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Bounds for the number of independent sets in some classes of graphs

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Contents

Introduction

Enumeration problems, related to counting the number of objects with given properties, have played an important role in combinatorics since its inception. Examples of such problems include estimating the number of integer solutions to systems of linear inequalities, counting the number of isomers of chemical compounds, and determining the number of graphs with certain properties. Another important class of combinatorial problems consists of extremal problems, related to describing the structure of objects from a given class that maximize or minimize certain parameters. As an example, one can cite Turán's famous theorem about the maximum number of edges in a graph that does not contain cliques of a given size. This dissertation addresses problems that lie at the intersection of these two areas of combinatorics. Upper and lower bounds are proved for the number of independent sets (that is, subsets of pairwise non-adjacent vertices) in graphs from various classes, and the structure of graphs that achieve these bounds is described.

Historical Background

The problem of enumerating independent sets in graphs has been studied since the middle of the last century and has become one of the classical areas in graph theory. This problem finds applications not only directly in mathematics (combinatorial number theory [17, 21], coding theory [14], theoretical computer science [26]), but also in other fields. For example, in theoretical chemistry, the parameter $i(G)$, equal to the number of independent sets in a graph G, is called the Merrifield-Simmons index [34], while the parameter $i'(G)$, equal to the number of independent sets in the line graph of G, is known as the Hosoya index [29]. Below is a brief review of works on the enumeration of independent sets.

The terminology used hereafter generally follows the book [13]. Only simple undirected graphs are considered below. A subset of pairwise non-adjacent vertices in a graph is called *independent*. By *maximal independent sets* (m.i.s.), we mean independent sets that are maximal with respect to inclusion. The maximum size of an independent set in a graph is called the *independence number* of the graph. We denote by $\alpha(G)$ the independence number of graph G, and by $n(G)$ — the number of vertices in G. We use $i(G)$ and $i_M(G)$ to denote the number of independent sets and the number of m.i.s. in G respectively. The notation $G' \simeq G''$ means that graphs G' and G'' are isomorphic.

Among the first works in the field of enumerating independent sets are papers [35] and [36], which independently proved the following fact.

Theorem 1 (R.E. Miller, D.E. Muller [35] and J.W. Moon, L. Moser [36]). *Let G be a graph on n vertices having the maximum number of m.i.s. among all n-vertex graphs. Then G is*

the union of $n/3$ copies of graph K_3 when $n \equiv 0 \pmod 3$,

the union of graph K_2 and $(n-2)/3$ copies of K_3 when $n \equiv 2 \pmod 3$,

the union of $(n-4)/3$ copies of graph K_3 and either graph K_4 or two graphs K_2 when $n \equiv 1 \pmod 3$.

The extremal graphs in theorem 1 are a special case of graphs $UK_{n,\alpha}$, defined as follows: $UK_{n,\alpha}$ is the union of $(\alpha \cdot (\lfloor n/\alpha \rfloor + 1) - n)$ cliques of size $\lfloor n/\alpha \rfloor$ and $(n - \alpha \cdot \lfloor n/\alpha \rfloor)$ cliques of size $\lceil n/\alpha \rceil$. One can verify that $n(UK_{n,\alpha}) = n$, $\alpha(UK_{n,\alpha}) = \alpha$.

Theorem 1 has been generalized in various directions by several authors. For example, C. Croitoru [25] considered the problem of upper-bounding the number of m.i.s. in the class of all graphs with a given independence number. J.M. Nielsen [37] obtained an achievable upper bound on the number of m.i.s. of a given size in graphs. In both of these problems, the maximum is achieved on the graph $UK_{n,\alpha}$. Such bounds are used to obtain estimates of running times for graph coloring algorithms and determining the size of maximum independent sets (see, for example, [26, 37]). This is enabled by the existence of algorithms that enumerate all m.i.s. in a graph in time proportional to the number of m.i.s. multiplied by a polynomial in the number of vertices of the graph [31, 43].

It is also interesting to obtain bounds on the number of m.i.s. in classes of graphs described in terms of forbidden subgraphs. M. Hujter and Z. Tuza [30] obtained a bound on the number of m.i.s. in triangle-free graphs (i.e., graphs not containing K_3 as a subgraph). In the work of V.E. Alekseev [1], the number of m.i.s. was studied in graphs that do not contain a "large" matching (union of K_2 graphs) as an induced subgraph.

Considerable attention has been paid to obtaining bounds on the number of independent sets in graphs with few cycles, primarily trees. In the work [40] of H. Prodinger and R.F. Tichy, upper and lower bounds were obtained for the number of independent sets in trees with a given number of vertices. Let ϕ_n denote the $(n+2)$-th Fibonacci number ($\phi_0 = 1$, $\phi_1 = 2$, $\phi_n = \phi_{n-1} + \phi_{n-2}$ for $n \geqslant 2$).

Theorem 2 (H. Prodinger, R. Tichy [40]). *Let T be a tree on n vertices. Then $\phi_n \leqslant i(T) \leqslant 2^{n-1}+1$, where equality $i(T)=\phi_n$ occurs only when T is a simple path, and equality $i(T)=2^{n-1}+1$ occurs only when T is a star.*

In the same paper, the number of independent sets in a cycle on n vertices was found. Apparently, the use of the term "Fibonacci number of a graph" as a synonym for the number of independent sets originates from Prodinger and Tichy's paper. In the work of S. Lin and C. Lin [33], trees were characterized whose number of independent sets differs by no more than 7 from the maximum possible value of $2^{n-1}+1$.

In the paper by H.S. Wilf [44], an upper bound was obtained for the number of maximal independent sets in trees with a given number of vertices:

Theorem 3 (H.S. Wilf [44]). *For any tree T on n vertices, the inequalities $i_M(T) \leqslant 2^{(n-1)/2}$ hold for odd n, and $i_M(T) \leqslant 1+2^{(n-2)/2}$ for even n.*

The original proof of theorem 3 was based on properties of partitions of natural numbers. B.E. Sagan in [41], using graph-theoretical reasoning, simplified the proof of theorem 3 and fully characterized the trees that achieve the upper bound. In paper [44], a question was posed about the number of m.i.s. in connected graphs with a given number of vertices. The answer was obtained in [28]. In work [42], Wilf's and Moon-Moser's theorems were simultaneously generalized by considering the class of connected graphs with a given number of cycles. For each fixed n and r, graphs achieving the maximum number of m.i.s. in the class of all connected n-vertex graphs with r cycles were identified in [42].

For further exposition, let us introduce several definitions. Let $U=\{u_1, \ldots, u_{d-1}\}$, $V=\{v_1, \ldots, v_p\}$, $W=\{w_1, \ldots, w_q\}$. Denote by $B_{d,p,q}$ a tree on the vertex set $U \cup V \cup W$, such that its subtrees induced by the sets $\{u_1\} \cup V$, $\{u_{d-1}\} \cup W$ and U represent stars $K_{1,p}$, $K_{1,q}$ and path P_{d-1} respectively. Note that $B_{d,1,1}$ is simply a path of length d. P.D. Vestergaard and A.S. Pedersen obtained the following upper bound on the number of independent sets in trees of given diameter:

Theorem (P.D. Vestergaard, A.S. Pedersen [39]). *For any n-vertex tree T of diameter d, the inequality $i(T) \leqslant i(B_{d,n-d,1})$ holds, with equality only when $T \simeq B_{d,n-d,1}$.*

In the same work [39], a question was posed about lower bounds on the number of independent sets in trees of given diameter. For trees of diameter 4, an exhaustive answer was given in work [27] (the theorem formulation is given in section 1.1). Also in work [27], the structure of extremal trees of diameter 5 was described for sufficiently large n. The Vestergaard problem (complete description of extremal trees for arbitrary given number of vertices and diameter) remains unsolved in the general case.

An important direction is obtaining asymptotic bounds on the number of independent sets in parametric classes of graphs. These include Hasse diagrams of partially ordered sets, planar rectangular lattices, and others. In work [14], A.D. Korshunov and A.A. Sapozhenko obtained the asymptotics for the number of independent sets in the graph of an n-dimensional Boolean cube (in the original, the result was formulated in terms of the number of binary codes with distance 2).

Theorem (A.D. Korshunov, A.A. Sapozhenko [14]). *For the graph of an n-dimensional Boolean cube B^n, the following asymptotics holds:*

$$i(B^n) \sim 2\sqrt{e}2^{2^{n-1}}.$$

For the number of independent sets in complete binary trees with n levels of edges, V.P. Voronin and E.V. Demakova obtained the following result.

Theorem 4 (V.P. Voronin, E.V. Demakova [2]). *Let ι_n denote the number of independent sets in a complete binary tree having k levels of edges. There exist constants β and γ such that as $n \to \infty$, the following asymptotics holds:*

$$\iota_n \sim \beta \cdot \gamma^{2^n}.$$

The question of asymptotics for the number of independent sets in planar rectangular grids — graphs $\Gamma_{m,n}$, defined by the relations $V(\Gamma_{m,n}) = \{1, \dots, m\} \times \{1, \dots, n\}$ and

$$E(\Gamma_{m,n}) = \{\{(i_1, j_1),\, (i_2, j_2)\} : \, |i_1 - i_2| + |j_1 - j_2| = 1\},$$

has also been actively studied. Among many works on this topic, we mention the paper by H. S. Wilf and N. Calkin [23], characterized by the application of the transfer matrix method, which proves the following

Theorem (H. S. Wilf, N. Calkin [23]). *There exists a double limit as $m, n \to \infty$*

$$i(\Gamma_{m,n})^{\frac{1}{mn}} \to \eta,$$

where $1.503 < \eta < 1.5035$.

Estimates of the number of independent sets in regular and "almost regular" graphs (that is, graphs where vertex degrees are either pairwise equal or lie within a relatively narrow range) are of significant interest. Some enumeration problems in number theory and group theory reduce to problems of this type. For example, the enumeration of sum-free sets (SFS) in abelian groups (that is, sets A such that $A \cap \{a+b \mid a, b \in A\} = \varnothing$) reduces to counting independent sets in Cayley graphs. This approach was used by N. Alon in [21] to obtain the asymptotics of the logarithm of the number of SFS in an interval of natural numbers. Later, also using graph theory, A.A. Sapozhenko [17] obtained the asymptotics of the number of SFS in an interval of natural numbers. The following estimate for the number of independent sets in regular graphs was a working tool in paper [21].

Theorem (N. Alon [21])**.** *For any k-regular graph G on n vertices, the number of independent sets $i(G)$ satisfies the inequality*

$$i(G) \leqslant 2^{\frac{n}{2}(1+f(k))}, \tag{1}$$

where $f(k) = O(k^{-0.1})$.

In the proof of this theorem, counting the number of independent sets in regular graphs was reduced to counting the number of independent sets in almost regular bipartite graphs. This possibility was provided by the following lemma.

Lemma 1 (N. Alon [21])**.** *For every k-regular n-vertex graph, there exists a spanning bipartite subgraph whose vertex degrees lie in the interval*

$$\left[k/2 - 2\sqrt{k \log_2 k},\ k/2 + 2\sqrt{k \log_2 k}\right].$$

Note that the problem of estimating the number of independent sets in bipartite graphs also arises in other circumstances, for example, in solving the Dedekind problem [19].

A.A. Sapozhenko proposed a simpler proof of estimate (1), while also improving the remainder term to $f(k) = O(\sqrt{k^{-1} \ln k})$ and extending the estimate to quasi-regular graphs [16].

In work [21], the following was proposed

Conjecture (N. Alon [21])**.** *Among k-regular graphs on n vertices where $2k \mid n$, the unique (up to isomorphism) graph that has the largest number of independent sets is one that represents the union of $\frac{n}{2k}$ disjoint complete bipartite graphs.*

The graph from the hypothesis formulation will be called the *Alon graph* hereafter.

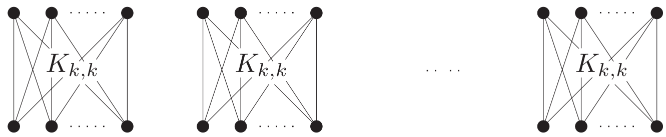

Figure 1. Alon graph

This hypothesis remains unproven to this day (April 2009), although most researchers do not doubt its validity. The truth of this hypothesis would imply, in particular, that in (1) there is an estimate $f(k) = O(k^{-1})$.

Using an information-theoretical approach, J. Kahn and A. Lawrenz in paper [32] obtained an achievable upper bound on the number of independent sets in bipartite regular graphs, which indirectly supports Alon's hypothesis.

Theorem 5 (J. Kahn, A. Lawrenz [32]). *Let G be a bipartite k-regular graph on n vertices. Then*

$$i(G) \leqslant (2^{k+1} - 1)^{\frac{n}{k}}.$$

Note that the question of uniqueness of the extremal graph in theorem 5 remains open to this day.

The question of the number of independent sets in graphs with known maximum independent set size is interesting. This is related to a fairly general approach in enumerative combinatorics, which can be called the *container method* [20]. The method is as follows. Let $\mathcal{A}$ and $\mathcal{B}$ be families of subsets of some set. We say that family $\mathcal{B}$ is a *system of containers* for $\mathcal{A}$ if for each $A \in \mathcal{A}$ there exists $B \in \mathcal{B}$ such that $A \subseteq B$. Then, obviously, the inequality holds

$$|\mathcal{A}| \leqslant \sum_{B \in \mathcal{B}} 2^{|B|}.$$

Such estimates, though seemingly crude at first glance, allow obtaining asymptotics with suitable choice of system $\mathcal{B}$. For example, this is how A.A. Sapozhenko obtained a solution to the Cameron-Erdős problem [17]. The question of applicability of the container method to the problem of estimating the number of independent sets in graphs is closely related to the above-mentioned problem of enumerating independent sets in graphs with fixed independence number, since the family of all m.i.s. of a graph is a system of containers for the family of all independent sets, and the independence number of a graph directly constrains the size of such containers.

In paper [1] the following was proved

Theorem 6 (V.E. Alekseev [1]). *For any graph G, the inequality holds*

$$i(G) \leqslant \left(\frac{n}{\alpha} + 1\right)^{\alpha}, \tag{2}$$

where $n = n(G)$, $\alpha = \alpha(G)$.

Inequality (2) was used in [1] to estimate the number of m.i.s. in graphs, and in work [18] — to obtain upper bounds on the number of independent sets in quasi-regular graphs with constraints on independence number and expanders. An achievable lower bound on the number of independent sets in graphs with fixed independence number was obtained in [38].

Brief Contents of the Dissertation

The dissertation consists of three chapters.

The first chapter is devoted to estimates of the number of independent sets in trees of fixed diameter. Section 1.1 introduces the key concept of graph *capacity* and provides several other definitions, proving auxiliary statements. Section 1.2 proves lower bounds on the number of independent sets in trees of diameter $6, 7, 8, 9$. In particular, the following theorems are proved:

Theorem (sect. 1.2, theorems 8, 9)**.** *Any tree of diameter* 6 *on* n *vertices contains at least* $35^{(n-1)/7}$ *independent sets. Any tree of diameter* 7 *on* n *vertices contains at least* $35^{(n-2)/7}$ *independent sets. Any tree of diameter* 8 *on* n *vertices contains at least* $35122^{(n-1)/21}$ *independent sets. Any tree of diameter* 9 *on* n *vertices contains at least* $35122^{(n-2)/21}$ *independent sets.*

Section 1.3 proves theorems characterizing the structure of extremal trees in the Vestergaard problem. A tree T is called (n, d)-minimal if it has the smallest number of independent sets among all trees of diameter d on n vertices. We denote by F_T the forest obtained from tree T by removing all central vertices.

Theorem (sect. 1.3, theorem 10)**.** *For any fixed* d*, there exists a finite set of trees* $\mathcal{M}_d$ *with the following property. For any* n *and any* (n, d)*-minimal tree* T*, each component of forest* F_T *is isomorphic to some tree from* $\mathcal{M}_d$*.*

Let T' denote a tree such that forest $F_{T'}$ is a matching on six vertices. Let T'' denote a tree of diameter 6 such that forest $F_{T''}$ is a union of four five-vertex paths.

Theorem (sect. 1.3, corollary from theorem 12)**.** *For* $d \in \{6, 7\}$ *and for all sufficiently large* n *of the form* $7k + d - 5$, $k \in \mathbb{N}$*, for any* (n, d)*-minimal tree* T*, all components of forest* F_T *are isomorphic to tree* T'*. For* $d \in \{8, 9\}$ *and for all* *sufficiently large n of the form $21k+d-7$, $k \in \mathbb{N}$, for any (n,d)-minimal tree T, all components of forest F_T are isomorphic to tree T''.*

Section 1.4 provides estimates of the number of independent sets in so-called radially regular trees, which are conjectured to be trees of minimal capacity.

Section 1.5 obtains a generalization of the Voronin-Demakova theorem to the case of q-ary trees for arbitrary q. Let $\iota_{q,\,k}$ denote the number of independent sets in a complete q-ary tree having k levels of edges, or equivalently, diameter $2k$. The following is proved

Theorem (sect. 1.5, theorem 15). *For $q \in \{2,3,4\}$, the following asymptotics holds for $\iota_{q,\,k}$ as $k \to \infty$:*

$$\iota_{q,\,k} \sim \beta_q \cdot \gamma_q^{q^k},$$

for some constants β_q and γ_q.

For $q \geqslant 5$, the following asymptotics holds as $k \to \infty$:

$$\begin{aligned} \iota_{q,\,2k} &\sim \alpha_{q,0} \cdot \gamma_q^{q^{2k}}, \\ \iota_{q,\,2k+1} &\sim \alpha_{q,1} \cdot \gamma_q^{q^{2k+1}}, \end{aligned}$$

where constants $\alpha_{q,0}$ and $\alpha_{q,1}$ satisfy the inequality $\alpha_{q,0} > \alpha_{q,1}$.

