ISSN 1990-4789, Journal of Applied and Industrial Mathematics, 2018, Vol. 12, No. 2, pp. 1–16. © Pleiades Publishing, Ltd., 2018.
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On Trees of Bounded Degree with Maximal Number of Greatest Independent Sets

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Received September 29, 2017

Abstract—For each n and d, we describe the structure of trees with the maximal possible number of greatest independent sets in the class of n-vertex trees of vertex degree at most d. We show that for all even n an extremal tree is unique but uniqueness may fail for odd n; moreover, for $d = 3$ and every odd $n \geq 7$, there are exactly $\lceil (n-3)/4 \rceil + 1$ extremal trees. In the paper, the problem of searching for extremal (n, d)-trees is also considered for 2-caterpillars, i.e., trees in which every vertex lies at distance at most two from some simple path. For each n and $d \in \{3, 4\}$, we completely reveal all extremal 2-caterpillars on n vertices each of which has degree at most d.

DOI: 10.1134/S1990478918020011

Keywords: *extremal combinatorics, tree, greatest independent set*

INTRODUCTION

An *independent set* in a graph is arbitrary set of its nonadjacent vertices. We assume that the empty set is also independent. An independent set is called *maximal* if it is inclusion maximal. A *greatest independent set* is an independent set of the greatest cardinality. The cardinality of the greatest independent set in a graph G is denoted by $\alpha(G)$. In what follows, we use the abbreviations "i.s.," "m.i.s.," and "g.i.s." for the terms "independent set," "maximal independent set," and "greatest independent set" respectively. The number of all i.s. (g.i.s.) in a graph G is denoted by $i(G)$ (respectively, $xi(G)$).

A vast literature is devoted to enumerating i.s. (m.i.s. or g.i.s.) in different classes of graphs. The bulk of the corresponding literature is constantly extending. In the famous article by Moon and Moser [8], the value of the maximal possible number of m.i.s. and g.i.s. in graphs with n vertices was given and all corresponding extremal graphs were described. They turned out to be disconnected. In [2], the analogous result was obtained for connected graphs. In [4, 5, 7, 9], the maximal possible numbers of m.i.s. were found in triangle-free graphs, unicyclic graphs, bipartite graphs, and in trees with n vertices respectively.

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Concerning g.i.s., their maximal possible number in trees with n vertices was found in the review [6]. Also in [6], the maximal values were given for the number of g.i.s. in n-vertex graphs of some classes (including connected graphs, unicyclic graphs, and triangle-free graphs).

In [3], for each d, there were completely described extremal trees maximizing the number of i.s. in the class of trees with degrees of all vertices at most d. Later in [1], a method was exposed for constructing n-vertex trees with maximal number of i.s. having a given sequence of degrees.

As usual, a *tree of maximal degree* d is a tree in which the degree of each vertex is at most d. The maximal possible number of i.s. and g.i.s. in n-vertex trees of maximal degree d will be denoted by $i_d(n)$ and $xi_d(n)$ respectively. A tree T of maximal degree d with n vertices will be called (i, d, n)-*maximal* if $i(T) = i_d(n)$. Refer to a tree T of maximal degree d with n vertices as (xi, d, n)-*maximal* if $xi(T) = xi_d(n)$.

The only tree of maximal degree is a simple path. All trees with at most three vertices are also simple paths. Therefore, in what follows, speaking of (i, d, n)-maximal trees or of (xi, d, n)-maximal trees, we mean $d \geq 3$ and $n \geq 4$.

The main result of this article is finding all (xi, d, n)-maximal trees for all values of d and n. It turned out that for all even n such a tree is unique and uniqueness may fail for odd n; moreover, for $d = 3$ and odd $n \geq 7$, there are exactly $\lceil (n-3)/4 \rceil + 1$ extremal trees.

Recall that a k-*caterpillar* is a tree whose each vertex is located at distance k from some its simple path, called the *ridge*. A tree is called an (i, d, n)-*maximal* k-*caterpillar* (respectively, the (xi, d, n)-*maximal* k-*caterpillar*) if it is a k-caterpillar on n vertices of maximal degree d and contains the greatest number of i.s. (respectively, of g.i.s.) among all trees of such kind. In the article, we find all $(xi, 3, n)$-maximal 2-caterpillars and all $(xi, 4, n)$-maximal 2-caterpillars for every n.

1. SOME NOTATIONS AND DEFINITIONS

We use the following notations:

P_n is a simple path on n vertices;

$K_{p,q}$ is a complete bipartite graph with p vertices in one part and q vertices in the other;

$G_1 \cup G_2$ is the disjoint union of graphs G_1 and G_2 with disjoint vertex sets;

kG is the disjoint union of k copies of a graph G;

$i_+(G, v)$ $(i_-(G, v))$ is the number of i.s. in a graph G containing (not containing) a vertex v;

$xi_+(G, v)$ $(xi_-(G, v))$ is the number of g.i.s. in a graph G containing (not containing) a vertex v;

$I(G)$ $(XI(G))$ is the number of i.s. (g.i.s.) in G.

We will use the following definitions: the *size of a graph* is the number of its vertices, an *even* (*odd*) *tree* is a tree having even (odd) number of vertices. A vertex in a tree is *adjacent to a subtree* if it has a neighbor in this subtree. A vertex in a k-caterpillar is *located on the level* s if its distance to the ridge of the k-caterpillar is equal to s.

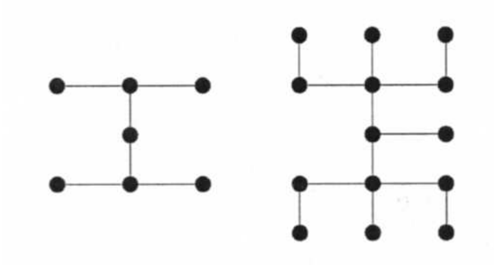

Fig. 1. A tree and its extension.

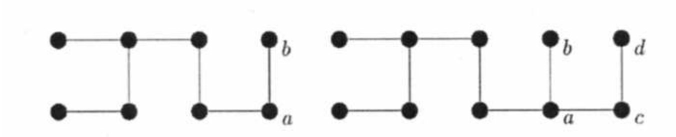

Fig. 2. A tree and one of its spreads.

