) \prod_{i=e+1}^{r} 2^{l_i}$$

$$= 2^{(n-2-r-e)/2} \max_{J(r,e,t)} \prod_{i=1}^{e} (1+2^{-(l_i-1)})$$

where (7a) was used in the last equality.

The following result will be useful in the sequel.

LEMMA 2. *Fix* $g, z \geqq 0$. *Let*

$$(9) \qquad G(g, z) = \max \prod_{i=1}^{g} (1+2^{-m_i})$$

where the max is over all g-tuples of nonnegative integers $m_1, \cdots, m_g$ *whose sum is z. Then*

$$(10) \qquad G(g, z) = 2^{g-1}(1+2^{-z})$$

and the maximum occurs when exactly one $m_i = z$ *and all* $m_j = 0$ $(j \neq i)$. □

It is now convenient to split up the maximization of (8) over $J(r, e, t)$ into two cases, first where $e = r$, so all parts of (7)(a) are even, and second where $e < r$, so odd parts then also occur in (7)(a).

Case I. $e = r$. In this case (7a) shows that n is even and

$$\sum_{i=1}^{r} l_i = n/2 - 1 = t$$

so we are in the class $J(e, e, n/2-1)$. If we use Lemma 2 with $g = e$, $z = n/2-1-e$, the maximum on the right side of (8) becomes just $2^{n/2-2}+2^{e-1}$. In this case, then, (6) takes the form

$$(11) \qquad h(n) \leqq \max_{e} \{2^{n/2-2}+2^{e-1}+2^{n/2-1-e}\}$$

where the maximum extends over $1 \leqq e \leqq n/2-1$. It is clear, from (11), that the maximum occurs at either endpoint $e = 1$ or $e = n/2-1$, of the interval. The maximum value is $1+2^{n/2-1} = f(n)$, as required.

Case II. $e < r$. Here we find, from Lemma 2 with $g = e$, $z = t-e$, that the maximum on the right side of (8) is

$$(12) \qquad \max_{J(r,e,t)} \{2^{(n-2-r-e)/2}\{2^{e-1}+2^{2e-t-1}\}\}.$$

The maximum over t occurs when t is as small as possible, viz. $t = e$ (see (7b, c)) and the maximum is $2^{(n-2-r+e)/2}$. Thus (6) now becomes

$$(13) \qquad h(n) \leqq \max_{(r,e)} \{2^{(n-2-r+e)/2}+2^{(n-2-r-e)/2}\}.$$

In (13) the "max" is taken over the set of (r, e) for which

$$(14)\quad \begin{array}{lll} \text{(a)} & 1 \leqq r \leqq n-2 & \text{(from (7a))} \\ \text{(b)} & 0 \leqq e < r & \text{(in Case II)} \\ \text{(c)} & e+r \leqq n-2 & \text{(from (7a, b))} \\ \text{(d)} & e+r \equiv n (\text{mod } 2) & \text{(from 7a)} \end{array}$$

Suppose n is odd. We claim that the "max" in (13) occurs at $r=1$, $e=0$. Indeed, if it occurs at (r, e) then surely $r=e+1$ or $r=e+2$, else we could reduce r by 2 to increase the maximum without violating any of the constraints (14). Hence $r=e+1$, by (14d), and (13) reads as

$$h(n) \leqq 2^{n/2-3/2} \max_e \{1+2^{-e}\} = 2^{(n-1)/2} = f(n)$$

so in Case II, n odd, we have established that $h(n) \leqq f(n)$.

Finally, in Case II, suppose n is even, and further suppose that the maximum in (13) occurs at (r, e). Again we must have $r=e+1$ or $r=e+2$, else we could reduce r by 2. Now $r=e+1$ is ruled out by (14d), so $r=e+2$. Therefore (13) reduces to

$$(15)\qquad h(n) \leqq 2^{n/2-2} \max_e \{1+2^{-e}\}$$

and the max occurs at $e=0$, the value being $2^{n/2-1} < f(n)$, completing the proof of Theorem 1. □

3. A linear time algorithm. In this section we give another algorithm for computing $\mu(T)$. It will easily be seen to operate in linear time.

Let the edges of T be oriented away from the root r, let x be some vertex, and let $\mathscr{C}(x)$, $\mathscr{G}(x)$ be the sets of children of x and of grandchildren of x, respectively. Let μ_x be the number of m.i.s. in the subtree rooted at x, and let ν_x be the number of those m.i.s. that do not contain x. Then it is easy to see that

$$(16)\qquad \nu_x = \prod_{y \in \mathscr{C}(x)} \mu_y - \prod_{y \in \mathscr{C}(x)} \nu_y, \qquad \mu_x = \nu_x + \prod_{z \in \mathscr{G}(x)} \mu_z.$$

These formulas permit the computation of the pairs (μ_x, ν_x) at each vertex of T, in descending order of distance from r. One would begin by introducing a new fictitious "child" of each leaf, and placing $(1, 0)$ at each such new vertex as well as at each leaf. The remaining vertices could then be done, in descending order, from (16). Therefore the number of maximal independent sets of vertices in a tree can be computed in linear time.

4. Remarks. In [1] E. Lawler discusses an algorithm for determining the chromatic number of a graph, and shows that its run time, in the worst case, is $O(mn(1+\sqrt[3]{3})^n)$ for graphs of m edges and n vertices.

The appearance of $\sqrt[3]{3}$ derives from a theorem of Moon and Moser [2] to the effect that a graph of n vertices cannot have more than $3^{n/3}$ maximal independent sets (they proved a sharper bound, but this one suffices for our present purpose). However, the extremal graphs of Moon and Moser are disconnected. They are essentially disjoint unions of triangles.

An improvement of Lawler's run time estimate might therefore result if we could solve the following problem:

What is the largest number of maximal independent sets that can occur in a connected graph of n vertices?

The present paper resulted from consideration of the above question. J. Griggs, C. Grinstead and D. Guichard (p.c.) have shown that if $c(n)$ denotes the answer to this question then lim $c(n)^{1/n} = 3^{1/3}$. *Note added in proof.* They and, independently, Z. Füredi, have now answered the above question.

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[2] J. MOON AND L. MOSER, *On cliques in graphs*, Israel J. Math., 3 (1965), pp. 23–28.