The different character of the asymptotics of $\iota_{q,\,k}$ for $q \leqslant 4$ and $q \geqslant 5$ deserves attention.

The results of the first chapter are published in [4, 8].

The second chapter of the dissertation is devoted to estimates of the number of maximal independent sets in graphs of given diameter. Section 2.1 introduces basic definitions and proves some auxiliary statements. Section 2.2 provides a complete description of graphs with given diameter that achieve the minimum number of m.i.s. Define the sequence ψ_n by the relation $\psi_n = \psi_{n-2} + \psi_{n-3}$ and initial conditions $\psi_0 = \psi_1 = 1$, $\psi_2 = 2$.

Theorem (sect. 2.2, theorem 16). *For any d, $d \geqslant 4$, and for any graph G of diameter d, the inequality $i_M(G) \geqslant \psi_{d+1}$ holds. If $i_M(G) = \psi_{d+1}$, then the set $V(G)$ can be partitioned into subsets $V_0, \ldots, V_d$, such that for any k, $2 \leqslant k \leqslant d$, and any i, $0 \leqslant i \leqslant d-k$, there are no edges in G between vertices from V_i and V_{i+k}, and for every i, $0 \leqslant i \leqslant d-1$, the subgraph of G induced by the set $V_i \cup V_{i+1}$ is complete bipartite with parts V_i and V_{i+1}.*

Section 2.3 provides a complete description of trees with given diameter and number of vertices that achieve the maximum number of m.i.s. This gives a substantial generalization of Wilf's [44] and Sagan's [41] theorems:

Theorem (sect. 2.3, theorem 17)**.** *For any n-vertex tree T of diameter d, the inequality $i_M(T) \leqslant M(n,d)$ holds, where*

$$M(n,d) = \begin{cases} \psi_{d-1} + (2^{(n-d+1)/2} - 1)\psi_{d-2}, & \text{for } d \geqslant 4,\ n-d = 2k+1,\ k \geqslant 0, \\ \psi_{d-2} + \psi_d, & \text{for } d \geqslant 4,\ n-d = 2, \\ 2^{(n-d)/2}\psi_{d-1}, & \text{for } d \geqslant 5,\ d \neq 7,\ n-d = 2k \geqslant 4, \\ 2^{(n-d)/2}\psi_{d-1} + 1, & \text{for } d \in \{4,7\},\ n-d = 2k \geqslant 4. \end{cases}$$

For $d \geqslant 9$ there exists a unique up to isomorphism tree on which this bound is achieved (see sect. 2.3 for complete description of extremal trees for all d).

The results of the second chapter are published in [9, 10, 11, 12].

The third chapter of the dissertation investigates the number of independent sets in graphs with given maximum independent set size. Inequality (2) becomes equality when $\alpha | n$ (the maximum number of independent sets is achieved on graph $UK_{n,\alpha}$). Theorem 18 proved in section 3.1 provides a refinement of estimate (2), making it achievable for all possible combinations of parameters n, α, and also describes the extremal graphs.

Theorem (sect. 3.1, theorem 18)**.** *For any graph G such that $n(G) = n$ and $\alpha(G) = \alpha$, the inequality $i(G) \leqslant i(UK_{n,\alpha})$ holds, becoming equality only for graphs isomorphic to $UK_{n,\alpha}$.*[1]

Section 3.2 provides estimates of the number of independent sets in trees and forests with given independence number.

Theorem (sect. 3.2, theorem 19)**.** *For any $n, \alpha\,(n \geqslant 2)$, among all trees on n vertices with independence number α, the maximum number of independent sets is*

[1] This theorem, as it turns out, is a special case of the following Erdős theorem (see, for example, Corollary VI.1.10 in B. Bollobás's book *Extremal graph theory*): for any p, α, n satisfying inequalities $2 \leqslant p \leqslant \alpha \leqslant n$, graph $UK_{n,\alpha}$ contains more independent sets of size p than any other (non-isomorphic to it) n-vertex graph with independence number α. See also the paper by Véronique Bruyére and Hadrien Mélot *Turán Graphs, Stability Number, and Fibonacci Index* in the collection *B. Yang, D.-Z. Du, and C.A. Wang (Eds.): Combinatorial Optimization and Applications: Second International Conference, COCOA 2008, LNCS 5165, pp. 127–138, 2008.*

achieved only by trees isomorphic to the tree obtained from star $K_{1,\alpha}$ *by subdividing* $(n-\alpha-1)$ *edges.*

Theorem (sect. 3.2, theorem 20)**.** *Among all forests on* n *vertices without isolated vertices with independence number* α*, the maximum number of independent sets is achieved only by forests that are unions of a matching on* $2(n-\alpha-1)$ *vertices and a star* $K_{1,2\alpha-n+1}$*.*

Section 3.3 is devoted to estimates of the number of independent sets in regular n-vertex graphs whose independence number is close to $n/2$ (that is, to the maximum possible).

Theorem (sect. 3.3, theorem 22)**.** *For arbitrarily large* K *and* N*, there exists a* k*-regular* n*-vertex graph* G *such that* $k > K$*,* $n > N$*, and*

$$\begin{aligned} \alpha(G) &< \frac{n}{2}\left(1-\Omega(k^{-1})\right), \\ \log_2(i(G)) &> \frac{n}{2}\left(1+\Omega(k^{-1})\right). \end{aligned}$$

On the other hand, for any constant $\theta \in (0, 1/2)$*, for any* k*-regular* n*-vertex graph* G *such that* $\alpha(G) < \frac{n}{2}(1-\Omega(k^{-\theta}))$*, the inequality holds*

$$\log_2(i(G)) < \frac{n}{2}(1-\Omega(k^{-\theta})).$$

Section 3.4 proves a generalization of theorem 5 to quasi-regular bipartite graphs:

Theorem (sect. 3.4, theorem 23)**.** *Let* G *be a bipartite graph with parts* A *and* B*. Let the degrees of vertices in* A *be bounded above by* k_2*, and the degrees of vertices in* B *be bounded below by* k_1*. Then*

$$i(G) \leqslant (2^{k_1}+2^{k_2}-1)^{\frac{|A|}{k_1}}.$$

The results of the third chapter are published in [3, 5, 6, 7].

Main Results of the Dissertation

1. For arbitrary d, the structure of (n, d)-minimal trees is described (theorems 10, 11, 12). As a consequence, asymptotically achievable lower bounds are obtained for the number of independent sets in trees of diameter 6, 7, 8, 9 (theorems 8, 9, 13).

2. An achievable lower bound is obtained for the number of maximal independent sets in graphs of fixed diameter, with a complete description of extremal graphs provided (theorem 16). An achievable upper bound is obtained for the number of maximal independent sets in trees of fixed diameter, with a complete description of extremal trees provided (theorem 17).
3. An achievable upper bound is obtained for the number of independent sets in graphs with given independence number, with a complete description of the graphs achieving this bound (theorem 18).
4. Estimates are obtained for the number of independent sets in regular graphs with independence number close to the maximum (theorem 22).

Chapter 1. Estimates of the Number of Independent Sets in Trees of Fixed Diameter

Lower bounds are proved for the number of independent sets in trees of diameter 6, 7, 8, 9. A description of the structure of extremal trees is provided for the general case.

The asymptotics of the number of independent sets in complete q-ary trees is established.

1.1 Basic Concepts

We denote by ∂v the set of all vertices adjacent to v. The sets of vertices and edges of graph G are denoted as $V(G)$ and $E(G)$ respectively. By $G \setminus S$ we denote the subgraph of graph G induced by the vertex set $V(G) \setminus S$. The union of graphs G' and G'' is a graph G such that $V(G) = V(G') \cup V(G'')$ and $E(G) = E(G') \cup E(G'')$ (notation: $G = G' \cup G''$). Hereafter, it is assumed that the vertex sets of graphs in the union do not intersect.

The *capacity* of graph G will be defined as the value

$$c(G) = (i(G))^{1/n(G)}.$$

The *length* of a path will mean the number of edges in it. The *distance* between vertices u and v of a graph is the smallest of the lengths of paths connecting these vertices (notation $\operatorname{dist}(u, v)$). The *diameter* of a connected graph G (notation $\operatorname{diam}(G)$) is the largest of the distances between vertices of G. The *eccentricity* of vertex v in graph G is the largest of the distances $\operatorname{dist}(v, u)$, where $u \in V(G)$. Any vertex of the graph having the smallest eccentricity is called the *center* of the graph. Let d, $n \in \mathbb{N}$, and let $d < n$. Any tree of diameter d on n vertices having the minimum (maximum) number of independent sets among all trees with given number of vertices and diameter will be called (n, d)*-minimal* (respectively, (n, d)*-maximal*).

For tree T, we denote by F_T the forest obtained by removing the central vertices from T. Let T be an arbitrary tree, and T' its subtree. Let $v \in V(T) \setminus V(T')$, $u \in V(T')$. We say that tree T' *adjoins* with vertex u to vertex v in T if $\{u, v\} \in E(T)$ and tree T' is a connected component of forest $T \setminus \{v\}$. For example, we can say that in any path of even diameter $2d$, exactly two paths of diameter $(d-1)$ adjoin to the central vertex with their end vertices. By P_t we denote a path on t vertices with a distinguished root vertex. In the case of $t \in \{4,5\}$, we consider the central vertex as the root, and for $t \in \{1,2,3\}$ — the end vertex.

By $T_{p,q,r}$ we denote such a rooted tree that exactly p, q and r paths on 3, 2 and 1 vertices respectively adjoin to its root v, where the paths on 3 vertices adjoin to v with their central vertices. Further, we write $T_{p,q}$ instead of $T_{p,q,0}$. One can verify that the following equalities hold

$$\begin{aligned} n(T_{p,q,r}) &= 3p+2q+r+1, \\ i(T_{p,q,r}) &= 5^p 3^q 2^r + 4^p 2^q. \end{aligned}$$

For natural d we define the value

$$\widehat{c}(d) = \inf_{\substack{T\text{-tree},\\ \operatorname{diam}(T)=d}} c(T). \tag{3}$$

Note that from theorem 2 and the well-known Binet formula for Fibonacci numbers it follows that

$$\lim_{d\to\infty} \widehat{c}(d) = \frac{1+\sqrt{5}}{2}.$$

Lemma 2. *For any graphs G_1, G_2, the inequality holds*

$$c(G_1 \cup G_2) \geqslant \min\{c(G_1),\, c(G_2)\}.$$

Proof. Let us show that for any positive numbers a, b, c, d, the inequality holds

$$(ab)^{1/(c+d)} \geqslant \min\{a^{1/c},\, b^{1/d}\}. \tag{4}$$

Without loss of generality, assume that $a^{1/c} \leqslant b^{1/d}$. Then $b \geqslant a^{d/c}$, whence $ab \geqslant a^{1+d/c}$. Raising both sides of the last inequality to the power of $1/(c+d)$, we get $(ab)^{1/(c+d)} \geqslant a^{1/c}$, which was required. We have

$$c(G_1 \cup G_2) = (i(G_1 \cup G_2))^{1/n(G_1 \cup G_2)} = (i(G_1)i(G_2))^{1/(n(G_1)+n(G_2))}.$$

It remains to apply inequality (4), setting $a = i(G')$, $b = i(G'')$, $c = n(G')$, and $d = n(G'')$. ☐

Lemma 3. *Let T be a tree of diameter d. Then if d is even (odd), each tree in forest F_T has diameter no greater than $d-2$ (respectively, $d-3$).*

Proof. Consider the case of even d; the reasoning for odd d is similar. Let T be a tree of diameter d, and let v be the unique central vertex in T. Let $u_1 \dots u_{d/2} v w_1 \dots w_{d/2}$ be a diametral path in T. Suppose that in F_T there is a connected component T' of diameter d', $d' > d-2$. Without loss of generality, we can assume that $V(T') \cap \{u_1, \dots, u_{d/2}\} = \varnothing$. Let s be a vertex of T' adjacent to v in T. If s' and s'' are the ends of any diametral path in T', then one of the paths $s' \dots s$ and $s'' \dots s$ contains no fewer than $\lfloor (d'+1)/2 \rfloor \geqslant d/2$ edges. Let this be path $s' \dots s$, then path $u_1 \dots u_{d/2} v s \dots s'$ in T contains no fewer than $(d+1)$ edges — a contradiction with $\operatorname{diam}(T) = d$. □

Lemma 4. *For any n, d such that $2 \leqslant d < n$, and any tree T of diameter d on n vertices, the inequality holds*

$$i(T) > \begin{cases} (\min_{m \leqslant d-2} \widehat{c}(m))^{n-1}, & \text{if } d \text{ is even} \\ (\min_{m \leqslant d-3} \widehat{c}(m))^{n-2}, & \text{if } d \text{ is odd} \end{cases}$$

Proof. Let T be a tree of even diameter d on n vertices. Let v be the center in T. By lemma 3, each tree from forest $F_T = T_n \setminus \{v\}$ has diameter no greater than $(d-2)$. Then, taking into account lemma 2, we have

$$i(T) > i(F) = (c(F))^{n-1} \geqslant \left(\min_{m \leqslant d-2} \widehat{c}(m) \right)^{n-1}.$$

The case of odd d is considered similarly. □

Lemma 5. *Let trees $T_1, \dots, T_k$ adjoin to vertex v in tree T with vertices $v_1, \dots, v_k$ respectively. Let trees $\widehat{T}_1, \dots, \widehat{T}_m$ be such that $V(T) \cap \bigcup_i V(\widehat{T}_i) = \varnothing$, and $V(\widehat{T}_i) \cap V(\widehat{T}_j) = \varnothing$ for $i \neq j$. Let $\widehat{T}$ be the tree obtained from T by removing subtrees $T_1, \dots, T_s$ and adding subtrees $\widehat{T}_1, \dots, \widehat{T}_m$ such that in $\widehat{T}$ trees $\widehat{T}_1, \dots, \widehat{T}_m$ adjoin to v with vertices $u_1, \dots, u_m$ respectively. Let the inequality hold*

$$i(\widehat{T}_1) \cdot \ldots \cdot i(\widehat{T}_m) < i(T_1) \cdot \ldots \cdot i(T_s).$$

1. *If*

$$i(\widehat{T}_1 \setminus \{u_1\}) \cdot \ldots \cdot i(\widehat{T}_m \setminus \{u_m\}) - i(T_1 \setminus \{v_1\}) \cdot \ldots \cdot i(T_s \setminus \{v_s\}) < \\ < i(T_1) \cdot \ldots \cdot i(T_s) - i(\widehat{T}_1) \cdot \ldots \cdot i(\widehat{T}_m),$$

then $i(\widehat{T}) < i(T)$.

2. *If*

$$i(\widehat{T}_1 \setminus \{u_1\}) \cdot \ldots \cdot i(\widehat{T}_m \setminus \{u_m\}) - i(T_1 \setminus \{v_1\}) \cdot \ldots \cdot i(T_s \setminus \{v_s\}) = \\ = i(T_1) \cdot \ldots \cdot i(T_s) - i(\widehat{T}_1) \cdot \ldots \cdot i(\widehat{T}_m)$$

and $s < k$, *then* $i(\widehat{T}) < i(T)$.

Proof. We have

$$\begin{aligned} & i(T) - i(\widehat{T}) = \\ & = i(T \setminus \{v\}) + i(T \setminus (\{v\} \cup \partial v)) - (i(\widehat{T} \setminus \{v\}) + i(\widehat{T} \setminus (\{v\} \cup \partial v))) = \\ & = i(T_1) \cdot \ldots \cdot i(T_k) + i(T_1 \setminus \{v_1\}) \cdot \ldots \cdot i(T_k \setminus \{v_k\}) - \\ & \qquad - i(\widehat{T}_1) \cdot \ldots i(\widehat{T}_m) \cdot i(T_{s+1}) \cdot \ldots \cdot i(T_k) - \\ & \quad - i(\widehat{T}_1 \setminus \{u_1\}) \cdot \ldots i(\widehat{T}_m \setminus \{u_m\}) \cdot i(T_{s+1} \setminus \{v_{s+1}\}) \cdot \ldots \cdot i(T_k \setminus \{v_k\}) = \\ & = \Big(i(T_1) \cdot \ldots \cdot i(T_s) - i(\widehat{T}_1) \cdot \ldots \cdot i(\widehat{T}_m) \Big) \cdot i(T_{s+1}) \cdot \ldots \cdot i(T_k) \times \\ & \quad \times \left(1 - \frac{i(T_{s+1} \setminus \{v_{s+1}\}) \cdot \ldots \cdot i(T_k \setminus \{v_k\})}{i(T_{s+1}) \cdot \ldots \cdot i(T_k)} \cdot \frac{i(\widehat{T}_1 \setminus \{u_1\}) \cdot \ldots \cdot i(\widehat{T}_m \setminus \{u_m\}) - i(T_1 \setminus \{v_1\}) \cdot \ldots \cdot i(T_s \setminus \{v_s\})}{i(T_1) \cdot \ldots \cdot i(T_s) - i(\widehat{T}_1) \cdot \ldots \cdot i(\widehat{T}_m)} \right). \end{aligned}$$

It is easy to see that under the conditions of the lemma, each of the factors in the last product is positive, from which the statement of the lemma follows. □

We will need two following statements from [27].

Lemma 6 (A. Frendrup et al. [27]). *Let tree* T *of diameter* d *have the minimum number of independent sets among trees of diameter* d *with the same number of vertices. Then no vertex in* T *is adjacent to more than two pendant vertices. If a vertex is adjacent to two pendant vertices, then each of them must lie on some diametral path in* T.