2. PRELIMINARY RESULTS

2.1. The Extension Operation

Given a graph G, denote by $\mathrm{ext}(G)$ the graph obtained by adding a leaf to each vertex of G. Refer to the graph $\mathrm{ext}(G)$ as the *extension* of G (see Fig. 1).

Lemma 1. *For every graph G and its extension* $\mathrm{ext}(G)$*, we have* $i(G) = xi(\mathrm{ext}(G))$.

Proof. Obviously, $\alpha(\mathrm{ext}(G)) = |V(G)|$. To a given set $I' \in I(G)$, add all elements of the vertex set $V(\mathrm{ext}(G)) \setminus V(G)$ whose neighbors do not occur in I'. Clearly, the so-obtained vertex set is a g.i.s. in G. Moreover, to different elements of $I(G)$ there correspond different elements of $XI(\mathrm{ext}(G))$. Conversely, removing all elements of $V(\mathrm{ext}(G)) \setminus V(G)$ from an element of the set $XI(\mathrm{ext}(G))$, we obtain a g.i.s. of G. Thus, there is a bijection between $I(G)$ and $XI(\mathrm{ext}(G))$. This implies Lemma 1. □

2.2. The Spread Operation

Two leaves are called *duplicate leaves* if they have a common neighbor. Refer as a *collection of duplicate leaves* of a graph to the set of its duplicate leaves adjacent to some common vertex. Note that each such set contains at least two elements. Obviously, we have

Lemma 2. *If we remove all vertices but one from each collection of duplicate leaves from a graph G then the obtained graph* G' *satisfies* $xi(G) \leq xi(G')$.

Refer as an *offshoot* of a tree T to its subgraph consisting of a vertex of degree 2 and a leaf adjacent to it. We will denote the offshoot with leaf v and adjacent vertex u by uv. Refer as a *spread* of a tree T to a tree T' obtained by adjoining a new offshoot cd adjacent to a vertex a, where ab is an offshoot of T (see Fig. 2). A tree for which we can construct a spread (i.e., containing at most one offshoot) will be called *spreadable*.

Lemma 3. *If* T' *is a spread of a tree* T *then* $xi(T') > xi(T)$.

Proof. Suppose that a tree T' is obtained from T by adding an offshoot cd adjacent to a vertex a, where ab is an offshoot of T. Clearly, $xi(T') = xi_+(T', c) + xi_+(T', d)$. Moreover, $xi_+(T', d) = xi(T)$ and $xi_+(T', c) = xi_+(T, b)$. Since

$$xi_+(T, a) + xi_+(T, b) = xi(T), \qquad xi_+(T, b) \geq xi_+(T, a),$$

we have $xi_+(T, b) \geq 1$. Lemma 3 follows. □

Lemma 4. *Every (xi, d, n)-maximal tree is spreadable.*

Proof. Show that if a tree is not spreadable then it has at least two collections of duplicate leaves. Assume that a (xi, d, n)-maximal tree T is not spreadable and consider an arbitrary path of greatest length in it. Denote the ends of this path by u_1 and u_2 (they are leaves in T) and designate the adjacent vertices as v_1 and v_2 respectively. Since T is (xi, d, n)-maximal, we have $v_1 \neq v_2$. All neighbors but one of each of the vertices v_1, v_2 are leaves. Since T is not spreadable, we have $\deg(v_1) \geq 3$ and $\deg(v_2) \geq 3$. Let $m \triangleq \min(\deg(v_1), \deg(v_2))$. Then, removing $m - 2$ leaves adjacent to v_1 and v_2, we obtain a spreadable tree T', and also $xi(T') \geq xi(T)$ by Lemma 2. Applying the spread operation to T' $m - 2$ times consecutively, we obtain a tree T''; moreover,

$$|V(T'')| = |V(T)|, \qquad xi(T'') > xi(T') \geq xi(T)$$

(by Lemma 3), which contradicts the (xi, d, n)-maximality of T. Lemma 4 is proved. □

Lemma 5. *For every $d \geq 3$, the sequences $xi_d(2k)$ and $xi_d(2k + 1)$ grow strictly monotonely.*

Proof. Suppose that we have a (xi, d, n)-maximal tree T that is spreadable by Lemma 4. Denote by T' an arbitrary spread of a tree T. Then Lemma 3 yields the double inequality

$$xi_d(n + 2) \geq xi(T') > xi(T) = xi_d(n).$$

Lemma 5 is proved. □

Corollary 1. *Every (xi, d, n)-maximal tree contains at most one collection of duplicate leaves, and this collection contains exactly two elements.*

3. PROPERTIES OF (xi, d, n)-MAXIMAL TREES

3.1. Absence of Fixed Vertices

Refer to a vertex v in a tree T as *xi_+-fixed* if it occurs in every its g.i.s.; i.e., if $xi_+(T, v) = xi(T)$. Call a vertex u in a tree T *xi_--fixed* if it occurs in none of its g.i.s.; i.e., if $xi_-(T, u) = xi(T)$. Obviously, all neighbors of a xi_+-fixed vertex are xi_--fixed. A path with $2m + 1$ vertices ($m \geq 1$) in a tree will be called a *xi-alternating chain* if it begins and ends in a xi_+-fixed leaf and also xi_+-fixed vertices alternate in it with xi_--fixed vertices.

It is not hard that, in every tree, duplicate leaves are always xi_+-fixed vertices. If each vertex in a tree is either xi_+-fixed or xi_--fixed then it contains a unique g.i.s. It is intuitively clear that the trees with maximal number of g.i.s. must contain as few such vertices as possible. Namely, the following assertions hold: Each $(xi, d, 2k)$-maximal tree does not contain xi_+-fixed vertices, and each $(xi, d, 2k + 1)$-maximal tree contains exactly two xi_+-fixed vertices—a pair of duplicate leaves. The proofs of these propositions will be given below.