Theorem 7 (A. Frendrup et al. [27]). *Let* T_n *be a tree of diameter* 4 *on* n *vertices having the minimum number of independent sets among* n*-vertex trees of diameter* 4. *Then* $T_5 \simeq P_5$, $T_6 \simeq T_{0,2,1}$. *For* $n > 6$, $T_n \simeq T_{p,q}$, *where* $q = 2n + 1 \pmod 3$ *for* $n \geqslant 26$, *and for* $7 \leqslant n \leqslant 25$ *the value of* q *is determined from Table 1.*

n	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
q	3	2	4	3	5	4	6	5	4	3	5	4	3	2	4	3	2	1	3

Table 1. Values of q in theorem 7

1.2 Number of Independent Sets in Trees of Diameter 6..9

Lemma 7. *The equalities* $\widehat{c}(d) = \phi_{d+1}^{1/(d+1)}$ *hold for* $d \leqslant 3$*, and* $\widehat{c}(4) = 35^{1/7}$*. Among trees of diameter* 4*, only tree* $T_{0,3}$ *has capacity equal to* $\widehat{c}(4)$*.*

Proof. Every path on $(d+1)$ vertices has ϕ_{d+1} independent sets, hence $\widehat{c}(d) \leqslant \phi_{d+1}^{1/(d+1)}$ for any d. For $d = 4$, we can specify tree $T_{0,3}$ of diameter 4, having 7 vertices and 35 independent sets, therefore $\widehat{c}(4) \leqslant 35^{1/7}$. Note that $\phi_1 > \phi_2^{1/2} > \phi_3^{1/3} > \phi_4^{1/4} > 35^{1/7}$.

To complete the proof, let us show that for any tree T of diameter d on n vertices, for $d = 4$ the inequality $i(T) \geqslant 35^{n/7}$ holds, and for $d \leqslant 3$ the inequality $i(T) \geqslant \phi_{d+1}^{n/(d+1)}$ holds. For trees of diameter 0 and 1 this holds. The statement also holds for trees where $n \leqslant d+1$, since in this case $i(T) \geqslant \phi_n \geqslant \phi_{d+1}^{n/(d+1)}$. Let us assume that $n \geqslant d+2$ and tree T contains the minimum number of independent sets among all trees with given n and d.

1. $d = 2$. Then T is a star, and $i(T) = 2^{n-1} + 1 > 5^{n/3}$ for $n \geqslant 4$.

2. $d = 3$. In this case

$$i(T) \geqslant 2^{n-2} + 2^{\lfloor n/2-1 \rfloor} + 2^{\lceil n/2-1 \rceil} > 8^{1/4}$$

   (for $5 \leqslant n \leqslant 8$ the inequality $i(T) > 8^{1/4}$ is verified directly, and for $n \geqslant 9$ the inequality $2^{(n-2)/n} > 8^{1/4}$ holds).

3. $d = 4$. Let us proceed by induction on n. The fact that for $n = \overline{6, 13}$ every n-vertex tree of diameter 4, not isomorphic to $T_{0,3}$, has capacity greater than $35^{1/7}$, is verified directly using theorem 7 (this forms the base case of induction). Let $n \geqslant 14$ and all trees T' of diameter d on $n' < n$ vertices contain no fewer than $35^{n'/7}$ independent sets. Since $n \geqslant 14$, from theorem 7 it follows that the tree achieving the minimum number of independent sets for given n and $d = 4$

contains two pendant vertices w and w' having a common neighbor v. Using the induction hypothesis, we get

$$\begin{aligned} i(T) &= i(T \setminus \{w\}) + 2i(T \setminus \{w, w', v\}) \geqslant \\ &\geqslant 35^{(n-1)/7} + 2 \cdot 35^{(n-3)/7} = \\ &= 35^{n/7}(35^{-1/7} + 2 \cdot 35^{-3/7}) > 35^{n/7}, \end{aligned}$$

which completes the inductive step. The lemma is proved.

□

Theorem 8. 1. *Every tree of diameter* 6 *on* n *vertices contains at least* $35^{(n-1)/7}$ *independent sets.*

2. *Every tree of diameter* 7 *on* n *vertices contains at least* $35^{(n-2)/7}$ *independent sets.*

Proof. The theorem follows from lemmas 4 and 7. □

Remark. *The bounds 1 and 2 of theorem 8 are asymptotically tight for* $n \equiv 1 (\mathrm{mod} 7)$ *and* $n \equiv 2 \pmod 7$ *respectively.*

Proof. Consider a tree T' on $(7t+1)$ vertices of diameter 6, such that t trees of type $T_{0,3}$ are adjacent to the central vertex. We have $i(T') = 35^t + 27^t \sim 35^t$. Similarly, we can consider a tree T'' of diameter 7 on $(7t+2)$ vertices, such that $\lfloor t/2 \rfloor$ trees $T_{0,3}$ are adjacent to one of the central vertices, and $\lceil t/2 \rceil$ trees $T_{0,3}$ are adjacent to the other central vertex. We have $i(T'') = 35^t + 27^{\lfloor t/2 \rfloor} 35^{\lceil t/2 \rceil} + 35^{\lfloor t/2 \rfloor} 27^{\lceil t/2 \rceil} \sim 35^t$. □

Let us denote by $\widetilde{T}_6$ such a tree of diameter 6 that when removing the central vertex from $\widetilde{T}_6$, the resulting forest consists of four five-vertex paths. We have $n(\widetilde{T}_6) = 21$, $i(\widetilde{T}_6) = 35122$, hence $c(\widetilde{T}_6) = 35122^{1/21}$. By definition, it follows that $\widehat{c}(6) \leqslant 35122^{1/21}$. Tree $\widetilde{T}_6$ is shown in Fig. 2.

Lemma 8. *For* $j \leqslant 5$, *the inequality* $\widehat{c}(j) > \widehat{c}(6)$ *holds.*

Proof. The inequalities $\widehat{c}(j) > \widehat{c}(6)$ for $j \leqslant 4$ follow from lemma 7 and inequalities $35^{1/7} > 35122^{1/21} \geqslant \widehat{c}(6)$.

Let us prove that $\widehat{c}(5) > \widehat{c}(6)$. Let T be an arbitrary $(n, 5)$-minimal tree. Consider two cases:

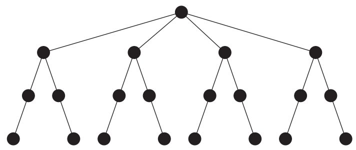

Figure 2. Tree $\widetilde{T}_6$

1. Let tree T have the following form: when removing from T two central vertices u, v and edges incident to them, the resulting forest consists of 2-vertex paths, where vertex u is adjacent to the ends of p paths, and vertex v to the ends of q paths, $p, q \geqslant 1$, $p+q = n/2-1$. Then

$$c(T) = (i(T))^{1/n(T)} = (3^{p+q} + 2^p 3^q + 3^p 2^q)^{\frac{1}{2(p+q+1)}}.$$

The minimum of expression $3^{p+q} + 2^p 3^q + 3^p 2^q$ under constraints $p+q = A$ and $p, q \geqslant 1$ is achieved at $p = q = A/2$. Hence

$$c(T) \geqslant \inf_{n \in \mathbb{N},\, n \geqslant 6} (3^{n/2-1} + 2 \cdot 6^{n/4-1/2})^{1/n}.$$

The inequality

$$(3^{n/2-1} + 2 \cdot 6^{n/4-1/2})^{1/n} > 35122^{1/21}$$

for $6 \leqslant n \leqslant 21$ is verified directly, and for $n \geqslant 22$ the inequality

$$(3^{n/2-1} + 2 \cdot 6^{n/4-1/2})^{1/n} > 3^{5/11} > 35122^{1/21}$$

holds.

2. Now consider the case when tree T has a form different from that considered in p. 1. Note that in this case there exists a vertex in T to which two paths are adjacent by their end vertices, where the first path contains one vertex and the second contains p vertices, where $p \in \{1, 2\}$. Let us replace them with one path on $(p+1)$ vertices. From p. 2 of lemma 5 it follows that for the obtained tree $\widehat{T}$ the relations $i(\widehat{T}) < i(T)$ and $n(\widehat{T}) = n(T)$ hold. Moreover, $\mathrm{diam}(\widehat{T}) \in \{5, 6\}$. If $\mathrm{diam}(\widehat{T}) = 5$, then tree T is not (n, d)-minimal — contradiction with the choice of T. If $\mathrm{diam}(\widehat{T}) = 6$, then $c(T) > i(\widehat{T}) > \widehat{c}(6)$.

□

Estimating the value of $\widehat{c}(6)$

Let T be some tree of diameter 6 on n vertices having the minimum number of independent sets among all n-vertex trees of diameter d. Let $T_1, \ldots, T_k$ be the trees adjacent to the central vertex v of tree T at vertices $v_1, \ldots, v_k$ respectively. We will consider $T_1, \ldots, T_k$ as rooted trees with roots $v_1, \ldots, v_k$. When speaking about replacing subtree T_i with rooted tree $\widehat{T_i}$ in tree T, we will assume that the replacement is done so that in the resulting tree, subtree $\widehat{T_i}$ is adjacent to vertex v at its root. We will call a replacement *reducing* if the conditions of lemma 5 are satisfied, that is, when under such replacement the number of independent sets in the resulting tree is strictly less than in the original one. Table 2 shows possible replacements and specifies the conditions under which they are reducing.

No.	T_i	$\widehat{T_i}$	Conditions
S1	$T_{0,q,1}$	$T_{1,q-1,0}$	$q \geqslant 3$
S2	$T_{p,q,1}$	$T_{p-1,q+2,0}$	$p \geqslant 1,\ q \geqslant 0$
S3	$T_{p,q},\ P_1$	$T_{p,q-1},\ P_3$	$\left[\begin{array}{l} p\geqslant 0, q\geqslant 2 \\ p\geqslant 1, q=1 \end{array}\right.$
S4	$T_{p,0},\ P_1$	$T_{p-2,2},\ P_3$	$p \geqslant 2$
S5	$P_2,\ P_1$	P_3	
S6	$P_3,\ P_1$	$P_2,\ P_2$	
S7	$P_4,\ P_1$	$P_3,\ P_2$	
S8	$T_{0,2,1},\ P_1$	$T_{0,3}$	
S9	$T_{1,0}$	P_4	
S10	$T_{0,q}$	$T_{2,q-3}$	$q \geqslant 7$
S11	$T_{0,6}$	$T_{0,3},\ T_{0,2,1}$	
S12	$P_2,\ P_2,\ P_3$	$P_2,\ P_5$	
S13	$P_2,\ P_2,\ P_2$	$P_3,\ P_3$	

Table 2. Reducing replacements in trees of diameter 6

Note that none of the specified reducing replacements can be performed in tree T (otherwise it would contradict the (n, d)-minimality of T). From lemmas 3 and 6 follows

Proposition 1. *Each of the trees $T_1, \ldots, T_k$ either has diameter no more than 3, or has the form $T_{p,q,r}$, where $r \leqslant 1$.*

[This is an automated translation of the original manuscript from Russian into English]

From the impossibility of performing replacements S1 and S2 follows the following fact.

Proposition 2. *Among the subtrees $T_1, \ldots, T_k$ of tree T for $r > 0$ there cannot be trees of type $T_{p,q,r}$ other than P_2, P_4 and $T_{0,2,1}$.*

From statement 2, lemma 6 and the impossibility of performing replacements S3-S9 follows

Proposition 3. *Among the subtrees $T_1, \ldots, T_k$ of tree T having diameter less than 4, there can only be trees P_2, P_3, P_4.*

The impossibility of performing replacements S10 and S11 implies the following

Proposition 4. *Among the subtrees $T_1, \ldots, T_k$ of tree T there cannot be trees $T_{0,q}$ for $q \geqslant 6$.*

From the impossibility of performing replacements S12 and S13 follows

Proposition 5. *Among the subtrees $T_1, \ldots, T_k$ of tree T there cannot be more than two trees of type P_2. If among $T_1, \ldots, T_k$ there is a tree P_3, then among $T_1, \ldots, T_k$ there are not more than one tree of type P_2.*

Lemma 9. *Every tree of diameter 6 on n vertices contains at least $35122^{n/21}$ independent sets. The capacity of every tree of diameter 6 not isomorphic to $\widetilde{T}_6$ is strictly greater than $35122^{1/21}$.*

Proof. Let us prove the lemma by induction on n. For $n = 7$ we have $i(T) = 34 > > 35122^{1/3}$, and the statement of the theorem holds. Let $n > 7$ and the statement of the lemma holds for all n', $n' < n$. Let T be a tree on n vertices having the minimum number of independent sets among trees of diameter 6 on n vertices. If $n \geqslant 54$, then from theorem 8 follows that

$$c(T) \geqslant 35^{\frac{n-1}{7n}} \geqslant 35^{53/378} > 35122^{1/21}.$$

Further assume $n \leqslant 53$. If T has two pendant vertices u, v with a common neighbor w, then, using the induction hypothesis and inequality $\widehat{c}(j) \geqslant 35122^{1/21}$, $j \leqslant 5$, we get

$$\begin{aligned} i(T) &= i(T \setminus \{u\}) + i(T \setminus \{u, w\}) \geqslant \\ &\geqslant 35122^{(n-1)/21} + 2 \cdot 35122^{(n-3)/21} = \\ &= 35122^{n/21}(35122^{-1/21} + 2 \cdot 35122^{-1/7}) > \\ &> 35122^{n/21}. \end{aligned}$$

Let $T_1, \ldots, T_k$ be the trees adjacent to the central vertex v of tree T. If among trees $T_1, \ldots, T_k$ there is a tree P_4, then, using the induction hypothesis, decomposing T by the pendant vertex adjacent to the root in P_4, we get

$$i(T) \geqslant 35122^{n/21}(35122^{-1/21} + 3 \cdot 35122^{-4/21}) > 35122^{n/21}.$$

Similarly, if among $T_1, \ldots, T_k$ there is a tree $T_{0,2,1}$, then, decomposing T by the pendant vertex adjacent to the root in $T_{0,2,1}$, we get

$$i(T) \geqslant 35122^{n/21}(35122^{-1/21} + 9 \cdot 35122^{-2/7}) > 35122^{n/21}.$$

From statements 1–5 it follows that it remains to consider the following cases:

1. $T_i \simeq T_{0,q_i}$ for $i = \overline{1, k}$, where $1 \leqslant q_i \leqslant 5$. Then $\frac{n-1}{11} \leqslant k \leqslant \frac{n-1}{3}$. We have

$$i(T) = (3^{q_1} + 2^{q_1}) \cdot \ldots \cdot (3^{q_k} + 2^{q_k}) + 3^{q_1 + \ldots + q_k}.$$

Function

$$f(x_1, \ldots, x_k) = \prod_{i=1}^{k} (3^{x_i} + 2^{x_i})$$

achieves on the set $\{(x_1, \ldots, x_k) \mid x_i \geqslant 0, \sum_{i=1}^k x_i = A\}$ its minimum at point $(A/k, \ldots, A/k)$. Therefore

$$i(T) \geqslant (3^{\frac{n-1-k}{2k}} + 2^{\frac{n-1-k}{2k}})^k + 3^{\frac{n-1-k}{2}}.$$

By enumeration over the set

$$M_1 = \left\{(n, k) \in \mathbb{N}^2 \mid n \in [7, 53],\, k \in [\tfrac{n-1}{11}, \tfrac{n-1}{3}]\right\}$$

one can verify that

$$\min_{(n,k) \in M_1} \left((3^{\frac{n-1-k}{2k}} + 2^{\frac{n-1-k}{2k}})^k + 3^{\frac{n-1-k}{2}} \right)^{1/n} = 35122^{1/21},$$

and the minimum is achieved only at point $n = 21$, $k = 4$.

2. $T_1 \simeq T_2 \simeq P_2$, and $T_j = T_{0,q_j}$, where $2 \leqslant q_i \leqslant 5$, for $j > 2$. Then $n \geqslant 15$ and $\frac{n+17}{11} \leqslant k \leqslant \frac{n+5}{5}$. In this case

$$c(T) \geqslant \left(9 \cdot \left(3^{\frac{n-3-k}{2k-4}} + 2^{\frac{n-3-k}{2k-4}}\right)^{k-2} + 4 \cdot 3^{\frac{n-3-k}{2}}\right)^{1/n}.$$

By enumeration over the set

$$M_2 = \left\{(n,k) \in \mathbb{N}^2 \mid n \in [15, 53],\ k \in [\tfrac{n+17}{11}, \tfrac{n+5}{5}]\right\}$$

one can verify that

$$\min_{(n,k)\in M_2} \left(9 \cdot \left(3^{\frac{n-3-k}{2k-4}} + 2^{\frac{n-3-k}{2k-4}}\right)^{k-2} + 4 \cdot 3^{\frac{n-3-k}{2}}\right)^{1/n} > 1.65 > 35122^{1/21},$$

(minimum is achieved at point $n = 22$, $k = 5$). In this case we have $c(T) > 35122^{1/21}$.

3. $T_1 \simeq P_2$, and $T_j = T_{0,q_j}$, where $1 \leqslant q_i \leqslant 5$, for $j > 1$. In this case $n \geqslant 9$ and $\frac{n+8}{11} \leqslant k \leqslant \frac{n}{3}$. We have

$$c(T) \geqslant \left(3 \cdot \left(3^{\frac{n-k}{2k-2}} + 2^{\frac{n-k}{2k-2}}\right)^{k-1} + 2 \cdot 3^{\frac{n-k}{2}}\right)^{1/n}.$$

By enumeration over the set

$$M_3 = \left\{(n,k) \in \mathbb{N}^2 \mid n \in [9, 53],\ k \in [\tfrac{n+8}{11}, \tfrac{n}{3}]\right\}$$

one can verify that

$$\min_{(n,k)\in M_3} \left(3 \cdot \left(3^{\frac{n-k}{2k-2}} + 2^{\frac{n-k}{2k-2}}\right)^{k-1} + 2 \cdot 3^{\frac{n-k}{2}}\right)^{1/n} > 1.68 > 35122^{1/21},$$

(minimum is achieved at point $n = 53$, $k = 9$). In this case again we get $c(T) > 35122^{1/21}$. The lemma is proved.

□

From lemmas 4, 8 and 9 follows the following statement.