Lemma 6. *Every odd tree contains a xi_+-fixed leaf.*

Proof. Prove the assertion by induction on the size of the tree $n = 2k + 1$. The induction base $k = 0$ is obvious. Suppose that the assertion holds for some tree of size $2k + 1$. Consider any tree T of size $2k + 3$. If it contains duplicate leaves then there is nothing to prove. Otherwise, it contains an offshoot uv, where the vertex u is adjacent to some subtree T' of size $2k + 1$, which, by the induction assumption, contains some xi_+-fixed leaf z. In T, the vertex z is either a leaf or is adjacent to the offshoot uv. In both cases, this vertex is xi_+-fixed since each i.s. of T not containing z contains less than $\alpha(T) = \alpha(T') + 1$ vertices and is not greatest. If z is not a leaf of T then it contains a xi_+-fixed leaf. If z is adjacent to u then v is the xi_+-fixed leaf. Lemma 6 is proved. □

Lemma 7. *In every tree with some xi_+-fixed vertex, there is a xi-alternating chain containing this vertex.*

Proof. Suppose that a tree T contains some xi_+-fixed vertex v. Consider the set of its neighbors $\{u_1, u_2, \dots, u_k\}$, which, obviously, are xi_--fixed vertices and show that each of them is adjacent to at least one more xi_+-fixed vertex. Assume that all neighbors of u_1 but v are not xi_+-fixed. Since T is a tree, there exists $I \in XI(T)$ containing exactly one neighbor of u_1, the vertex v. Consider the set $(I \setminus \{v\}) \cup \{u_1\}$ and again obtain a g.i.s. of T. Hence, there exists some xi_+-fixed vertex v_1 different from v and adjacent to u_1.

If v_1 is not a leaf then consider its neighbor v' different from u_1 and, arguing by analogy, verify that this vertex is adjacent to a xi_+-fixed vertex v_2 different from v_1. Continuing these arguments, we will sooner or later show the existence of a xi_+-fixed leaf. If the initial vertex v is also a leaf then the lemma is proved. If not then, considering its one more neighbor u_2 and conducting analogous arguments, show the existence of a second xi_+-fixed leaf. Lemma 7 is proved. □

Lemma 8. *If some (xi, d, n)-maximal tree T contains a xi-alternating chain then it does not contain xi_+-fixed vertices outside this chain.*

Proof. Suppose that we have a chain $P \triangleq (z_1, \dots, z_{2k+1})$ and one of the inclusion maximal subtrees adjacent to the vertices of the chain and not containing its vertices contains a xi_+-fixed vertex u. Then, by Lemma 7, there exists a xi-alternating chain passing through u, and hence there exists a xi_+-fixed leaf w outside P. Remove from the chain the vertex z_1 and adjoin it to w. Denote the new tree by T'. Show that, in result of our actions, the number of g.i.s. increased.

It is not hard to see that $\alpha(T') = \alpha(T) - 1$. Thus, every i.s. of T' containing $\alpha(T) - 1$ vertices is the greatest. Construct a mapping

$$F\colon XI(T) \to XI(T')$$

taking the g.i.s. I of T into the g.i.s. $I \setminus \{w\}$ of T'. The mapping is clearly injective. Moreover, for some $I' \in XI(T')$, we have $w \in I'$. Therefore, I' does coincides with no $F(I), I \in XI(T)$. Then

$$xi(T') > xi(T);$$

a contradiction. Lemma 8 is proved. □

Lemma 9. *Every (xi, d, n)-maximal tree does not contain xi-alternating chains of length four or more.*

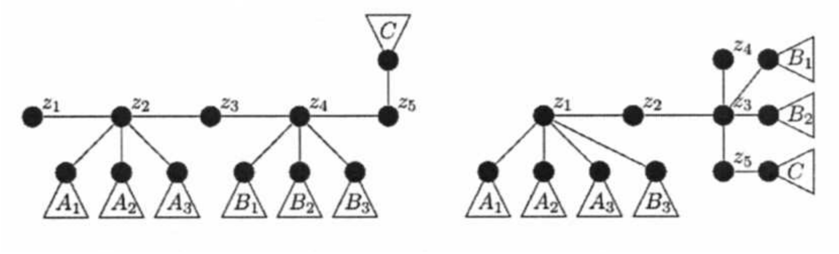

Fig. 3. An example of a transformation in the case of $d = 5$.

Proof. Suppose that some (xi, d, n)-maximal tree T contains a xi-alternating chain P of length at least four. Consider its initial part $(z_1, z_2, z_3, z_4, z_5)$. The vertex z_1 is a leaf of T. Recall that, in the proof of Lemma 7, it was shown that, in every tree with at least two vertices, every neighbor b of an arbitrary xi_+-fixed vertex a has a xi_+-fixed neighbor $c_b \neq a$. Then $\deg(z_3) = 2$ and $\deg(z_5) = 2$ (if the length of P is at least five) by Lemma 8. Denote by C an inclusion maximal subtree in T adjacent to z_5 and not containing z_4. The vertices z_2 and z_4 are adjacent to more than $d - 2$ inclusion maximal subtrees not containing the vertices z_1–z_5 each, which we will denote by A_i and B_j respectively (Fig. 3).

Remove from T the edge z_4z_5 and add the edge z_3z_5. Adjoin all subtrees A_i to the vertex z_1 and all subtrees B_j, to the vertex z_3. If the degree of z_3 exceeds d then adjoin one of the subtrees to z_1.

It is not hard that the degrees of all vertices in the obtained tree T' are at most d. Recall that the vertices z_1, z_3, and z_5 in T are xi_+-fixed. Therefore, each its g.i.s. I is representable as

$$I = \{z_1, z_3, z_5\} \cup I_A \cup I_B \cup I_C,$$

where

$$I_C \triangleq I \cap (V(C) \setminus \{z_6\}), \qquad I_A \triangleq I \cap \bigcup_i V(A_i), \qquad I_B \triangleq I \cap \bigcup_j V(B_j).$$

Denote by T'' the subtree in T' generated by the vertices $z_1, \dots, z_5$. Clearly, $\alpha(T'') = 3$ and each its g.i.s. contains z_5. Moreover,

$$|\{z_2, z_4, z_5\}| + |I_A| + |I_B| + |I_C| \leq \alpha(T') \leq \alpha(T'') + |I_A| + |I_B| + |I_C|;$$

therefore, $\alpha(T') = \alpha(T)$. Suppose that a mapping $F\colon XI(T) \to XI(T')$ takes the g.i.s.

$$\{z_1, z_3, z_5\} \cup I_A \cup I_B \cup I_C$$

of the tree T to the g.i.s. $\{z_2, z_4, z_5\} \cup I_A \cup I_B \cup I_C$ of T'. Moreover, there exists at least one g.i.s. in T' containing the vertices z_1, z_4, and z_5 since the subtrees A_i and B_j of T do not contain xi_+-fixed vertices by Lemma 8. Thus, $xi(T') > xi(T)$; a contradiction. Lemma 9 is proved. $\square$

Lemmas 7 and 9 imply that each xi_+-fixed leaf of every (xi, d, n)-maximal tree belongs to a xi-alternating chain of length two. Hence, the other end of the chain is the duplicate of this leaf.

Corollary 2. *Each xi_+-fixed leaf of every (xi, d, n)-maximal tree has a duplicate leaf.*

Theorem 1. *The following assertions hold:*

(A) *Every $(xi, d, 2k + 1)$-maximal tree contains exactly two xi_+-fixed vertices—a pair of duplicate leaves.*

(B) *Every $(xi, d, 2k)$-maximal tree does not contain xi_+-fixed vertices.*

Proof. (A) By Lemma 6, each $(xi, d, 2k+1)$-maximal tree contains a xi_+-fixed leaf, which, by Corollary 2, has a duplicate leaf. Hence, by Corollary 1, the corresponding collection contains exactly two duplicate leaves. These leaves are the ends of a xi-alternating chain of three vertices, outside which, by Lemma 8, there are no other xi_+-fixed vertices.

(B) If a $(xi, d, 2k)$-maximal tree contains xi_+-fixed vertices then, by Lemma 7, it also contains xi_+-fixed leaves. By Lemma 8 and Corollaries 1 and 2, the tree contains a unique pair of duplicate leaves. Then there exists a tree of size $2k-1$ containing at least the same number of g.i.s.; i.e., $xi_d(2k-1) \geq xi_d(2k)$. On the other hand, a $(xi, d, 2k+1)$-maximal tree also contains a pair of duplicate leaves (see (A)). Hence, we have the double inequality

$$xi_d(2k-1) \geq xi_d(2k) \geq xi_d(2k+1),$$

which contradicts Lemma 5. Theorem 1 is proved. □

3.2. Extendability of $(xi, d, 2k)$-Maximal Trees

Prove the most important property of $(xi, d, 2k)$-maximal trees, which enables us to reduce our problem to the problem for i.s. already solved in [3].

Lemma 10. *The vertices of every tree of size $2k$ not containing xi_+-fixed vertices can be uniquely partitioned into k pairs $A_1, \dots, A_k$ of adjacent vertices so that every g.i.s. of the tree contain exactly one vertex from each pair.*

Proof. We carry out the proof by unduction on the size of the tree.

The induction base $k = 1$ is obvious. Suppose that T is arbitrary tree without xi_+-fixed vertices of size $2k$ and the lemma holds for every tree of size $2k-2$. The tree T contains no duplicate leaves (otherwise they would be xi_+-fixed vertices). Consequently, it contains some offshoot uv. Denote by T' the result of the removal of the vertices u and v from T. Clearly, $\alpha(T') = \alpha(T) - 1$ and each g.i.s. in T contains either v or u; moreover, there exist g.i.s. of the tree T of both types; otherwise, u or v would be a xi_+-fixed point. Therefore, no neighbor of u is a xi_+-fixed vertex in T'. Obviously, no other vertex in T' is xi_+-fixed. By the induction hypothesis, $V(T')$ can be partitioned into pairs $A_1, \dots, A_{k-1}$ in a unique way. Putting $A_k = \{u, v\}$, we obtain a desired partition, which is also unique. Lemma 10 is proved. □

Throughout the rest of the present section, by a vertex pair we mean one of the pairs with the property of the statement of Lemma 10.

Lemma 11. *For every offshoot uv of an arbitrary tree T, there holds $xi_-(T, u) \geq xi(T)/2$.*

Proof. Since each g.i.s. of T contains exactly one of the vertices u and v, we have

$$xi_-(T, u) + xi_-(T, v) = xi(T).$$

Clearly,

$$xi_-(T, u) + xi_+(T, u) = xi_-(T, v) + xi_+(T, v) = xi(T).$$

Since v is a leaf vertex, $xi_+(T, v) \geq xi_+(T, u)$. Hence,

$$xi_-(T, u) \geq xi_-(T, v),$$

which implies the lemma. □

Suppose that T is an arbitrary $(xi, d, 2k)$-maximal tree. Then, by Theorem 1, it does not contain xi_+-fixed vertices. Let $\{u, v\}$ be a vertex pair of T. Denote by $A_1, \dots, A_l$ all inclusion maximal subtrees adjacent to u and not containing v and designate as $B_1, \dots, B_r$ all inclusion maximal subtrees adjacent to v and not containing u. Since $\{u, v\}$ is a pair, by Lemma 10, each of the trees $A_1, \dots, A_l, B_1, \dots, B_r$ is even. Each of them contains no duplicate leaves; otherwise, T would contain duplicate leaves, which would have to be its xi_+-fixed vertices. Therefore, each of them must contain an offshoot.

For a tree T^*, denote by r_{T^*} its root and denote by $p(T^*)$ the quantity

$$\frac{xi(T^* \setminus \{r_{T^*}\})}{xi(T^*)}.$$

Define the following quantities:

$$a \triangleq \prod_{i=1}^{l} xi(A_i), \qquad a_0 \triangleq \prod_{i=1}^{l} xi(A_i \setminus \{r_{A_i}\}), \qquad p(a) \triangleq \prod_{i=1}^{l} \frac{xi(A_i \setminus \{r_{A_i}\})}{xi(A_i)} = \prod_{i=1}^{l} p(A_i),$$

$$b \triangleq \prod_{i=1}^{r} xi(B_i), \qquad b_0 \triangleq \prod_{i=1}^{r} xi(B_i \setminus \{r_{B_i}\}), \qquad p(b) \triangleq \prod_{i=1}^{r} \frac{xi(B_i \setminus \{r_{B_i}\})}{xi(B_i)} = \prod_{i=1}^{r} p(B_i).$$

Since each g.i.s. of T contains only one of the vertices u and v, we have

$$xi(T) = a_0 \cdot b + a \cdot b_0.$$

Thus, $p(a) > 0$ and $p(b) > 0$; otherwise, u or v is a xi_+-fixed vertex of T. Assume without loss of generality that $p(a) \geq p(b)$. The tree A constituted by the vertex u and the vertices of the even trees $A_1, \dots, A_l$ is odd. By Lemma 6, A contains a xi_+-fixed leaf. If $p(a) = 1$ then it must be a xi_+-fixed leaf of T; therefore, $p(a) < 1$. By analogy, $p(b) < 1$. Refer to a subtree A_i as *suitable* if $p(A_i) < 1$. Obviously, there is a suitable subtree among $A_1, \dots, A_l$.