Theorem 9. 1. *Every tree of diameter* 8 *on* n *vertices contains at least* $35122^{(n-1)/21}$ *independent sets.*

2. *Every tree of diameter* 9 *on* n *vertices contains at least* $35122^{(n-2)/21}$ *independent sets.*

The bounds 1 *and* 2 *for* $n \equiv 1 \pmod{21}$ *and* $n \equiv 2 \pmod{21}$ *respectively are asymptotically tight.*

1.3 Structure of (n, d)-minimal trees

Lemma 10. *Let d be an even positive number, and let there exist a tree T of diameter d or $(d-1)$, such that $c(T) = \min_{m \leqslant d} \widehat{c}(m)$. Let $n = n(T)$.*

1. *There exists a tree $\widehat{T}'$ of diameter $(d+2)$, for which $c(\widehat{T}') < c(T)$ and $n(\widehat{T}') < 2^n$. For every tree T' of diameter $(d+2)$ with number of vertices exceeding $2^{n+1}n$, the inequality holds*
$$c(T') > \left(1 + \frac{1}{5 \cdot 2^n n}\right) c(\widehat{T}').$$

2. *There exists a tree $\widehat{T}''$ of diameter $(d+3)$, for which $c(\widehat{T}'') < c(T)$ and $n(\widehat{T}'') < 2^n$. For every tree T'' of diameter $(d+3)$ with number of vertices exceeding $2^{n+1}n$, the inequality holds*
$$c(T'') > \left(1 + \frac{1}{100 \cdot 2^n n}\right) c(\widehat{T}'').$$

Proof. Let T be the tree from the lemma's conditions. Let $n(T) = n$, $i(T) = i$. For $d \leqslant 4$ the validity of the lemma's statement is easily verified. Further assume that $d \geqslant 6$ and $n \geqslant 10$. Moreover, since $c(T) \leqslant \widehat{c}(6) = 35122^{1/21} < 5/3$, then $i < (5/3)^n$. Let u be the central vertex in T; we will consider it as the root vertex of T. Let $i_0 = i(T \setminus \{u\})$. Let $k \geqslant 2$, $T_1, \ldots, T_k$ be copies of tree T, and let $v \notin \bigcup_j V(T_j)$. By connecting the roots of trees $T_1, \ldots, T_k$ with vertex v, we get a tree $\widehat{T}'$ having diameter $(d+2)$. Let's find k for which inequality $c(\widehat{T}') < c(T)$ holds:

$$\begin{aligned} c(\widehat{T}) < c(T) \ &\Leftrightarrow (i^k + i_0^k)^{1/(1+kn)} < i^{1/n} \Leftrightarrow \\ &\Leftrightarrow \left((i_0/i)^k + 1\right)^n < i \ \Leftrightarrow \ k > \frac{\ln \frac{1}{i^{1/n}-1}}{\ln(i/i_0)}. \end{aligned} \tag{5}$$

From theorem 2 it directly follows that $i^{1/n} \geqslant (\phi_n)^{1/n} > \frac{1+\sqrt{5}}{2}$, hence

$$\ln \frac{1}{i^{1/n} - 1} < \ln \frac{1}{\frac{1+\sqrt{5}}{2} - 1} < \frac{1}{2}. \tag{6}$$

Since for tree T the equality $c(T) = \widehat{c}(d)$ holds, then

$$i \leqslant \widehat{c}(6)^n < (5/3)^n.$$

Further, from inequalities $i_0 < i < (5/3)^n$, and from inequality $\ln(1+x) \geqslant \frac{x}{2}$, which holds for $x \in (0,1)$, follows

$$\frac{1}{\ln(i/i_0)} = \frac{1}{\ln\left(1+\frac{i-i_0}{i_0}\right)} \leqslant \frac{2i_0}{i-i_0} \leqslant 2\cdot(5/3)^n. \tag{7}$$

From (6) and (7) follows that

$$\frac{\ln\frac{1}{i^{1/n}-1}}{\ln(i/i_0)} < (5/3)^n,$$

therefore for $k > (5/3)^n$, considering (5), the inequality $c(\widehat{T}') < c(T)$ will hold. Further assume that $k = 2^n - 1$, and $\widehat{T}'$ is the tree corresponding to such k. From what was said above follows that $c(\widehat{T}') < c(T)$. Moreover, $n(\widehat{T}') = 1+n(2^n-1) < 2^n$. From this follows the first statement of the first part of the lemma.

Consider an arbitrary tree T' of diameter $(d+2)$ on n' vertices, where $n' \geqslant 2kn$. By lemma 4, inequality $c(T') > i^{(n'-1)/n}$ holds. Let's estimate the ratio $\alpha = \frac{c(T')}{c(\widehat{T}')}$:

$$\begin{aligned}\alpha &> 1+\ln\alpha > \\ &> 1+\ln\frac{i^{\frac{n'-1}{n'n}}}{(i^k+i_0^k)^{1/(1+kn)}} = \\ &= 1+\frac{n'-1-kn}{n'n(1+kn)}\ln i - \frac{1}{1+kn}\ln\left(1+(i_0/i)^k\right).\end{aligned}$$

From this, considering inequality $\frac{i_0}{i} \leqslant 1-\frac{1}{i}$, using inequalities $(1-1/x)^x < e^{-1}$ (for $x>1$) and $\ln(1+x) < x$ (for $x>0$), we get

$$\begin{aligned}\alpha &> 1+\frac{n'-1-kn}{n'n(1+kn)}\ln i - \frac{1}{1+kn}\ln\left(1+e^{-k/i}\right) > \\ &> 1+\frac{1}{(1+kn)}\left(\frac{n'-1-kn}{n'n}\ln i - e^{-k/i}\right).\end{aligned}$$

From inequalities $\left(\frac{1+\sqrt{5}}{2}\right)^n < i < (5/3)^n$ and equality $k = 2^n-1$, considering $n \geqslant 10$, follows that $\ln i > 6n/25$ and $e^{-k/i} < 1/400$. Hence

$$\alpha > 1+\frac{1}{(1+kn)}\left(\frac{6(n'-1-kn)}{25n'} - \frac{1}{400}\right).$$

It's easy to verify that the last inequality for $n' \geqslant 2kn$ and $kn > 100$ implies inequality $\alpha > 1+\frac{1}{5kn}$, which completes the proof of the first part of the lemma.

Similarly we prove the second part of the lemma, concerning trees of diameter $(d+3)$. For even k we consider tree $\widehat{T}''$ on $(kn+2)$ vertices, such that to each of its two central vertices are adjacent $k/2$ trees isomorphic to T. Similarly we establish that for $k > 5 \cdot (5/3)^n$ the inequality $c(\widehat{T}'') < c(T)$ holds. Further, for $k = 2^n - 2$, the corresponding tree $\widehat{T}''$, and every tree T'' of diameter $(d+3)$ on n'' vertices, where $n'' \geqslant 2kn$, the relations hold

$$\begin{aligned}\frac{c(T'')}{c(\widehat{T}'')} &> 1 + \ln \frac{i^{\frac{n'-2}{n'n}}}{\left(i^k + i^{k/2} \cdot i_0^{k/2}\right)^{1/(2+kn)}} > \\ &> 1 + \frac{1}{2+kn}\left(\frac{2n' - 2kn - 4}{n'n} \ln i - 2e^{-k/(2i)}\right) > \\ &> 1 + \frac{1}{2+kn}\left(\frac{12(n' - kn - 2)}{25n'} - \frac{1}{10}\right) > 1 + \frac{1}{100kn}.\end{aligned}$$

□

Proposition 6. *Let natural numbers a, b, x, y satisfy inequalities a, $b \leqslant M$, x, $y \leqslant N$ and $a^{1/x} > b^{1/y}$. Then $\frac{a^{1/x}}{b^{1/y}} > 1 + \frac{1}{MN(2M)^N}$.*

Proof. We have

$$\frac{a^{1/x}}{b^{1/y}} = \left(1 + \frac{a^{y/x} - b}{b}\right)^{1/y} > 1 + \frac{a^{y/x} - b}{yb}. \tag{8}$$

Two cases are possible:

1. $a^{y/x} \in \mathbb{N}$. Then, since $a^{y/x} > b$, from (8) follows that

$$\frac{a^{1/x}}{b^{1/y}} > 1 + \frac{1}{yb} > 1 + \frac{1}{MN}.$$

2. $a^{y/x} \notin \mathbb{N}$. Let $\rho = a^{y/x} - \lfloor a^{y/x} \rfloor$. Then

$$\begin{aligned}\mathbb{N} \ni \left(\left\lfloor a^{y/x} \right\rfloor + \rho\right)^x &= \sum_{k=0}^{x} \binom{x}{k} \left\lfloor a^{y/x} \right\rfloor^{x-k} \rho^k = \\ &= \left\lfloor a^{y/x} \right\rfloor^x + \rho \sum_{k=1}^{x} \binom{x}{k} \left\lfloor a^{y/x} \right\rfloor^{x-k} \rho^{k-1}.\end{aligned}$$

From this and from inequalities $0 < \rho < 1$ follows that

$$\rho \geqslant \left(\sum_{k=1}^{x} \binom{x}{k} \left\lfloor a^{y/x} \right\rfloor^{x-k} \rho^{k-1}\right)^{-1} > \frac{1}{(a^{y/x} + 1)^x} > \frac{1}{2^x a^y}. \tag{9}$$

Using (8) and (9), we get

$$\frac{a^{1/x}}{b^{1/y}} > 1 + \frac{\rho}{yb} > 1 + \frac{1}{2^x a^y yb} > 1 + \frac{1}{MN(2M)^N}.$$

□

Lemma 11. *If T_1 and T_2 are trees on n_1 and n_2 vertices, $n_1, n_2 \leqslant N$, and $c(T_1) > c(T_2)$, then $c(T_1)/c(T_2) > 1 + 3^{-N^2-2}$.*

Proof. Let's apply statement 6, setting $a = i(T_1)$, $b = i(T_2)$, $x = n_1$, $y = n_2$. From constraints n_1, $n_2 \leqslant N$ and $i(T_1)$, $i(T_2) < 2^N$, follows

$$\frac{c(T_1)}{c(T_2)} > 1 + \frac{1}{2^N \cdot N(2^{N+1})^N} > 1 + \frac{1}{3^{N^2+2}}.$$

□

Let's define function $\mathrm{TOW}(x)$ of natural argument x as follows: $\mathrm{TOW}(1) = 2$ and $\mathrm{TOW}(x+1) = x \cdot 2^{\mathrm{TOW}(x)}$ for $x \geqslant 1$.

Lemma 12. *In the definition of value $\widehat{c}(d)$ (in the right part of (3)) the exact lower bound is achieved, and only on trees with no more than $\mathrm{TOW}(d)$ vertices. For every tree T of diameter d with more than $\mathrm{TOW}(d)$ vertices inequality $c(T) > \left(1 + \frac{1}{100 \cdot \mathrm{TOW}(d)}\right)\widehat{c}(d)$ holds. For every tree T of diameter d such that $c(T) > \widehat{c}(d)$, inequality $c(T) > \left(1 + \frac{1}{3^{(\mathrm{TOW}(d))^2}}\right)\widehat{c}(d)$ holds.*

Proof. The lemma's statement follows by induction from lemmas 10 and 11. □

Theorem 10. *Let d be an arbitrary natural number. There exists such a finite set of trees $\mathcal{M}_d$ that for any n and any (n, d)-minimal tree T each component of forest F_T is isomorphic to some tree from $\mathcal{M}_d$. It is possible to choose set $\mathcal{M}_d$ so that $|\mathcal{M}_d| < 4^{200(\mathrm{TOW}(d))^2}$.*

Proof. Let T be an arbitrary tree of diameter d. Let's show that each connected component of F_T has no more than $200(\mathrm{TOW}(d))^2$ vertices, from which the theorem's statement will follow.

Suppose in F there is a tree T' on n' vertices, and $n' > 200(\mathrm{TOW}(d))^2$. By lemma 12, there exists a tree T_d such that $n(T_d) = n < \mathrm{TOW}(d)$ and $c(T_d) = \widehat{c}(d)$. By lemma 12, inequality holds

$$i(T') > \left(1 + \frac{1}{100 \cdot \mathrm{TOW}(d)}\right)^{n'} (c(T))^{n'}.$$

From this and from inequality $(1 + 1/x)^x > 2$ (for $x > 1$) follows that

$$i(T') > 2^{n'/(100 \cdot \mathrm{TOW}(d))}(c(T))^{n'}.$$

Let's replace in F_T tree T' with $\lfloor n'/n \rfloor$ copies of tree T_d and $n' - n \cdot \lfloor n'/n \rfloor$ isolated vertices. For the obtained forest $\widehat{F}$ inequalities will hold

$$\begin{aligned} \frac{i(\widehat{F})}{i(F_T)} &< \frac{(c(T))^{n'-n} \cdot 2^n}{2^{n'/(100 \cdot \mathrm{TOW}(d))}(c(T))^{n'}} < \\ &< 2^{\mathrm{TOW}(d) - n'/(100 \cdot \mathrm{TOW}(d))} < \\ &< 2^{-\mathrm{TOW}(d)}. \end{aligned}$$

For tree $\widehat{T}$ obtained from T by replacing forest F_T with forest $\widehat{F}$, by lemma 5, inequality $i(\widehat{T}) < i(T)$ will hold, while, by construction of $\widehat{T}$, equalities $n(\widehat{T}) = n(T)$ and $\mathrm{diam}(\widehat{T}) = \mathrm{diam}(T)$ hold. This contradicts (n, d)-minimality of T. The obtained contradiction completes the proof. □

Similarly we prove

Theorem 11. *Let d be an even number, and $\mathcal{M}_d$ be the set of all trees T' for which $c(T') = \min_{m \leqslant d} \widehat{c}(m)$. Then for $d' \in \{d+2,\ d+3\}$, arbitrary natural number n, and arbitrary (n, d')-minimal tree T in forest F_T no more than $2 \cdot 3^{(\mathrm{TOW}(d))^2}$ vertices lie in connected components not isomorphic to trees from $\mathcal{M}_d$.*

Theorem 12. *Let d be an even natural number, and $\mathcal{M}_d$ be the set of all trees T' for which $c(T') = c_d = \min_{m \leqslant d} \widehat{c}(m)$. Let $d' \in \{d + 2,\ d + 3\}$. Consider the set*

$$\mathcal{J}_d = \{j \in \mathbb{N} \mid \exists T' \in \mathcal{M}_d,\ |V(T')| = j\}.$$

We call number q decomposable by $\mathcal{J}_d$ if $q = \sum_{s=1}^{l} j_s$ for some (not necessarily distinct) numbers $j_1, \ldots, j_l \in \mathcal{J}_d$. There exists such constant N that for all n, $n \geqslant N$, *such that $(n-d'+d+1)$ is decomposable by $\mathcal{J}_d$, and arbitrary (n,d')-minimal tree T, each component of forest F_T is isomorphic to some tree from $\mathcal{M}_d$.*

Proof. The proof is generally similar to the proof of previous theorems. Consider the case $d' = d+2$. Let

$$\begin{aligned} \delta &= \inf_{T' \notin \mathcal{M}_d} \frac{c(T')}{c_d}, \\ m &= \min_{T' \in \mathcal{M}_d} n(T'), \\ t &= \max_{\substack{T' \in \mathcal{M}_d, \\ v \in V(T')}} \frac{i(T' \setminus \{v\})}{i(T')}. \end{aligned}$$

Obviously, $t < 1$ and $m \geqslant 2$. Moreover, from lemma 12 follows that $\delta > 1$. Let $\widehat{T}$ be an arbitrary n-vertex tree of diameter d' such that each component of $F_{\widehat{T}}$ is isomorphic to some tree from $\mathcal{M}_d$ (due to decomposability of number $(n-1)$ by $\mathcal{J}_d$, at least one such tree $\widehat{T}$ exists). We have $i(\widehat{(T)}) \leqslant (t^{(1-1/m)(n-1)}+1)c_d^{n-1}$. Since $t^{(1-1/m)} < 1$, then for all sufficiently large n inequality $t^{(1-1/m)(n-1)} < \delta - 1$ holds, and therefore inequality $i(\widehat{(T)}) < \delta c_d^{n-1}$ holds. Then for all sufficiently large n for any (n,d')-minimal tree T each component of F_T must be isomorphic to a tree from $\mathcal{M}_d$, because otherwise inequality $i(T) > \delta c_d^{n-1} > i(\widehat{(T)})$ would hold. □

From theorem 12 follows, in particular

Corollary. *For $d \in \{6,7\}$ and for all sufficiently large n of the form $7k+d-$ -5, $k \in \mathbb{N}$, for any (n,d)-minimal tree T all components of forest F_T are isomorphic to tree $T_{0,3}$. For $d \in \{8,9\}$ and for all sufficiently large n of the form $21k+d-$ -7, $k \in \mathbb{N}$, for any (n,d)-minimal tree T all components of forest F_T are isomorphic to tree $\widetilde{T}_6$.*

From lemmas 7, 9, 12 follows

Theorem 13. *There exists such number N' that for $d \in \{6,7\}$ and every (n,d)-minimal tree T' the number of vertices in $F_{T'}$ not lying in connected components isomorphic to $T_{0,3}$ does not exceed N'. There exists such number N'' that for $d \in \{8,9\}$ and every (n,d)-minimal tree T'' the number of vertices in $F_{T''}$ not lying in connected components isomorphic to $\widetilde{T}_6$ does not exceed N''.*

1.4 Radially Regular Trees

For $d \leqslant 6$ trees of even diameter d having minimal capacity possess a certain symmetry, which is expressed in the following definition. We call a tree of even diameter *radially regular* if the degrees of all vertices of the tree located at the same distance from the center of the tree coincide. We find plausible the following statement.