Theorem 2. *The tree T is an extension of some tree of size k.*

Proof. Show that each of the k pairs contains a leaf of T. This will imply the theorem. Suppose that both vertices in the pair $\{u, v\}$ are nonleaf vertices.

Denote by X one of the suitable trees. An arbitrary inclusion maximal subtree adjacent to v and not containing u will be denoted by Y. The remaining subtrees adjacent to u or to v are again denoted by $A_1, \dots, A_l$ and $B_1, \dots, B_r$, where $l \geq 0$ and $r \geq 0$. For $A_1, \dots, A_l$ and $B_1, \dots, B_r$, the notations a, b, a_0, b_0, $p(a)$, and $p(b)$ have the same sense as above. Introduce the notations

$$x \triangleq xi(X), \qquad y \triangleq xi(Y), \qquad x_0 \triangleq xi(X \setminus \{r_X\}), \qquad y_0 \triangleq xi(Y \setminus \{r_Y\}).$$

It is easy to see that

$$xi(T) = b \cdot y \cdot a_0 \cdot x_0 + a \cdot x \cdot b_0 \cdot y_0.$$

Consider the tree T' obtained from T by removing the subtree X and attaching it to some offshoot wt of the subtree Y (Fig. 4).

Let $y^+ \triangleq xi_+(Y, w)$ and $y^- \triangleq xi_-(Y, w)$. Denote by y_0^+ the number of the g.i.s. in Y simultaneously containing the vertex w and not containing r_Y. Denote by y_0^- the number of g.i.s. in Y simultaneously not containing w and r_Y.

Show that $xi(T') > xi(T)$. It is not hard to check that

$$xi(T') = a_0 \cdot b \cdot (y^+ \cdot x_0 + y^- \cdot x) + a \cdot b_0 \cdot (y_0^+ \cdot x_0 + y_0^- \cdot x).$$

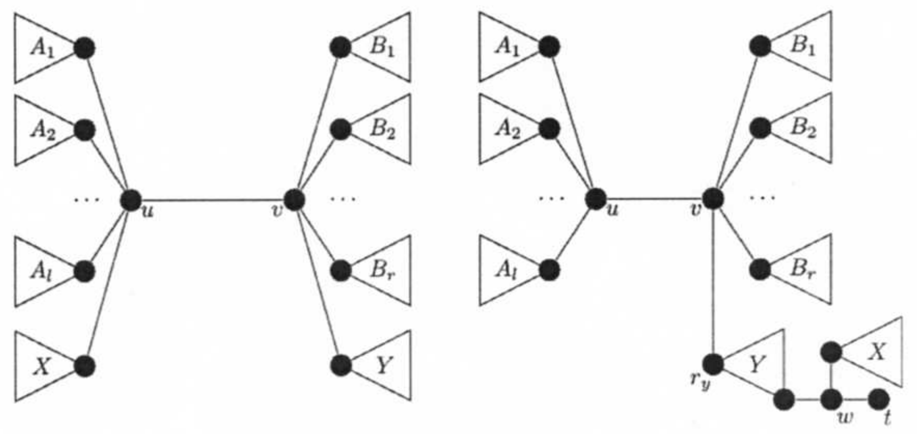

Fig. 4. Displacement of the subtree X.

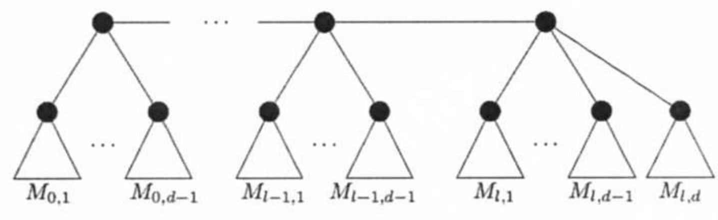

Fig. 5. The structure of the tree $T_{d+1,n}$.

Then

$$xi(T') - xi(T) = a_0 \cdot b \cdot y^- \cdot (x - x_0) - a \cdot b_0 \cdot y_0^+ \cdot (x - x_0)$$
$$= (x - x_0) \cdot (a_0 \cdot b \cdot y^- - a \cdot b_0 \cdot y_0^+).$$

Since X is suitable, $x > x_0$. Since $p(a) \geq p(b)$, we have $a_0 \cdot b \geq b_0 \cdot a > 0$. By Lemma 11, $y^- \geq 1/2$. By analogy with the proof of Lemma 11, we can show that $y_0^+ \leq y_0/2$. Since $p(Y) > 0$, we have $y_0^+ < 1/2$. Hence, $xi(T') > xi(T)$; a contradiction. Theorem 2 is proved. □

4. THE STRUCTURE OF (xi, d, n)-MAXIMAL TREES

4.1. The Even Case

Denote the complete d-ary tree of height $h - 1$ by $C_{d,h}$. In particular, $C_{d,0}$ is the empty tree, and $C_{d,1}$ consists of a single vertex for arbitrary d. The following assertion was proved in [3]:

Theorem 3. *For every $d \geq 2$ and $n \geq 1$, there exists a unique $(i, d+1, n)$-maximal tree $T_{d+1,n}$ which is representable in the form given in Fig. 5, where $M_{k,1}, \dots, M_{k,d-1} \in \{C_{d,k}, C_{d,k+2}\}$ for $0 \leq k \leq l - 1$ and either $M_{l,1} = \dots = M_{l,d} = C_{d,l-1}$ or $M_{l,1} = \dots = M_{l,d} = C_{d,l}$ or*

$$M_{l,1}, \dots, M_{l,d} \in \{C_{d,l}, C_{d,l+1}, C_{d,l+2}\},$$

where at least two of the subtrees $M_{l,1}, \dots, M_{l,d}$ are equal to $C_{d,l+1}$.

Theorem 4. *There exists a unique $(xi, d, 2k)$-maximal tree. It is isomorphic to the tree* $\mathrm{ext}(T_{d-1,k})$.

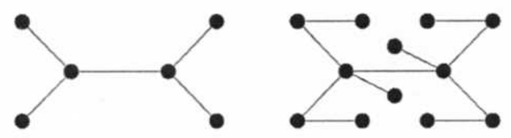

Fig. 6. The trees $T_{3,6}$ and $\mathrm{ext}(T_{3,6})$.