Conjecture 1. *Any tree of even diameter having minimal capacity is radially regular.*

Proving hypothesis 1 would provide an opportunity for substantial reduction in enumeration when searching for trees minimal by capacity, since radially regular trees of diameter d are uniquely determined by $\frac{d-2}{2}$ parameters — degrees of vertices at the same distance from the center. Let q_j be the degree of vertices of a radially regular tree of diameter d located at distance j from the center, $0 \leqslant j \leqslant \frac{d-2}{2}$. Then, if the number of vertices in the tree does not exceed n, the q_j must satisfy constraints

$$1 + \sum_{k=1}^{d/2} \prod_{j=0}^{k-1} q_j \leqslant n. \tag{10}$$

Through q_j the number $i_{q_0, \ldots, q_{d/2-1}}$ of independent sets in the corresponding tree can be calculated using the recurrent relation

$$\begin{aligned} i_{q_{d/2-1}} &= 2^{q_{d/2-1}} + 1, \\ i_{q_{d/2-2}, q_{d/2-1}} &= i_{q_{d/2-1}}^{q_{d/2-2}} + 2^{q_{d/2-2} q_{d/2-1}}, \\ i_{q_j, \ldots, q_{d/2-1}} &= i_{q_{j+1}, \ldots, q_{d/2-1}}^{q_j} + i_{q_{j+2}, \ldots, q_{d/2-1}}^{q_j q_{j+1}}. \end{aligned}$$

Similarly to lemma 4 we establish the following fact.

Proposition 7. *If T is a tree having minimal capacity among radially regular trees of diameter $(d-2)$, then for any radially regular n-vertex tree T' of diameter d inequality $c(T') > c(T)^{(n-1)/n}$ holds.*

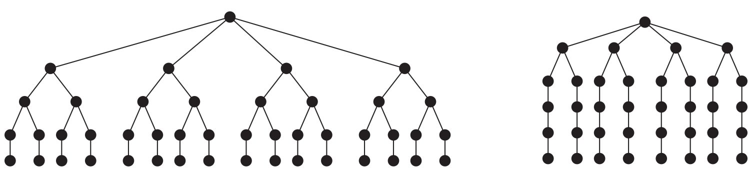

Figure 3. Trees $\widetilde{T}_8$ and $\widetilde{T}_{10}$

From statement 7 and equality $\widehat{c}(6) = 35122^{1/21}$ follows

Proposition 8. *Among radially regular trees of diameter* 8 *only tree* $\widetilde{T}_8$ *has minimal capacity (Fig. 3).*

Proof. We have $c(\widetilde{T}_8) = 4721980721^{1/45}$. For any tree T of diameter 8 with number of vertices $n \geqslant 147$, by statement 7, inequality holds

$$c(T) > 35122^{146/(21\cdot 147)} > c(\widetilde{T}_8)$$

. Consequently, it is sufficient to restrict consideration to trees with $n \leqslant 146$. For such n there exist only 1552 sequences $q_0, \ldots, q_{d/2-1}$ satisfying condition (10). By enumeration over all these sequences the validity of the statement is established. □

Similarly, minimal capacity radially regular trees of diameter $10 \div 26$ are found. Their parameters are given in Table 3. The extremal tree $\widetilde{T}_{10}$ of diameter 10 is also shown in Fig. 3. From the definition of value $\widehat{c}(d)$ it follows that upper bounds for the number of independent sets in radially regular trees of diameter d are upper bounds for $\widehat{c}(d)$.

Diameter	Number of vertices	Sequence $q_0, \ldots, q_{d/2-1}$	Capacity (upper bound)
8	45	$4, 2, 2, 1$	1.6405163
10	37	$4, 2, 1, 1, 1$	1.6350322
12	45	$4, 2, 1, 1, 1, 1$	1.6322615
14	53	$4, 2, 1, 1, 1, 1, 1$	1.6300187
16	201	$5, 3, 2, 1, 1, 1, 1, 1$	1.6282445
18	231	$5, 3, 2, 1, 1, 1, 1, 1, 1$	1.6269451
20	261	$5, 3, 2, 1, 1, 1, 1, 1, 1, 1$	1.6259081
22	291	$5, 3, 2, 1, 1, 1, 1, 1, 1, 1, 1$	1.6250981
24	321	$5, 3, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1$	1.6244353
26	351	$5, 3, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1$	1.6238877

Table 3. Extremal radially regular trees

1.5 Asymptotics of the Number of Independent Sets in Complete q-ary Trees

Consider sequence $\{\iota_{q,k}\}_{k=1}^{\infty}$, where $\iota_{q,k}$ is the number of independent sets in a q-ary tree having k levels of edges, or, equivalently, diameter $2k$. Note that complete

q-ary trees are a special case of radially regular trees. In this section we prove a generalization of theorem 4 for arbitrary q (theorem 15).

Further through $\{x_{q,k}\}_{k=0}^{\infty}$ we will denote the sequence defined by relations

$$\begin{aligned} x_{q,0} &= 2, \\ x_{q,k+1} &= 1 + x_{q,k}^{-q} \quad \text{for } k \geqslant 0. \end{aligned}$$

Let's prove several auxiliary statements.

Proposition 9. *Let q, t, s be arbitrary positive numbers such that $t \in [1,2]$ and $s = 1 + t^{-q}$.*

1. *If $t > 1 + t^{-q}$ and $t > 1 + (1 + t^{-q})^{-q}$, then $s < 1 + s^{-q}$ and $s < 1 + (1 + s^{-q})^{-q}$.*

2. *If $t < 1 + t^{-q}$ and $t < 1 + (1 + t^{-q})^{-q}$, then $s > 1 + s^{-q}$ and $s > 1 + (1 + s^{-q})^{-q}$.*

Proof. Let's prove the first part of the statement, the second is proved similarly. We have

$$\begin{aligned} t > 1 + t^{-q} &\Leftrightarrow t^{-q} < (1 + t^{-q})^{-q} \Leftrightarrow \\ &\Leftrightarrow 1 + t^{-q} < 1 + (1 + t^{-q})^{-q} \Leftrightarrow \\ &\Leftrightarrow s < 1 + s^{-q}, \end{aligned}$$

$$\begin{aligned} t > 1 + (1 + t^{-q})^{-q} &\Leftrightarrow 1 + t^{-q} < 1 + (1 + (1 + t^{-q})^{-q})^{-q} \Leftrightarrow \\ &\Leftrightarrow s < 1 + (1 + s^{-q})^{-q}. \end{aligned}$$

□

Proposition 10. *Let q be an arbitrary positive constant. Equation $x = 1 + x^{-q}$ has on interval $[1,2]$ a unique real root ξ_q. For $x \in [1,2]$ inequality $x > 1 + x^{-q}$ $(x < 1 + x^{-q})$ is equivalent to inequality $x > \xi_q$ (respectively, $x < \xi_q$).*

Proof. The statement follows from the strict increase and continuity of function $f(x) = x^{q+1} - x^q - 1$ on interval $[1,2]$, and inequalities $f(1) < 0 < f(2)$. □

Throughout the remainder of this section, we will denote by ξ_q the unique real root of equation $x^{q+1} - x^q - 1 = 0$ lying on interval $[1,2]$.

Proposition 11. *For any $q \geqslant 5$ there exists such positive $\widehat{\varepsilon} = \widehat{\varepsilon}(q)$ that for any $\varepsilon \in (0, \widehat{\varepsilon})$ inequalities hold*

$$\varepsilon < \xi_q - (1 + (\xi_q + \varepsilon)^{-q}) < q\varepsilon, \tag{11}$$

$$\varepsilon < (1 + (\xi_q - \varepsilon)^{-q}) - \xi_q < q\varepsilon. \tag{12}$$

Proof. First let's show that for $q \geqslant 5$ inequalities hold

$$1 < \frac{q}{\xi_q^{q+1}} < q. \tag{13}$$

Inequality $\frac{q}{\xi_q^{q+1}} < q$ is obvious. Let's prove inequality $1 < \frac{q}{\xi_q^{q+1}}$. For this it is sufficient to show that $q^{1/(q+1)} > \xi_q$, which, in turn, by statement 10, is equivalent to inequality $q - q^{q/(q+1)} - 1 > 0$. We have

$$\begin{aligned} & q - q^{q/(q+1)} - 1 > 0 \Leftrightarrow \\ \Leftrightarrow\ & (q-1)^{q+1} > q^q \Leftrightarrow \\ \Leftrightarrow\ & (q+1)\ln(q-1) - q\ln q > 0. \end{aligned} \tag{14}$$

Function $f(q) = (q+1)\ln(q-1) - q\ln q$ has derivative

$$f'(q) = \frac{2}{q-1} - \ln\left(1 + \frac{1}{q-1}\right),$$

positive for $g > 1$. Therefore $f(q)$ increases on interval $[5, +\infty)$, from which, considering inequality $f(5) > 0$, follows that for all $q \geqslant 5$ inequality $f(q) > 0$ holds. From this and from (14) follows (13).

Consider function

$$g(\varepsilon) = \xi_q - (1 + (\xi_q + \varepsilon)^{-q}) = \xi_q^{-q} - (\xi_q + \varepsilon)^{-q}.$$

We have $g(0) = 0$ and $g'(0) = \frac{q}{\xi^{q+1}}$. Thus, due to (13), we get $g'(0) \in (1, q)$. From this follows that for sufficiently small values of ε we have $g(\varepsilon) \in (\varepsilon, q\varepsilon)$, which is equivalent to (11). Similarly we establish the validity of inequalities (12) for sufficiently small ε. □

We will need the following classical result due to Sturm (see, for example, [15, §4.2]):

Theorem 14 (C. Sturm)**.** *Let $f(x)$ be a polynomial of degree k over $\mathbb{R}$. Let sequence of polynomials $f_0, \ldots, f_k$ be constructed by the following rule: $f_0 = f$, $f_1 = f'$, and f_j equals the remainder from division of f_{j-2} by f_{j-1}, taken with opposite sign, for $j \geqslant 2$. Denote by $\omega_f(x)$ the number of sign changes in sequence*

$$f_0(x), \ldots, f_k(x)$$

. Then for any real numbers a and b such that $f(a) \neq 0$, $f(b) \neq 0$ and $a < b$, the number of roots of f on interval $[a, b]$ equals $\omega_f(a) - \omega_f(b)$.

The sequence $f_0, \ldots, f_k$ in theorem 14, as well as any sequence whose polynomials differ from f_j by positive factors, is called a *Sturm sequence* for polynomial $f(x)$.

Proposition 12. *For $q \in \{2, 3, 4\}$ equation*

$$x = 1 + (1 + x^{-q})^{-q} \tag{15}$$

has on interval $[1, 2]$ a unique real root.

Proof. Equation (15) is equivalent to equation $f(x) = 0$, where $f(x) = (x-1)(x^q+1)^q - x^{q^2}$. For all positive q, obviously, inequalities $f(1) < 0 < f(2)$ hold.

1. $q = 2$. It suffices to show that $f(x)$ is convex on interval $[1, 2]$. Considering derivative $f''(x) = 20x^3 - 24x^2 + 12x - 4$, for $x \in [1,\ 1.5]$ we have

$$f''(x) \geqslant -4x^2 + 12x - 4 \geqslant 9x - 4 > 0,$$

and for $x \in [1.5,\ 2]$ we get $20x^3 \geqslant 30x^2$ and $f''(x) \geqslant 6x^2 + 12x - 4 > 0$.

2. $q = 3$. In this case $f(x) = x^{10} - 2x^9 + 3x^7 - 3x^6 + 3x^4 - 3x^3 + x - 1$. For $x \in [1, \frac{9}{8}]$ we have

$$f(x) \leqslant -\frac{7}{8}x^9 + \frac{3}{8}x^6 + \frac{3}{8}x^3 + x - 1 \leqslant -\frac{1}{8}x^9 + x - 1 < 0.$$

Thus, on interval $[1,\ \frac{9}{8}]$ equation $f(x) = 0$ has no roots. Now it suffices to show that $f(x)$ is convex on interval $[\frac{9}{8},\ 2]$. We have

$$f^{(5)}(x) = 30240(x^5 - x^4) + 7560x^2 - 2160x > 0$$

for $x > 1$. Moreover, the second, third and fourth derivatives of $f(x)$ at point $x = \frac{9}{8}$ are positive. From this follows the convexity of function $f(x)$ for $x \geqslant \frac{9}{8}$.

3. $q = 4$. Let's use Sturm's theorem. In Appendix A a Sturm sequence for $f(x)$ is given. From it we can determine that

$$\begin{aligned}
(\operatorname{sign} f_0(1), \ldots, \operatorname{sign} f_{17}(1)) &= (-\ 0 + - - + - - - + + + - + - - - +), \\
(\operatorname{sign} f_0(2), \ldots, \operatorname{sign} f_{17}(2)) &= (+ + + - - + - - + + - - + + - + + +),
\end{aligned}$$

hence $\omega_f(1) = 9$, $\omega_f(2) = 8$. Consequently, by theorem 14, equation $f(x) = 0$ has on interval $[1, 2]$ a unique real root. □

Lemma 13. *Let $q \in \mathbb{N}$, $q \geqslant 2$. Then*

1. *Sequence $\{x_{q,\,2k}\}_{k=0}^{\infty}$ monotonically decreases, while sequence $\{x_{q,\,2k+1}\}_{k=0}^{\infty}$ monotonically increases. Moreover, for each k inequalities hold*

$$x_{q,\,2k+1} < \xi_q < x_{q,\,2k}.$$

2. *For $q \in \{2, 3, 4\}$ sequence $\{x_{q,\,k}\}_{k=0}^{\infty}$ converges to ξ_q. For $q \geqslant 5$ sequence $\{x_{q,\,2k}\}_{k=0}^{\infty}$ converges to ζ_q, while sequence $\{x_{q,\,2k+1}\}_{k=0}^{\infty}$ converges to η_q, where η_q and ζ_q are roots of equation $x = 1 + (1 + x^{-q})^{-q}$ such that $1 < \eta_q < \xi_q < \zeta_q < 2$.*

Proof. Statement p. 1 of the lemma directly follows from statements 9 and 10 by induction, with the base of induction being obvious relations $\xi_q < x_{q,\,0}$ and $x_{q,\,2} = 1 + (1 + 2^{-q})^{-q} < 2 = x_{q,\,0}$.

Convergence of sequences $\{x_{q,\,2k}\}_{k=0}^{\infty}$ and $\{x_{q,\,2k+1}\}_{k=0}^{\infty}$ to finite limits immediately follows from boundedness and monotonicity of these sequences. Let's denote by ζ_q and η_q respectively $\lim_{k\to\infty} x_{q,\,2k}$ and $\lim_{k\to\infty} x_{q,\,2k+1}$. Obviously, η_q and ζ_q are roots of equation (15). Moreover, from inequalities

$$x_{q,\,2k+1} < \xi_q < x_{q,\,2k},$$

which hold for any k, follows that $\eta_q \leqslant \xi_q \leqslant \zeta_q$. According to statement 12, for $q \in \{2, 3, 4\}$ equation (15) has on interval $[1, 2]$ a unique real root. This root, obviously, coincides with ξ_q. Therefore for $q \in \{2, 3, 4\}$ we have $\eta_q = \zeta_q = \xi_q$.

Let's show that for $q \geqslant 5$ strict inequalities $\eta_q < \xi_q < \zeta_q$ hold. Assume that $\zeta_q = \xi_q$, that is $x_{q,\,2k} \downarrow \xi_q$ as $k \to \infty$. Let $\widehat{\varepsilon}$ be the constant from statement 11. By assumption, there exists such k_0 that $x_{q,\,2k_0} - \xi_q < \widehat{\varepsilon}/q$. But then, applying statement 11 twice, we get $x_{q,\,2k_0} - \xi_q < \xi_q - x_{q,\,2k_0+1} < \widehat{\varepsilon}$ and

$$x_{q,\,2k_0} - \xi_q < \xi_q - x_{q,\,2k_0+1} < x_{q,\,2k_0+2} - \xi_q,$$

which contradicts monotonicity of sequence $\{x_{q,\,2k}\}$. Thus, $\zeta_q > \xi_q$. Similarly the validity of inequality $\eta_q < \xi_q$ is established. □

For $q \geqslant 2$ let

$$\gamma_q = \exp\left(\sum_{j=0}^{\infty} q^{-j} \ln x_{q,\,j}\right).$$

Value γ_q is correctly defined due to convergence of series $\sum_{j=1}^{\infty} q^{-j} \ln x_{q,j}$, which directly follows from inequalities $0 \leqslant \ln x_{q,j} \leqslant \ln 2$ for all j.