Proof. By Theorem 2, every $(xi, d, 2k)$-maximal tree is an extension of some tree of maximal degree $d-1$ on k vertices. But then $xi_d(2k) = i_{d-1}(k)$ by Lemma 1. Hence, every $(xi, d, 2k)$-maximal tree is isomorphic to $\mathrm{ext}(T_{d-1,k})$ by Theorem 3. □

Fig. 6 contains a $(xi, 4, 12)$-maximal tree obtained from a $(i, 3, 6)$-maximal tree.

4.2. The Odd Case

Lemma 12. *Every $(xi, d, 2k+1)$-maximal tree T satisfies*

$$xi(T) = \prod_{i=1}^{d'} xi(T_i),$$

where the tree T_i is $(xi, d, 2k_i)$-maximal and

$$\sum_{i=1}^{d'} k_i = k - 1, \qquad d' \le d - 2.$$

Proof. By Theorem 1, T contains xi_+-fixed duplicate leaves u and v and also their common xi_--fixed neighbor w. Then w is adjacent to $d' \le d-2$ inclusion maximal subtrees $T_1, \dots, T_{d'}$ each of which contains neither v nor u. Then

$$xi(T) = \prod_{i=1}^{d'} xi(T_i).$$

By Theorem 1, T contains exactly two xi_+-fixed vertices and exactly one xi_--fixed vertex, and all subtrees $T_1, \dots, T_{d'}$ are even. Since T is $(xi, d, 2k+1)$-maximal, each of the subtrees $T_1, \dots, T_{d'}$ is $(xi, d, 2k_i)$-maximal. Lemma 12 is proved. □

By Theorem 4 and Lemma 12, we have

$$\bigcup_{i=1}^{d'} T_i = \mathrm{ext}(F),$$

where F is a forest of size $k-1$ of maximal degree $d-1$. Thus, the problem of the maximization of the number of g.i.s. in a tree of size $2k+1$ of maximal degree d is reduced to the problem of maximizing the number of all i.s. in a forest of size $k-1$ consisting of more than $d-2$ connected components of maximal degree $d-1$ each.

Let T_1 and T_2 be the trees each of which has at least two vertices. Refer as the *splice* of T_1 and T_2 to the tree T obtained by identifying some leaf of T_1 and some leaf of T_2.

Lemma 13. *Given arbitrary trees T_1 and T_2 consisting of more than one vertex and any their splice T, we have*

$$2i(T) > i(T_1) \cdot i(T_2).$$

Proof. Suppose that a leaf v of T_1 and a leaf u of T_2 are identified. Put

$$A \triangleq i_-(T_1, v), \qquad A' \triangleq i_+(T_1, v), \qquad B \triangleq i_-(T_2, u), \qquad B' \triangleq i_+(T_2, u).$$

Here $A > A'$ and $B > B'$ because each of the trees T_1 and T_2 consists of more than one vertex (recall that the empty set is also an i.s.). It is not hard to see that

$$i(T_1) \cdot i(T_2) = (A + A') \cdot (B + B'), \qquad 2i(T) = 2 \cdot A \cdot B + 2 \cdot A' \cdot B'.$$

Then

$$2i(T) - i(T_1) \cdot i(T_2) = 2 \cdot A \cdot B + 2 \cdot A' \cdot B' - A \cdot B - A' \cdot B - A \cdot B' - A' \cdot B'$$
$$= A \cdot B + A' \cdot B' - A' \cdot B - A \cdot B' = (A - A')(B - B') > 0.$$

Lemma 13 is proved. □

Lemma 14. *Among all forests of maximal degree d and size n consisting of at most $s \le n$ connected components, the maximal number of all i.s. is possessed by the forest*

$$(s-1)P_1 \cup T_{d,n-s+1}.$$

Proof. Suppose that there exists an optimal forest F containing two connected components T_1 and T_2 each of which differs from P_1. Construct a tree T as an arbitrary split of T_1 and T_2 and replace $T_1 \cup T_2$ by $P_1 \cup T$. Clearly,

$$i(P_1 \cup T) = 2i(T) \quad \text{and} \quad i(T_1 \cup T_2) = i(T_1) \cdot i(T_2).$$

Therefore, by Lemma 13, the new forest F' satisfies the inequality $i(F') > i(F)$; a contradiction to the optimality of the forest F.

Prove that, for every d' and n', there holds the inequality $2i(T_{d',n'}) > i(T_{d',n'+1})$. Since it implies that for every $s' < s$ we have

$$i((s-1)P_1 \cup T_{d,n-s+1}) > i((s'-1)P_1 \cup T_{d,n-s'+1}),$$

this is insufficient for proving the lemma. Let x be a leaf of the tree $T_{d',n'+1}$. Then

$$i_-(T_{d',n'+1}, x) > i_+(T_{d',n'+1}, x);$$

therefore, we have the inequality

$$i(T_{d',n'+1}) = i_-(T_{d',n'+1}, x) + i_+(T_{d',n'+1}, x) < 2i_-(T_{d',n'+1}, x) \le 2i(T_{d',n'}).$$

Lemma 14 is proved. □

Denote by S_p the graph obtained by subdividing $p-2$ edges of the graph $K_{1,p}$. Refer as a *d-build-up of a tree T* to a tree obtained by joining the central vertex of the graph S_{d-1} to some vertex of $\mathrm{ext}(T)$ of degree at most $d-1$.

Theorem 5. *If $k \ge d-1$ then the set of $(xi, d, 2k+1)$-maximal trees coincides with the set of all possible d-build-ups of the tree $T_{d-1,k-d+2}$. If $1 \le k < d-1$ then the only $(xi, d, 2k+1)$-maximal tree is S_{k+1}.*

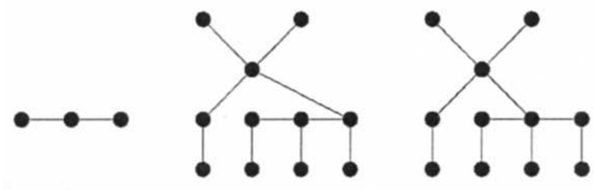

Fig. 7. The path P_3 and its two different 4-build-ups.

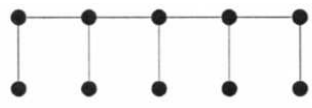

Fig. 8. The graph R_5.