Theorem 15. *For fixed q, $q \in \{2, 3, 4\}$, the following asymptotics holds as $k \to \infty$:*

$$\iota_{q,\,k} \sim \beta_q \cdot \gamma_q^{q^k},$$

where β_q is defined from Table 4.

q	β_q	$\approx$
2	$\sqrt[3]{\frac{\sqrt{93}}{18}+\frac{1}{2}} - \sqrt[3]{\frac{\sqrt{93}}{18}-\frac{1}{2}}$	0.6823278
3	$\sqrt{\sqrt{\frac{\sqrt[3]{12\sqrt{849}+108}-\sqrt[3]{12\sqrt{849}-108}}{24}} \cdot \left(\sqrt{\frac{18\left(\sqrt[3]{12\sqrt{849}+108}+\sqrt[3]{12\sqrt{849}-108}\right)}{\sqrt[3]{12\sqrt{849}+108}-\sqrt[3]{12\sqrt{849}-108}}-1}-1\right)}$	0.8511709
4	$\sqrt[3]{\frac{\sqrt[3]{100+12\sqrt{69}}}{6}+\frac{\sqrt[3]{100-12\sqrt{69}}}{6}-\frac{1}{3}}$	0.9105257

Table 4. Values of β_q in theorem 15

For fixed q, $q \geqslant 5$, the following asymptotics holds as $k \to \infty$:

$$\iota_{q,\,2k} \sim \alpha_{q,0} \cdot \gamma_q^{q^{2k}},$$

$$\iota_{q,\,2k+1} \sim \alpha_{q,1} \cdot \gamma_q^{q^{2k+1}},$$

where constants $\alpha_{q,0}$ and $\alpha_{q,1}$ satisfy inequality $\alpha_{q,0} > \alpha_{q,1}$ and are defined by relations

$$\alpha_{q,0} = \left(1 - \left(\lim_{k\to\infty} x_{q,\,2k}\right)^{-1}\right)^{1/(q^2-1)},$$

$$\alpha_{q,1} = \left(1 - \left(\lim_{k\to\infty} x_{q,\,2k+1}\right)^{-1}\right)^{1/(q^2-1)}.$$

Proof. Obviously, $\iota_{q,\,0} = 2$, $\iota_{q,\,1} = 2^q + 1$. Formally setting $\iota_{q,\,-1} = 1$, for $k \geqslant 1$ we have $\iota_k = \iota_{q,\,k-1}^q + \iota_{q,\,k-2}^{q^2}$. Consider sequence $\{\iota_{q,\,k}/\iota_{q,\,k-1}^q\}_{k=0}^{\infty}$. Since $\iota_{q,\,0}/\iota_{q,\,-1}^q = 2$, and for $k \geqslant 1$ equalities hold

$$\frac{\iota_{q,\,k}}{\iota_{q,\,k-1}^q} = \frac{\iota_{q,\,k-1}^q + \iota_{q,\,k-2}^{q^2}}{\iota_{q,\,k-1}^q} = 1 + \left(\frac{\iota_{q,\,k-1}}{\iota_{q,\,k-2}^q}\right)^q,$$

sequence $\{\iota_{q,k}/\iota_{q,k-1}^q\}_{k=0}^{\infty}$ coincides with $\{x_{q,k}\}_{k=0}^{\infty}$.

Let $y_{q,k} = \ln \iota_{q,k}$. For $k \geqslant 1$ we have

$$\begin{aligned} y_{q,k} &= \ln\left(\iota_{q,k-1}^q + \iota_{q,k-2}^{q^2}\right) = \\ &= q \ln \iota_{q,k-1} + \ln\left(1 + \iota_{q,k-2}^{q^2}/\iota_{q,k-1}^q\right) = \\ &= q y_{k-1} + \ln\left(1 + x_{q,k-1}^{-q}\right) = \\ &= q y_{q,k-1} + \ln x_{q,k}. \end{aligned}$$

From this by induction we conclude that

$$y_{q,k} = q^k y_{q,0} + \sum_{j=1}^{k} q^{k-j} \ln x_{q,j} = \sum_{j=0}^{k} q^{k-j} \ln x_{q,j}. \tag{16}$$

Let's denote $r_q(k) = \sum_{j=1}^{\infty} q^{-j} \ln x_{q,k+j}$. Let's transform the sum in the right part of (16) as follows:

$$\begin{aligned} \sum_{j=0}^{k} q^{k-j} \ln x_{q,j} &= \sum_{j=0}^{\infty} q^{k-j} \ln x_{q,j} - \sum_{j=k+1}^{\infty} q^{k-j} \ln x_{q,j} = \\ &= q^k \sum_{j=0}^{\infty} q^{-j} \ln x_{q,j} - \sum_{j=1}^{\infty} q^{-j} \ln x_{q,k+j} = \\ &= q^k \ln \gamma_q - r_q(k). \end{aligned} \tag{17}$$

From (16) and (17) follows

$$\iota_{q,k} = \exp\left(q^k \ln \gamma_q - r_q(k)\right) = \gamma_q^{q^k} \cdot e^{-r_q(k)}. \tag{18}$$

For $q \in \{2, 3, 4\}$ from lemma 13, due to monotonic convergence of $x_{q,k}$, follows that as $k \to \infty$

$$r_q(k) \to (\ln \xi_q) \cdot \sum_{j=1}^{\infty} q^{-j} = \frac{\ln \xi_q}{q-1}. \tag{19}$$

From (18) and (19) for $q \in \{2, 3, 4\}$ follows the asymptotics

$$\iota_{q,k} \sim \gamma_q^{q^k} \cdot (\xi_q^{-1})^{1/(q-1)}.$$

It remains to note that ξ_q is a root of equation $x = 1 + x^{-q}$, and therefore value ξ_q^{-1} is a root of equation $x^{q+1} + x - 1 = 0$. For $q \in \{2, 3, 4\}$ the latter equation is solvable in radicals. Solving it, and setting

$$\beta_q = (\xi_q^{-1})^{1/(q-1)},$$

we obtain the theorem's statement for the case $q \leqslant 4$.

Now let's consider the case $q \geqslant 5$. We have

$$\begin{aligned} r_q(2k) &= \sum_{j=1}^{\infty} q^{-j} \ln x_{q,\,2k+j} = \\ &= q \cdot \sum_{j=1}^{\infty} q^{-2j} \ln x_{q,\,2k+2j-1} + \sum_{j=1}^{\infty} q^{-2j} \ln x_{q,\,2k+2j}. \end{aligned}$$

From this and from lemma 13 follows that as $k \to \infty$

$$r_q(2k) \to (q \ln \eta_q + \ln \zeta_q) \cdot \sum_{j=1}^{\infty} q^{-2j} = \frac{\ln(\eta_q^q \zeta_q)}{q^2 - 1}. \tag{20}$$

Similarly it is proved that as $k \to \infty$

$$r_q(2k+1) \to \frac{\ln(\zeta_q^q \eta_q)}{q^2 - 1}. \tag{21}$$

From obvious equalities $\eta_q = 1 + \zeta_q^{-q}$ and $\zeta_q = 1 + \eta_q^{-q}$ follows that

$$(\eta_q^q \zeta_q)^{-1} = 1 - \zeta_q^{-1}, \qquad (\zeta_q^q \eta_q)^{-1} = 1 - \eta_q^{-1}. \tag{22}$$

From (18), (20), (21), (22) follows the theorem's statement for $q \geqslant 5$. □

Chapter 2. Estimates of the Number of Maximal Independent Sets in Graphs of Fixed Diameter

We establish a lower bound on the number of maximal independent sets in graphs of fixed diameter, as well as an upper bound on the number of maximal independent sets in trees of fixed diameter. We provide a complete description of the structure of graphs on which these bounds are achieved.

2.1 Basic Concepts

Let $d, n \in \mathbb{N}$, and let $d < n$. Any tree of diameter d on n vertices having the minimum (maximum) number of m.i.s. among all trees with the given number of vertices and diameter will be called $(n, d)_{\text{m.i.s.}}$–*minimal* (respectively, $(n, d)_{\text{m.i.s.}}$–*maximal*). The distance from a vertex $v \in V(G)$ in graph G to a subgraph G' will be called the minimum of the distances from v to vertices in $V(G')$.

Let $U = \{u_1, \ldots, u_{d-1}\}$, $V = \{v_1, \ldots, v_p\}$, $W = \{w_1, \ldots, w_q\}$. Let us denote by $B_{d,p,q}$ a tree of diameter d on the vertex set $U \cup V \cup W$, such that its subtrees induced by sets $\{u_1\} \cup V$, $\{u_{d-1}\} \cup W$ and U represent stars $K_{1,p}$, $K_{1,q}$ and path P_{d-1} respectively. Trees $B_{d,p,q}$ are called *brooms* (see, for example, [39]).

A *pendant edge* in a graph will mean any edge incident to a pendant vertex (vertex of degree 1).

We will say that graph G' is obtained by *subdivision* of edge $e = (v_1, v_2)$ of graph G if $V(G') = V(G) \cup \{v'\}$ and $E(G') = (E(G) \setminus \{e\}) \cup \{\{v_1, v'\}, \{v_2, v'\}\}$.

Let us denote by ψ_n the number of m.i.s. in a path on n vertices. The sequence ψ_n obviously satisfies the relation $\psi_n = \psi_{n-2} + \psi_{n-3}$ and initial conditions $\psi_0 = \psi_1 = 1$, $\psi_2 = 2$. Values of numbers ψ_n for small n are given in table 5.

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
ψ_n	1	1	2	2	3	4	5	7	9	12	16	21	28	37	49	65

Table 5. Values of ψ_n

A graph G will be called *quasi-path* if the set $V(G)$ admits a partition

$$V(G) = V_0 \sqcup V_2 \sqcup \ldots \sqcup V_d$$

with the following properties:

1. For any k, $2 \leqslant k \leqslant d$, and any i, $0 \leqslant i \leqslant d-k$, there are no edges in G of the form $\{u, u'\}$, where $u \in V_i$, $u' \in V_{i+k}$.
2. For each i, $0 \leqslant i \leqslant d-1$, the subgraph of graph G induced by set $V_i \cup V_{i+1}$ is a complete bipartite graph with parts V_i and V_{i+1}.

Any partition of the vertex set of a quasi-path having the properties specified above will be called *proper*.

In what follows, we will use without special mention the fact that the number of m.i.s. in a graph is not less than the number of m.i.s. in any of its induced subgraphs.

Proposition 13. *Let T be an arbitrary tree. Let T have a vertex adjacent to two or more leaves, and let u be one of these leaves. Then for tree T' obtained from T by deleting vertex u, the equality $i_M(T') = i_M(T)$ holds.*

Proof. It suffices to note that if $u_1, \ldots, u_r$ are leaves having a common neighbor in T, then in any m.i.s. in T either all vertices $u_1, \ldots, u_r$ are included simultaneously, or none of them is included. □

Lemma 14. *For any n and d such that $4 \leqslant d < n$, in $(n, d)_{\text{m.i.s.}}$–maximal trees each vertex is adjacent to at most one leaf.*

Proof. Suppose that $d \geqslant 4$ and there exists a $(n, d)_{\text{m.i.s.}}$–maximal tree T in which there is a vertex adjacent to two or more leaves. After removing one of these leaves, we obtain a tree T' for which, by statement 13, the equality $i_M(T') = i_M(T)$ holds. Moreover, obviously, $\mathrm{diam}(T') = \mathrm{diam}(T)$ and $n(T') = n(T) - 1$. In any tree of diameter at least four, there exists a vertex that is either not adjacent to any leaves or is a leaf not lying on the diametral path. Let v be such a vertex in tree T'. By adding a new leaf vertex u to T' and connecting it to v, we obtain a tree T'' for which $n(T'') = n(T)$, $\mathrm{diam}(T'') = \mathrm{diam}(T)$ and $i_M(T'') > i_M(T)$. But this contradicts the choice of T as a $(n, d)_{\text{m.i.s.}}$–maximal tree. This contradiction completes the proof. □

2.2 Lower Bounds on the Number of Maximal Independent Sets in Graphs of Fixed Diameter

Proposition 14. *Every quasi-path graph of diameter d contains ψ_{d+1} maximal independent sets.*

Proof. Cases $d \leqslant 2$ are trivial. Let $d \geqslant 3$. Let G be a quasi-path graph of diameter d, and $V_1 \sqcup \ldots \sqcup V_{d+1}$ be a proper partition of its vertex set. Let $P_{d+1} = v_1 v_2 \ldots v_{d+1}$ be a path on $(d+1)$ vertices. Note that for each i, $1 \leqslant i \leqslant d+1$, and each $A \in \mathcal{I}_M(G)$, one of the equalities $A \cap V_i = \varnothing$, $A \cap V_i = V_i$ holds. Therefore, to each m.i.s. A in G we can bijectively associate a m.i.s. A' in path $v_1 v_2 \ldots v_{d+1}$ by the rule $v_i \in A' \Leftrightarrow V_i \cap A = V_i$. Consequently, $i_M(G) = i_M(P_{d+1}) = \psi_{d+1}$. □

Theorem 16. *For any d, $d \geqslant 4$, and for any graph G of diameter d, the inequality $i_M(G) \geqslant \psi_{d+1}$ holds, turning into equality only for quasi-path graphs.*

Proof. Let G be an arbitrary graph of diameter d. The inequality $i_M(G) \geqslant \psi_{d+1}$ immediately follows from the fact that G contains an induced path on $(d+1)$ vertices (such is, for example, any diametral path in G).

Suppose that $i_M(G) = \psi_{d+1}$, and let us show that in this case G is a quasi-path graph. Consider arbitrary vertices v_0, $v_d \in V(G)$ at distance d. Let $P = v_0 v_1 \ldots v_d$ be a diametral path in G. We will assume that G has vertices not belonging to P. Let u be an arbitrary vertex of graph G at distance 1 from path P (such a vertex exists due to the connectivity of G and strict inclusion $V(P) \subsetneq V(G)$). Without loss of generality, we will assume that the distance from vertex v_i of path P adjacent to u to vertex v_d is not less than the distance to vertex v_0. Consider the subgraph G_u of graph G induced by set $V(P) \cup \{u\}$. Note that if $(u, v_i) \in E(G)$ for some vertex $v_i \in V(P)$, then $\{\{u, v_{i-k}\}, \{u, v_{i+k}\}\} \cap E(G) = \varnothing$ for any $k \geqslant 2$ (otherwise this would contradict the diametrality of path P). From this it follows that G_u is isomorphic to one of the graphs in Fig. 4a–4i. It is easy to show that for each of the graphs $\widehat{G}$ in Fig. 4d–4i with $d \geqslant 4$, strict inequalities $i_M(\widehat{G}) > i_M(P) = \psi_{d+1}$ hold (since for each m.i.s. A in P there exists such m.i.s. $A' \in \widehat{G}$ that $A = A' \cap V(P)$,

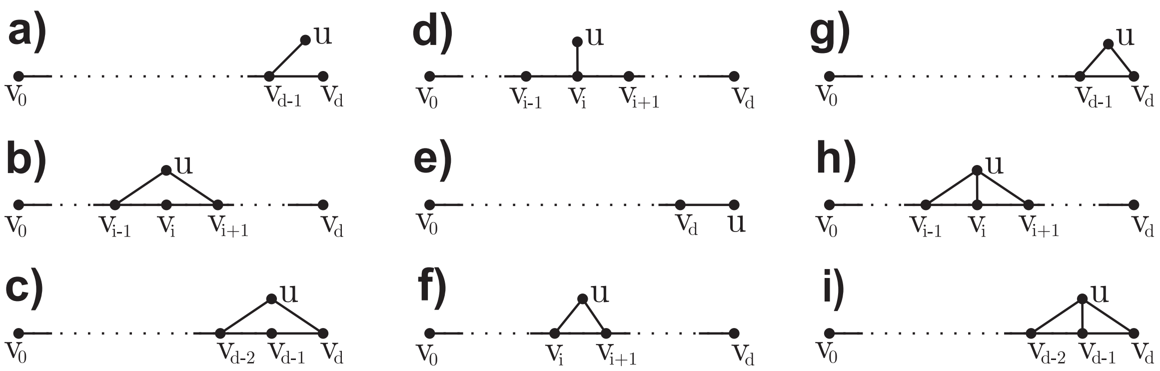

Figure 4. To the proof of theorem 16

but one can specify such m.i.s. A' in $\widehat{G}$ that $A' \cap V(P)$ is not a m.i.s. in P). From this and from the assumption $i_M(G) = \psi_{d+1}$ it follows that G_u must be isomorphic to one of the graphs in Fig. 4a–4c.

Let us now show that any vertex from $V(G) \setminus V(P)$ is at distance 1 from P. Suppose this is not the case. Then in G there exists a vertex w at distance 2 from P. Let u be a vertex adjacent to w at distance 1 from P. The subgraph $G_{u,w}$ of graph G induced by set $V(P) \cup \{u, w\}$ is isomorphic to one of the graphs in Fig. 5a–5c. But then, as can be easily shown, $i_M(G_{u,w}) > i_M(P)$, and thus $i_M(G) > \psi_{d+1}$ — a

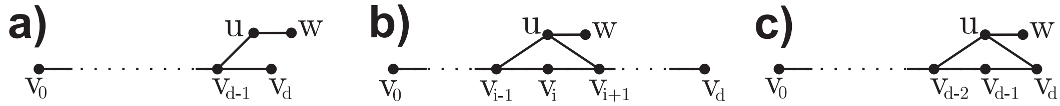

Figure 5. To the proof of theorem 16

contradiction with the choice of G.

From the above reasoning it follows that for any diametral path P in G and any vertex $u \in V(G) \setminus V(P)$ the subgraph G_u of graph G induced by set $V(P) \cup \{u\}$ is isomorphic to one of the graphs in Fig. 4a–4c. Let us construct sets $V_0, \ldots, V_d$ as follows. Set V_i for $1 \leqslant i \leqslant d-1$ contains exactly those vertices u from $V(G)$ for which $\{\{v_{i-1}, u\}, \{v_{i+1}, u\}\} \subseteq E(G)$. Set V_0 consists of all those vertices $u \in V(G)$ for which $\{v_1, u\} \in E(G)$ and $\{v_3, u\} \notin E(G)$. Set V_d consists of all those vertices $u \in V(G)$ for which $\{v_{d-1}, u\} \in E(G)$ and $\{v_{d-3}, u\} \notin E(G)$.

Let us show that G is a quasi-path graph, and $\{V_i\}_{i=0}^{d}$ is the corresponding proper partition of its vertices. Note that for the constructed sets V_i for each i, $0 \leqslant i \leqslant d$, we have $v_i \in V_i$. Moreover, any vertex $u \in V(G) \setminus V(P)$ belongs to exactly one of the sets V_i because graph G_u is isomorphic to one of the graphs in Fig. 4a–4c. Therefore, sets $\{V_i\}_{i=0}^{d}$ form a partition of set $V(G)$. Note that if u' and u'' are different vertices from the same set V_i, then $\{u', u''\} \notin E(G)$ (otherwise the subgraph of G induced by set $(P(V) \setminus \{v_i\}) \cup \{u', u''\}$ would be isomorphic to one of the graphs in Fig. 4g–4i, and we would have $i_M(G) > \psi_{d+1}$). Consequently, each set V_i is independent in G.

Now let us show that $\{u', u''\} \notin E(G)$ for any vertices $u' \in V_i$ and $u'' \in V_j$ with $|i - j| \geqslant 2$. If $2 \leqslant i + 1 < j < d$, then the existence of edge $\{u', u''\}$ in G would contradict the fact that v_0, v_d are at distance d. For the same reason, when $d \geqslant 6$, G cannot have an edge $\{u', u''\}$ such that $u' \in V_0$, $u'' \in V_d$. If $d \in \{4, 5\}$ and $\{u', u''\} \in E(G)$ for some $u' \in V_0$, $u'' \in V_d$, then G contains an induced subgraph isomorphic to the graph in Fig. 6a (for $d = 4$) or Fig. 6b (for $d = 5$), from which follows $i_M(G) > \psi_{d+1}$, contradicting the choice of G. It remains to consider the

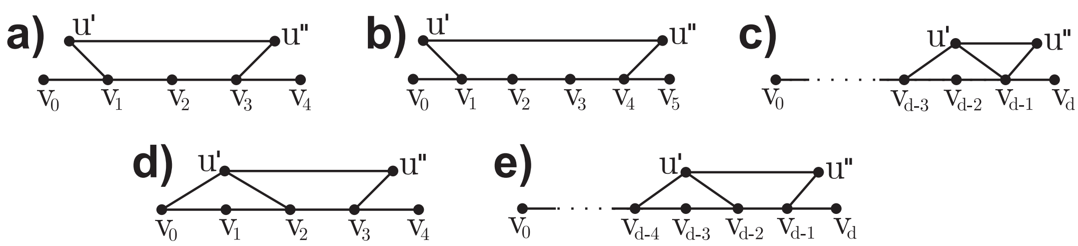

Figure 6. To the proof of theorem 16

case when $\{u', u''\} \in E(G)$ for vertices $u' \in V_i$, $u'' \in V_d$, where $1 \leqslant i \leqslant d - 2$. For $i \leqslant d - 4$ we get a contradiction with the fact that the distance between v_0 and v_d equals d. For $i = d - 2$ graph G would contain an induced subgraph isomorphic to the graph in Fig. 6c, the number of m.i.s. in which is strictly greater than ψ_{d+1}. Similarly, for $i = d - 3$ graph G would contain an induced subgraph isomorphic to one of the graphs in Fig. 6d,6e, and the strict inequality $i_M(G) > \psi_{d+1}$ would hold.

It only remains to note that $\{u', u''\} \in E(G)$ for any u', u'' such that $u' \in V_i$, $u'' \in V_{i+1}$ (otherwise G would have an induced subgraph isomorphic to one of the graphs in Fig. 7, and inequality $i_M(G) > \psi_{d+1}$ would hold). Thus, G has all

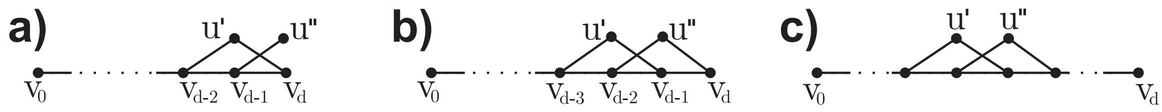

Figure 7. To the proof of theorem 16

properties of a quasi-path graph with proper partition $\{V_i\}_{i=0}^{d}$, and the theorem is proved. □

Corollary. *Let $d \geqslant 3$ and let tree T be $(n, d)_{\text{m.i.s.}}$–minimal. Then $T \simeq B_{d,p,q}$ for some natural numbers p, q.*

The following statement is proved completely analogously to theorem 16.

Proposition 15. *For any graph G of diameter 2, inequality $i_M(G) \geqslant 2$ holds, turning into equality only for complete bipartite graphs. For any graph G of diameter 3, inequality $i_M(G) \geqslant 3$ holds, with equality achieved only if set $V(G)$ can be partitioned into subsets $V' \sqcup V_0 \sqcup V_1 \sqcup V_2 \sqcup V_3$ (set V' may be empty) such that the subgraph induced by set $V(G) \setminus V'$ is quasi-path with proper partition $\{V_i\}_{i=0}^{3}$, set V' is independent in G, and*

$$V' \times (V_1 \cup V_2) \subset E(G),$$
$$(V' \times (V_0 \cup V_3)) \cap E(G) = \varnothing.$$

2.3 Upper Bounds on the Number of Maximal Independent Sets in Trees of Fixed Diameter

Let us introduce several notation for trees of special types. Let $\widetilde{B}_{4,n}$ denote the tree obtained from star $K_{1,\frac{n-1}{2}}$ by subdividing all edges. Let $\widetilde{B}'_{4,n}$ denote the tree obtained from star $K_{1,\frac{n}{2}}$ by subdividing $\frac{n-2}{2}$ edges. Trees $\widetilde{B}_{4,n}$ and $\widetilde{B}'_{4,n}$ are shown in Fig. 8.

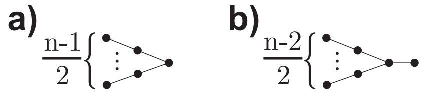

Figure 8. Trees $\widetilde{B}_{4,n}$ (a) and $\widetilde{B}'_{4,n}$ (b)

Let $\widetilde{B}'_{5,n}$ denote the tree obtained from broom $B_{3,\frac{n-5}{2},2}$ by subdividing all pendant edges except one edge incident to the vertex of degree 3. Let $\widetilde{B}_{5,n,p}$ denote the tree obtained from $B_{3,p,\frac{n-5-2p}{2}}$ by subdividing all pendant edges. Let $\widehat{B}'_{5,n,p}$ denote the tree obtained by attaching a pendant vertex to that central vertex of tree $\widetilde{B}_{5,n-1,p}$ which has degree $(p+1)$. Let $\widehat{B}''_{5,n,p}$ denote the tree obtained by attaching a pendant vertex to each central vertex of tree $\widetilde{B}_{5,n-2,p}$. Trees $\widetilde{B}'_{5,n}$, $\widetilde{B}_{5,n,p}$, $\widehat{B}'_{5,n,p}$ and $\widehat{B}''_{5,n,p}$ are shown in Fig. 9.

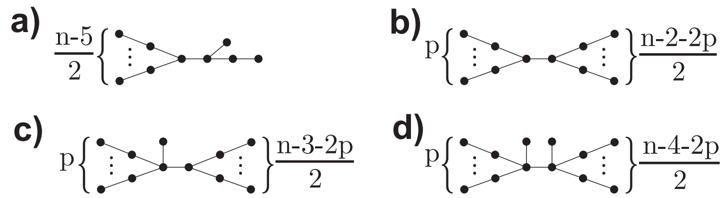

Figure 9. Trees $\widetilde{B}'_{5,n}$ (a), $\widetilde{B}_{5,n,p}$ (b), $\widehat{B}'_{5,n,p}$ (c) and $\widehat{B}''_{5,n,p}$ (d)

Let $\widehat{B}_{6,n,p}$ denote the tree obtained from $B_{4,p,\frac{n-3-2p}{2}}$ by subdividing all pendant edges. Let $\widetilde{B}'_{6,n,p}$ denote the tree obtained by attaching a pendant vertex to the central vertex of tree $\widehat{B}_{6,n-1,p}$. Let $\widehat{B}_{6,n,p,q}$ denote the tree obtained by attaching q pendant vertices to the center of $B_{4,p,\frac{n-3-2p-2q}{2}}$ and then subdividing all pendant edges. Let $\widehat{B}'_{6,n,p,q}$ denote the tree obtained by attaching a pendant vertex to the central vertex of tree $\widehat{B}_{6,n-1,p,q}$. Trees $\widehat{B}_{6,n,p,q}$, $\widehat{B}'_{6,n,p,q}$, $\widehat{B}_{6,n,p}$ and $\widetilde{B}'_{6,n,p}$ are shown in Fig. 10.

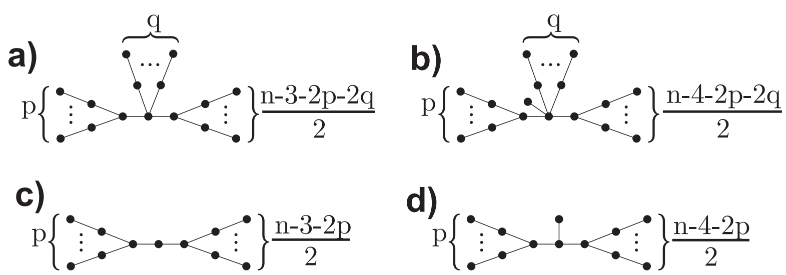

Figure 10. Trees $\widehat{B}_{6,n,p,q}$ (a), $\widehat{B}'_{6,n,p,q}$ (b), $\widehat{B}_{6,n,p}$ (c) and $\widetilde{B}'_{6,n,p}$ (d)

Let $\widetilde{B}'_{7,n}$ denote the tree obtained from $B_{5,\frac{n-7}{2},2}$ by subdividing all pendant edges except one edge incident to the vertex of degree 3. Let $\widetilde{B}_{7,n}$ denote the tree obtained from $B_{5,p,\frac{n-4-2p}{2}}$ by subdividing all pendant edges. Let $\widehat{B}_{7,n,p,q,r}$ denote the tree obtained by attaching $(q+1)$ and r pendant vertices respectively to the central vertices of tree $B_{5,p,\frac{n-5-2p-2q-2r}{2}}$ adjacent to vertices of degree $(p+1)$ and $\frac{n-3-2p-2q-2r}{2}$, and then subdividing all pendant edges except one incident to the central vertex adjacent to vertices of degree $(p+1)$ and $(r+2)$. Trees $\widetilde{B}'_{7,n}$, $\widetilde{B}_{7,n}$ and $\widehat{B}_{7,n,p,q,r}$ are shown in Fig. 11.

Let $\widehat{B}_{8,n}$ denote the tree obtained from $\widetilde{B}_{4,n-4}$ by double subdivision of two pendant edges. Let $\widehat{B}'_{8,n}$ denote the tree obtained by attaching a pendant vertex

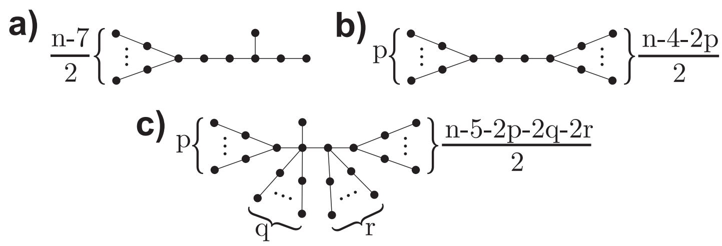

Figure 11. Trees $\widetilde{B}'_{7,n}$ (a), $\widetilde{B}_{7,n}$ (b) and $\widehat{B}_{7,n,p,q,r}$ (c)

to the center of tree $\widehat{B}_{8,n-1}$. Trees $\widehat{B}_{8,n}$ and $\widehat{B}'_{8,n}$ are shown in Fig. 12. Let $\widehat{B}_{9,n,p}$ denote the tree obtained from tree $\widetilde{B}_{5,n-4,p+1}$ by double subdivision of two pendant edges located at opposite ends of the tree. Let $\widehat{B}'_{9,n,p}$ denote the tree obtained by attaching a pendant vertex to the central vertex of degree $(p+2)$ of tree $\widehat{B}_{9,n-1,p}$. Let $\widehat{B}''_{9,n,p}$ denote the tree obtained by attaching pendant vertices to each of the central vertices of tree $\widehat{B}_{9,n-2,p}$. Trees $\widehat{B}_{9,n,p}$, $\widehat{B}'_{9,n,p}$ and $\widehat{B}''_{9,n,p}$ are shown in Fig. 12.

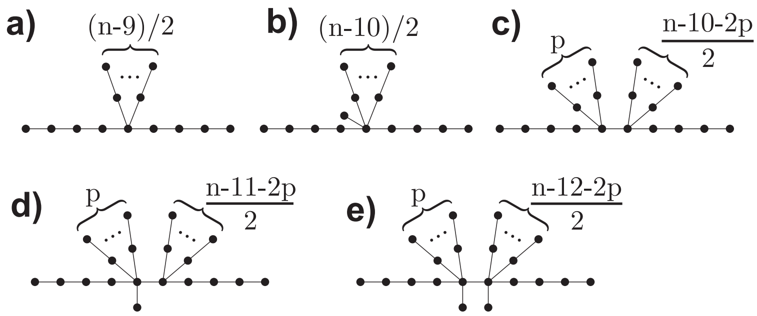

Figure 12. Trees $\widehat{B}_{8,n}$ (a), $\widehat{B}'_{8,n}$ (b), $\widehat{B}_{9,n,p}$ (c), $\widehat{B}'_{9,n,p}$ (d) and $\widehat{B}''_{9,n,p}$ (e)

Let $\widetilde{B}'_6$ denote the tree obtained from $K_{1,3}$ by double subdivision of two edges. Let $\widetilde{B}'_8$ denote the tree obtained by attaching a pendant vertex to the fourth from end vertex of path P_9. Let $\widetilde{B}_d$ denote the tree obtained by attaching a pendant vertex to the third from end vertex of path P_{d+1}. Trees $\widetilde{B}'_6$, $\widetilde{B}'_8$ and $\widetilde{B}_d$ are shown in Fig. 13.

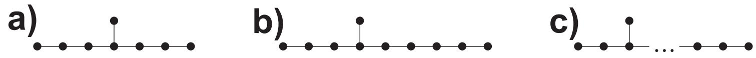

Figure 13. Trees $\widetilde{B}^*_6$ (a), $\widetilde{B}^*_8$ (b) and $\widetilde{B}''_n$ (c)

Let $\check{B}_{d,n}$ denote the tree obtained from $B_{d-2,\frac{n-d+1}{2},1}$ by subdividing all pendant edges. Let $\check{B}'_{d,n}$ denote the tree obtained by attaching a pendant vertex to that vertex of tree $\check{B}_{d,n-1}$ which is not adjacent to pendant vertices but is adjacent to a vertex of degree $\frac{n-d}{2}$. Trees $\check{B}_{d,n}$ and $\check{B}'_{d,n}$ are shown in Fig. 14.

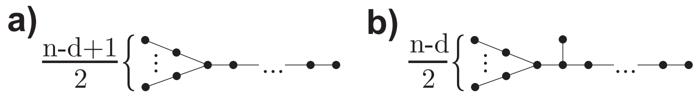

Figure 14. Trees $\check{B}_{d,n}$ (a) and $\check{B}'_{d,n}$ (b)

Finally, let $\widehat{B}^*_{d,k}$ denote the tree obtained by attaching a pendant vertex to the k-th vertex of the diametral path of tree $\check{B}_{d,d+3}$, counting from that end of the diametral path which is furthest from the vertex of degree 3. Trees $\widehat{B}^*_{d,k}$ for $k = 3$, $k = 4$ and $k \geqslant 5$ are shown in Fig. 15.

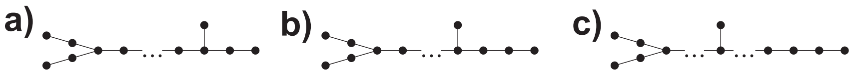

Figure 15. Trees $\widehat{B}^*_{d,k}$ with $k = 3$ (a), $k = 4$ (b) and $k \geqslant 5$ (c)

For natural numbers n, d such that $4 \leqslant d \leqslant n-1$, define the value $M(n,d)$:

$$M(n,d) = \begin{cases} \psi_{d-1} + (2^{(n-d+1)/2} - 1)\psi_{d-2}, & \text{for } d \geqslant 4,\ n-d = 2k+1,\ k \geqslant 0, \\ \psi_{d-2} + \psi_d, & \text{for } d \geqslant 4,\ n-d = 2, \\ 2^{(n-d)/2}\psi_{d-1}, & \text{for } d \geqslant 5,\ d \neq 7,\ n-d = 2k \geqslant 4, \\ 2^{(n-d)/2}\psi_{d-1} + 1, & \text{for } d \in \{4,7\},\ n-d = 2k \geqslant 4. \end{cases}$$

[This is an automated translation of the original manuscript from Russian into English]

Proposition 16.

1. *For* $d \geqslant 4$ *and any* n, $n \geqslant d+3$, *such that* $2 \nmid (n-d)$, *inequality* $M(n,d) > M(n,d+1)$ *holds.*

2. *For* $d \geqslant 4$ *and any* n, $n \geqslant d+2$, *such that* $2 \mid (n-d)$, *inequality* $M(n,d) \leqslant M(n,d+1)$ *holds, with* $M(n,d) = M(n,d+1)$ *only if* $d = 4$.

3. *For* $d \geqslant 4$ *and any* n, $n \geqslant d+3$, *inequality* $M(n,d) \geqslant M(n,d+2)$ *holds, with equality* $M(n,d) = M(n,d+2)$ *occurring only if both* $d = 5$ *and* n *is even.*

Proof.

1. Let $4 \leqslant d \leqslant n-3$ and $2 \nmid (n-d)$. If $n = d+3$, then

$$M(n,d) - M(n,d+1) = 2\psi_{d-2} - \psi_{d-1} > 0.$$

If $n \geqslant d+5$ and $d \neq 6$, then

$$\begin{aligned} M(n,d) - M(n,d+1) &= \psi_{d-1} - \psi_{d-2} + 2^{(n-d-1)/2}(2\psi_{d-2} - \psi_d) \geqslant \\ &\geqslant \psi_{d-1} + 7\psi_{d-2} - 4\psi_d > 0. \end{aligned}$$

If $n \geqslant d+5$ and $d = 6$, then $M(n,d) - M(n,d+1) = 2^{(n-7)/2} > 0$.