Proof. By Lemma 14, the forest

$$F \triangleq (d-3)P_1 \cup T_{d-1,k-d+2}$$

has the maximal number of i.s. among all forests of maxial degree $d-1$ of size $k-1$ and at most $d-2$ connected components. But then

$$\bigcup_{i=1}^{d-2} T_i = \mathrm{ext}(F)$$

(in the notations of the proof of Lemma 12). Removing the central vertex and its two adjacent leaves of S_{d-1} from an arbitrary d-build-up of the tree $T_{d-1,k-d+2}$, we obtain exactly the forest $\mathrm{ext}(F)$. This implies the theorem for $k \geq d-1$.

The validity of the assertion for $1 \leq k < d-1$ stems from Lemmas 12–14.

Theorem 5 is proved. □

Thus, a $(xi, d, 2k+1)$-maximal tree can be nonunique. In Fig. 7, we consider the case of $d = 4$, $k = 5$, and two 4-build-ups of the optimal forest $T_{3,3} = P_3$.

4.3. The Case of $d = 3$

For $d = 3$, the structure of extremal trees is rather simple and it is possible to enumerate them completely. Therefore, in our opinion, this case deserves a separate consideration. Introduce the renotation $R_k \triangleq \mathrm{ext}(P_k)$ (Fig. 8).

Lemma 15. *The following hold:*

(1) *There exists a unique $(xi, 3, 2k)$-maximal tree, and it is isomorphic to R_k.*

(2) *Given $k \geq 3$, there exist exactly $\lceil (k-1)/2 \rceil + 1$ pairwise nonisomorphic $(xi, 3, 2k+1)$-maximal trees.*

Proof. By Theorem 4, every $(xi, 3, 2k)$-maximal tree is isomorphic to the graph

$$\mathrm{ext}(T_{2,k}) = \mathrm{ext}(P_k) = R_k.$$

Theorem 5 implies that each $(xi, 3, 2k+1)$-maximal tree is obtained from R_{k-1} by adding a vertex x, two leaves adjacent to x, and an edge xy, where y is some vertex of the tree R_{k-1} of degree less than three. If $\deg(y) = 2$ then two possible candidates for y give isomorphic trees. If $\deg(y) = 1$ then the $k-1$ possible candidates for y partition into pairs according to the axisymmetry of R_{k-1}. Every such a pair generates its own $(xi, 3, 2k+1)$-maximal tree. Lemma 15 is proved. □

5. THE STRUCTURE OF $(xi, 4, n)$-MAXIMAL 2-CATERPILLARS

Lemma 15 implies that all $(xi, 3, n)$-maximal trees are 2-caterpillars. In this section, we completely describe all $(xi, 4, n)$-maximal 2-caterpillars. Let us first prove that all assertions analogous to Theorems 1 and 2 are also valid for the class of 2-caterpillars.

Lemma 16. *The following hold:*

(A) *Every $(xi, d, 2k+1)$-maximal 2-caterpillar contains exactly two xi_+-fixed vertices, i.e., a pair of duplicate leaves.*

(B) *Every $(xi, d, 2k)$-maximal 2-caterpillar does not contain xi_+-fixed vertices.*

Proof. It is not hard to check that all assertions of Section 2 are carried over unchanged also to the case of k-caterpillars for $k \geq 1$. Lemmas 6 and 7 are also carried over without changes.

Validate Lemma 8. Suppose that there exists a xi_+-fixed point outside a xi-alternating chain P. Hence, there also exists a xi_+-fixed leaf v outside P. If v is on the ridge or on the first level then adjoin the end of P to this leaf (similarly to the adjunction in the proof of Lemma 8) and obtain a 2-caterpillar with a greater number of g.i.s. If the leaf v is on the second level then consider a neighboring vertex u. If $\deg(u) = 2$ then, removing the offshoot uv, we obtain a 2-caterpillar with the same number of g.i.s. and the number of vertices less by two, which contradicts Corollary 1. Otherwise (when u is a neighborhodd of duplicate leaves) consider one of the ends of P, which we denote by w. The vertex w cannot be on the second level since otherwise it would be contained in some offshoot or there would exist two collections of duplicate leaves, which is impossible by Corollary 1. Attaching the leaf v to w, we obtain a 2-caterpillar with a greater number of g.i.s.

Let us now validate Lemma 9. Suppose that at least one end of a xi-alternating chain P' is on the second level. Then either its neighbor has degree two, which is impossible because then these two vertices could be removed without changing the number of g.i.s., or this leaf is a duplicate, but then the only xi-alternating chain in the tree has length 3, which was required. If both sides of P' are on the first level then it is easy to check that, after their removal, the number of g.i.s. remains the same, which contradicts the (xi, d, n)-maximality of the 2-caterpillar. If at least one of the ends of P' is an end of the ridge then consider an initial segment of P' starting from it and apply the arguments of Lemma 9.

As is easy to check, the arguments of Theorem 1 are also carried over without change. Lemma 16 is proved. □

Lemma 17. *Every $(xi, d, 2k)$-maximal 2-caterpillar is an extension of some 1-caterpillar of size k of maximal degree $d-1$.*

Proof. Assume that there exists a pair of nonleaf vertices $\{u, v\}$ in some $(xi, d, 2k)$-maximal 2-caterpillar. Show that then they both lie on the ridge of the 2-caterpillar. Suppose the contrary; then u lies on the first level and v lies on the ridge. But then the neighbors of u lying on the second level have no pairs. Thus, both vertices u and v lie on the ridge.

Denote by X and Y some inclusion maximal subtrees with roots at neighbors of u and v, where X is suitable. After that act by analogy to Theorem 2. It is not hard to see that the resulting tree is also a 2-caterpillar since we can always choose an offshoot of Y lying on the ridge (if there is no such offshoot then the the tree contains duplicate leaves, which is impossible by the previous lemma).

Lemma 17 is proved. □

Denote by R'_k the graph obtained by adding a leaf to each vertex of degree two of the graph R_k (Fig. 9) and designate as R''_k the result of the addition of a leaf to one of its vertices of degree two. Denote by $R'_{k,s}$ the result of the removal of the vetex v_s from R'_k.

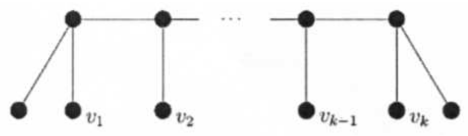

Fig. 9. The graph R'_k.

Lemma 18. *For each $k \geq 2$, the only $(i, 3, 2k+2)$-maximal 1-caterpillar is the tree R'_k. For each $k \geq 2$, the only $(i, 3, 2k+1)$-maximal 1-caterpillar is the tree $R'_{k,2}$.*

Proof. By Remark 4.2 in [3], every $(i, 3, n)$-maximal 1-caterpillar has at most one vertex of degree two. Therefore, every $(i, 3, n)$-maximal 1-caterpillar is isomorphic to one of the graphs R'_k, $R'_{k,s}$ for some k and $1 \leq s \leq \lceil k/2 \rceil$. Thus, the only $(i, 3, 2k+2)$-maximal 1-caterpillar is the tree R'_k.

Now, let $n = 2k+1$. Obviously, the equality

$$i(R'_k) = i_-(R'_k, v_s) + i_+(R'_k, v_s) = i(R'_{k,s}) + i(R''_{s-1}) \cdot i(R''_{k-s})$$

holds for all $3 \leq s \leq k$ (putting $i(R''_0) = 2$ and $i(R''_1) = 5$, we may assume it fulfilled also for $s \in \{1, 2\}$). Therefore,

$$\arg \max_{1 \leq s \leq k} i(R'_{k,s}) = \arg \min_{1 \leq s \leq \lceil k/2 \rceil} \big(i(R''_{s-1}) \cdot i(R''_{k-s}) \big).$$

Introduce $i_k \triangleq i(R''_k)$; then $i_k = 2i_{k-1} + 2i_{k-2}$ $(k \geq 2)$ and $i_0 = 2$, $i_1 = 5$. Put $\Phi_{k,s} \triangleq i_{s-1} \cdot i_{k-s}$. Prove by induction that

$$\arg \min_{1 \leq s \leq \lceil k/2 \rceil} \Phi_{k,s} = \{2\}.$$

This is not hard to check for all $2 \leq k \leq 5$. Suppose that $k \geq 6$ and for all $k' < k$ we have the equality

$$\arg \min_{1 \leq s \leq \lceil k'/2 \rceil} \Phi_{k',s} = \{2\}.$$

Using the equality $\Phi_{k,2} = 2\Phi_{k-1,2} + 2\Phi_{k-2,2}$ and the inequality

$$\min(a_1, b_1, c_1) + \min(a_2, b_2, c_2) \leq \min(a_1 + a_2, b_1 + b_2, c_1 + c_2),$$

valid for all its real arguments, we can easy validate the inequality $\Phi_{k,2} < \min(\Phi_{k,1}, \Phi_{k,3}, \Phi_{k,4})$ by induction. Assume from now on that $4 \leq s \leq \lceil k/2 \rceil$. Then $k - s - 1 \geq 2$.

We have

$$\Phi_{k,s} - \Phi_{k,s+1} = i_{s-1} \cdot i_{k-s} - i_s \cdot i_{k-s-1}$$
$$= i_{s-1} \cdot (2i_{k-s-1} + 2i_{k-s-2}) - (2i_{s-1} + 2i_{s-2}) \cdot i_{k-s-1} = 2(i_{s-1} \cdot i_{k-s-2} - i_{s-2} \cdot i_{k-s-1})$$
$$= 2((2i_{s-2} + 2i_{s-3}) \cdot i_{k-s-2} - i_{s-2} \cdot (2i_{k-s-2} + 2i_{i-s-3}))$$
$$= 4(i_{s-3} \cdot i_{k-s-2} - i_{s-2} \cdot i_{k-s-3}) = 4(\Phi_{k-4,s-2} - \Phi_{k-4,s-1}).$$

Thus, for $4 \le s' \le s \le \lceil k/2 \rceil$, we have

$$\Phi_{k,s'} - \Phi_{k,s} = 4(\Phi_{k-4,s'-2} - \Phi_{k-4,s-2}).$$

Putting $s' = 4$ and using the induiction assumption, we infer

$$\Phi_{k,4} - \Phi_{k,s} = 4(\Phi_{k-4,2} - \Phi_{k-4,s-2}) \le 0;$$

i.e., $\Phi_{k,4} \le \Phi_{k,s}$ for $s \ge 4$. This and $\Phi_{k,2} < \min(\Phi_{k,1}, \Phi_{k,3}, \Phi_{k,4})$ imply that

$$\arg \min_{1 \le s \le \lceil k/2 \rceil} \Phi_{k,s} = \{2\}.$$

Hence, the only $(i, 3, 2k + 1)$-maximal 1-caterpillar is the tree $R'_{k,2}$.

Lemma 18 is proved. □

Let $n \ge 5$. By Lemma 18, there exists a unique $(i, 3, n)$-maximal 1-caterpillar T^*_n that is isomorphic to the tree $R'_{n/2-1}$ for even n and to the tree $R'_{(n-1)/2,2}$ for odd n. There are exactly two nonisomorphic trees with four vertices, i.e., P_4 and $K_{1,3}$; moreover, $i(P_4) = 8$ and $i(K_{1,3}) = 9$. Therefore, put $T^*_4 \triangleq K_{1,3}$ and $T^*_n \triangleq P_n$ if $1 \le n \le 3$ and $T^*_0 \triangleq P_1$. By Lemma 17, there exists a unique $(xi, 4, 2k)$-maximal 2-caterpillar, and it is isomorphic to the tree $\mathrm{ext}(T^*_k)$. Using Lemma 16, by analogy with Lemmas 12–14 and Theorem 5, we can prove that every $(xi, 4, 2k + 1)$-maximal 2-caterpillar is a 4-build-up of T^*_{k-2}. Thus, we have

Theorem 6. *There exists a unique $(xi, 4, 2k)$-maximal 2-caterpillar, and it is isomorphic to the tree $\mathrm{ext}(T^*_k)$. Each $(xi, 4, 2k + 1)$-maximal 2-caterpillar is a 4-build-up of T^*_{k-2}.*

ACKNOWLEDGMENTS

The authors were supported by the Russian Science Foundation (Sections No. 2–4, project no. 17–11–01336), the Russian Foundation for Basic Research (Section 5, project no. 16–31–60008–mol-a-dk), and the Laboratory of Algorithms and Technologies for Networks Analysis of the National Research University Higher School of Economics.

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