2. For $d = 4$ and even n equality $M(n,d) = M(n,d+1)$ is easily verified. Let $5 \leqslant d \leqslant n-2$ and $2 \mid (n-d)$. If $n = d+2$, then

$$M(n,d+1) - M(n,d) = \psi_{d-1} - \psi_{d-2} > 0.$$

If $d \neq 7$ and $n \geqslant d+4$, then

$$M(n,d+1) - M(n,d) = \psi_d - \psi_{d-1} > 0.$$

If $d = 7$ and $n \geqslant d+4$, then $M(n,d+1) - M(n,d) = 1 > 0$.

3. For $4 \leqslant d \leqslant n-3$ and $2 \nmid (n-d)$ we have

$$M(n,d) - M(n,d+2) = (2^{(n-d-1)/2} - 1)(2\psi_{d-2} - \psi_d),$$

from which it follows that $M(n,5) = M(n,7)$, and $M(n,d) > M(n,d+2)$ for $d \neq 5$.

If $d = 4$ and n is even, then $M(n,d) - M(n,d+2) = 1 > 0$. Let $5 \leqslant d \leqslant n-3$. If $n = d+4$, then $M(n,d) - M(n,d+2) \geqslant 3\psi_{d-1} - 2\psi_d > 0$. If $n \geqslant d+6$ and $2 \mid (n-d)$, then

$$M(n,d) - M(n,d+2) \geqslant 2^{(n-d-2)/2}(2\psi_{d-1} - \psi_{d+1}) - 1 > 0.$$

□

From statement 16 the following fact follows directly.

Lemma 15. *If $4 \leqslant d' < d'' \leqslant n-1$, then*

1. $$\operatorname*{Argmax}_{d' \leqslant d \leqslant d''} M(n,d) = \begin{cases} \{d'+1\}, & \text{for } d' \geqslant 5,\ 2 \mid (n-d'), \\ \{4,5,7\} \cap [d', d''], & \text{for } d' \leqslant 5,\ 2 \mid n, \\ \{d'\}, & \text{for } d' \geqslant 4,\ d' \neq 5,\ 2 \nmid (n-d'). \end{cases}$$

2. $$\max_{d' \leqslant d \leqslant d''} M(n,d) = \begin{cases} M(n,d'+1), & \text{for } 2 \mid (n-d'), \\ M(n,d'), & \text{for } 2 \nmid (n-d'). \end{cases}$$

3. $\max_{d \geqslant d'} M(n,d) \leqslant M(n,4)$.

Lemma 16. *For $n-2 = d \geqslant 5$ any $(n,d)_{\text{m.i.s.}}$–maximal tree T is isomorphic to one of the trees $\widetilde{B}^*_6$, $\widetilde{B}^*_8$, $\widetilde{B}''_n$. Moreover, $i_M(T) = M(n,d)$.*

Proof. Let us prove the lemma by induction on d. For $5 \leqslant d \leqslant 8$ the statement of the lemma is verified by enumeration. Let $d \geqslant 9$ and assume the lemma holds for trees of diameter not exceeding $(d-1)$. Let T be a $(d+2,d)_{\text{m.i.s.}}$–maximal tree. Let v be the only vertex not lying on the diametral path of T. Denote by u that end vertex of the diametral path which is at the greatest distance from v. Let u' be the vertex adjacent to u, and u'' be the vertex at distance 2 from u. Then, using the induction hypothesis, we can estimate $i_M(T)$:

$$\begin{aligned} i_M(T) &= i_M(T \setminus \{u,u'\}) + i_M(T \setminus \{u,u',u''\}) \leqslant \\ &\leqslant M(n-2,d-2) + M(n-3,d-3) = \\ &= M(n,d), \end{aligned}$$

with equality $i_M(T) = M(n,d)$ possible only if trees $T \setminus \{u,u'\}$ and $T \setminus \{u,u',u''\}$ are isomorphic to some of the trees $\widetilde{B}_6^*$, $\widetilde{B}_8^*$, $\widetilde{B}''_{n-2}$, $\widetilde{B}''_{n-3}$. But then tree T itself is isomorphic to tree $\widetilde{B}''_n$. □

Lemma 17. *Any* $(n,5)_{\text{m.i.s.}}$*–maximal tree is isomorphic to one of the trees* $\widetilde{B}'_{5,n}$, $\widetilde{B}_{5,n,p}$ *(for some* p*).*

Proof. Let T be an arbitrary $(n,5)_{\text{m.i.s.}}$–maximal tree. If tree T is isomorphic to one of the trees $\widetilde{B}'_{5,n}$ or $\widetilde{B}_{5,n,p}$, then, as is easily verified, $i_M(T) = M(n,5)$. Suppose T is not isomorphic to any of the trees $\widetilde{B}'_{5,n}$, $\widetilde{B}_{5,n,p}$. Then from lemma 14 it follows that only the following cases are possible:

1. T has the form $\widehat{B}'_{5,n,p}$, where $n \geqslant 9$ and $p \geqslant 2$. Then

$$i_M(T) = 2^{(n-5)/2}(2 + 2^{1-p}) < 3 \cdot 2^{(n-5)/2} = M(n,5).$$

2. T has the form $\widehat{B}''_{5,n,p}$, where $n \geqslant 8$. Then

$$i_M(T) = 2^{(n-4)/2} + 2^p + 2^{(n-2p-4)/2} \leqslant 2 + 3 \cdot 2^{(n-6)/2} < 1 + 4 \cdot 2^{(n-6)/2} = M(n,5).$$

Thus, in both cases considered we get a contradiction with the $(n,5)_{\text{m.i.s.}}$–maximality of T, which completes the proof of the lemma. □

It is obvious that any tree of diameter 1 or 2 contains two m.i.s., and any tree of diameter 3 contains three m.i.s. For $d \geqslant 4$, a complete description of $(n,d)_{\text{m.i.s.}}$–maximal trees is given by the following theorem.

Theorem 17. *For $4 \leqslant d \leqslant n-2$, any $(n,d)_{\text{m.i.s.}}$–maximal tree T satisfies the equality $i_M(T) = M(n,d)$, and the tree T itself is isomorphic to one of the trees listed in the table:*

d	$(n-d)$	extremal trees
4	$2k+1$ $(k \geqslant 1)$	$\widetilde{B}_{4,n}$
4	$2k$ $(k \geqslant 1)$	$\widetilde{B}'_{4,n}$
5	$2k+1$ $(k \geqslant 1)$	$\widetilde{B}_{5,n,p}$ $(1 \leqslant p \leqslant \frac{n-4}{2})$
5	$2k$ $(k \geqslant 1)$	$\widetilde{B}'_{5,n}$
6	$2k+1$ $(k \geqslant 1)$	$\check{B}_{6,n}$
6	2	$\widetilde{B}^*_6$, $\widetilde{B}''_8$
6	$2k$ $(k \geqslant 2)$	$\widetilde{B}'_{6,n,p}$ $(1 \leqslant p \leqslant \frac{n-6}{2})$
7	$2k+1$ $(k \geqslant 1)$	$\widetilde{B}_{7,n}$ $(1 \leqslant p \leqslant \frac{n-6}{2})$
7	$2k$ $(k \geqslant 1)$	$\widetilde{B}'_{7,n}$
8	$2k+1$ $(k \geqslant 1)$	$\check{B}_{8,n}$
8	2	$\widetilde{B}^*_8$, $\widetilde{B}''_{10}$
8	$2k$ $(k \geqslant 2)$	$\check{B}'_{8,n}$
$\geqslant 9$	$2k+1$ $(k \geqslant 1)$	$\check{B}_{d,n}$
$\geqslant 9$	2	$\widetilde{B}''_n$
$\geqslant 9$	$2k$ $(k \geqslant 2)$	$\check{B}'_{d,n}$

Proof. The validity of the theorem for $d = 4$ follows directly from lemma 14, and for $d = 5$ it is ensured by lemma 17. Moreover, for $n = d+2$, the statement of the theorem follows from lemma 16.

Let $d \geqslant 6$, $n \geqslant d+3$, and assume the theorem holds for all pairs (n'', d) such that $n'' < n$, as well as for all pairs (n', d') such that $d' \leqslant d-1$. Let us prove that then the statement of the theorem is also valid for the pair (n,d). Let T be an arbitrary $(n,d)_{\text{m.i.s.}}$–maximal tree, and P be an arbitrary diametral path in T. Let us show that for any vertex v not lying on path P, the minimum distance from v

to vertices of P does not exceed 2. Suppose the contrary and show that under this assumption, the strict inequality $M(n,d) - i_M(T) > 0$ holds, which contradicts the choice of T. From lemma 14 it follows that only the following cases are possible:

A. Tree T has the form shown in Fig. 16a, where $\mathrm{diam}(T') = d$ and $1 \leqslant t \leqslant \frac{n-d-2}{2}$. In this case $M(n,d) - i_M(T) \geqslant D_1(n,d)$, where

$$D_1(n,d) = M(n,d) - M(n-2,d) - M(n-2t-1,d) \cdot 2^{t-1}.$$

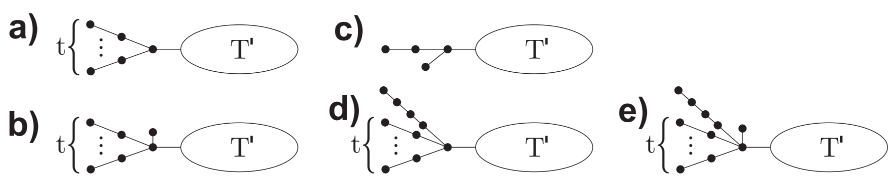

Figure 16. To the proof of theorem 17

Let us consider several subcases:

A1. $n = d+4$. Then $t = 1$ and $D_1(n,d) \geqslant 4\psi_{d-1} - \psi_{d-2} - \psi_d - \psi_{d+1} > 0$.

A2. $n = d+2k$, where $k \geqslant 3$. Then

$$\begin{aligned} D_1(n,d) &= 2^{(n-d)/2}\psi_{d-1} - 2^{(n-d-2)/2}(\psi_{d-1} + \psi_{d-2}) - 2^{t-1}(\psi_{d-1} - \psi_{d-2}) \geqslant \\ &\geqslant 2^{(n-d)/2}\psi_{d-1} - 2^{(n-d-2)/2}(\psi_{d-1} + \psi_{d-2}) - \\ &-2^{(n-d-4)/2}(\psi_{d-1} - \psi_{d-2}) = 2^{(n-d-4)/2}(\psi_{d-1} - \psi_{d-2}) > 0. \end{aligned}$$

A3. $n = d+2k+1$, where $k \geqslant 2$, and $t = \frac{n-d-3}{2}$. Then

$$D_1(n,d) = 2^{(n-d-5)/2}(3\psi_{d-2} - \psi_d) > 0.$$

A4. $n = d+2k+1$, where $k \geqslant 3$, and $t \leqslant \frac{n-d-5}{2}$. Then

$$D_1(n,d) \geqslant 2^{(n-d-7)/2}(8\psi_{d-2} - 4\psi_{d-1} - 1) > 0.$$

B. Tree T has the form shown in Fig. 16b, where $\mathrm{diam}(T') = d$ and $1 \leqslant t \leqslant \frac{n-d-3}{2}$. In this case $M(n,d) - i_M(T) \geqslant D_2(n,d)$, where

$$D_2(n,d) = M(n,d) - M(n-2,d) - M(n-2t-2,d) \cdot 2^{t-1}.$$

Let us consider several subcases:

B1. $n = d + 2k + 1$, where $k \geqslant 2$. Then

$$\begin{aligned} D_2(n,d) &= 2^{(n-d-3)/2}\psi_{d-2} - 2^{t-1}(\psi_{d-1} - \psi_{d-2}) \geqslant \\ &\geqslant 2^{(n-d-3)/2}\psi_{d-2} - 2^{(n-d-5)/2}(\psi_{d-1} - \psi_{d-2}) = \\ &= 2^{(n-d-5)/2}(3\psi_{d-2} - \psi_{d-1}) > 0. \end{aligned}$$

B2. $n = d + 2k$, where $k \geqslant 3$ and $t = \frac{n-d-4}{2}$. Then

$$D_2(n,d) = 2^{(n-d-6)/2}(4\psi_{d-1} - \psi_d - \psi_{d-2}) > 0.$$

B3. $n = d + 2k$, where $k \geqslant 3$ and $t \leqslant \frac{n-d-6}{2}$. Then

$$D_2(n,d) > 2^{(n-d-4)/2}(\psi_{d-1} - 1) > 0.$$

Thus, in any case, the existence of vertices at a distance greater than two from path P contradicts the $(n,d)_{\text{m.i.s.}}$–maximality of T. From this and from lemma 14 it follows that every vertex in T is at a distance of no more than 2 from the diametral path, and any vertex of T is adjacent to at most one leaf.

Let us separately consider the cases when tree T has diameter 6 and 7.

C. $\operatorname{diam}(T) = 6$. Suppose tree T is not isomorphic to any of the trees $\breve{B}_{6,n}$, $\widetilde{B}'_{6,n,p}$. Then the following cases are possible:

C1. T has the form shown in Fig. 16b, where $1 \leqslant t \leqslant \frac{n-6}{2}$ and $\operatorname{diam}(T') \geqslant 3$. If T' has exactly four vertices, then

$$i_M(T) = 2 + 3 \cdot 2^{(n-6)/2} < M(n,6).$$

Let T' have at least 5 vertices. Then from lemma 15 and the induction hypothesis it follows that

$$M(n,6) - i_M(T) \geqslant M(n,6) - \max_{d\in\{5,6\}} M(n-2,d) - 2^{t-1}M(n-2t-2,4).$$

If n is even, then $\max_{d\in\{5,6\}} M(n-2,d) = M(n-2,5)$ and

$$\begin{aligned} M(n,6) - i_M(T) &\geqslant M(n,6) - M(n-2,5) - 2^{t-1}M(n-2t-2,4) \geqslant \\ &\geqslant 2^{(n-8)/2} - 1 > 0. \end{aligned}$$

If n is odd, then $\max_{d\in\{5,6\}} M(n-2,d) = M(n-2,6)$ and

$$M(n,6) - i_M(T) \geqslant M(n,6) - M(n-2,6) - 2^{t-1}M(n-2t-2,4) = \\ = 2^{(n-7)/2} > 0.$$

C2. T is either isomorphic to one of the trees $\widehat{B}_{6,n,p,q}$, $\widehat{B}'_{6,n,p,q}$, or is isomorphic to tree $\widehat{B}_{6,n,p}$ where $2 \leqslant p \leqslant \frac{n-7}{2}$. From the table below, it is evident that in all these cases $i_M(T) < M(n,6)$.

T	$i_M(T)$	lower bound for $(M(n,6) - i_M(T))$
$\widehat{B}_{6,n,p,q}$	$2^{(n-3)/2} + 2^p + 2^{(n-3-2p-2q)/2} - 1$	$2^{(n-7)/2}$
$\widehat{B}'_{6,n,p,q}$	$2^{(n-4)/2} + 2^{(n-4-2q)/2}$	$2^{(n-6)/2}$
$\widehat{B}_{6,n,p}$	$2^{(n-3)/2} + 2^p + 2^{(n-3-2p)/2} - 1$	$2^{(n-7)/2} - 2$

D. $\mathrm{diam}(T) = 7$. The following subcases are possible:

D1. T has the form shown in Fig. 16b, where $1 \leqslant t \leqslant \frac{n-7}{2}$ and $\mathrm{diam}(T') \geqslant 4$. Then from lemma 15 and the induction hypothesis it follows that

$$M(n,7) - i_M(T) \geqslant M(n,7) - \max_{d\in\{6,7\}} M(n-2,d) - 2^{t-1}M(n-2t-2,4).$$

If n is even, then $\max_{d\in\{6,7\}} M(n-2,d) = M(n-2,7)$ and

$$M(n,7) - i_M(T) \geqslant M(n,7) - M(n-2,7) - 2^{t-1}M(n-2t-2,4) \geqslant 3\cdot 2^{(n-10)/2} > 0.$$

If n is odd, then $\max_{d\in\{6,7\}} M(n-2,d) = M(n-2,6)$ and

$$M(n,7) - i_M(T) \geqslant M(n,7) - M(n-2,6) - 2^{t-1}M(n-2t-2,4) = 0,$$

where from lemma 15 and the induction hypothesis it follows that the equality $M(n,7) - i_M(T) = M(n,7) - M(n-2,6) - 2^{t-1}M(n-2t-2,4)$ is possible only if $t = 1$ and tree T' has the form $\widetilde{B}_{4,n'}$, which is possible only if T is isomorphic to tree $\widetilde{B}'_{7,n}$.

D2. T has the form shown in Fig. 16a, where $1 \leqslant t \leqslant \frac{n-6}{2}$. If n is even, then from the induction hypothesis and lemma 15 we obtain

$$i_M(T) \leqslant M(n-2,5) + 2^{t-1}M(n-2t-1,4) = M(n,7),$$

where the equality $i_M(T) = M(n,7)$ is possible only if subtree T' of tree T is isomorphic to tree $\widetilde{B}_{4,n'}$, and thus tree T itself is isomorphic to tree $\widetilde{B}_{7,n}$.

Now suppose that n is odd, and T is not isomorphic to tree $\widetilde{B}'_{7,n}$, and also cannot be represented in the form described in item D1. Then T is isomorphic to tree $\widehat{B}_{7,n,p,q,r}$ for some $q, r \geqslant 0$, and the following relations hold

$$i_M(T) = 2^{(n-5)/2} + 2^{p+q} + 2^{(n-2q-5)/2} \leqslant 5 \cdot 2^{(n-7)/2} < M(n,7).$$

All cases where $d = \operatorname{diam}(T) \leqslant 7$ have been examined above, and for the remainder of the theorem's proof we will assume that $d \geqslant 8$. Let us fix some diametral path P in tree T. Denote by w, w', u, u', u'' the consecutive vertices of P, where w is an end vertex of P. In doing so, we will assume that if $\tilde{w}$, $\tilde{w}'$, $\tilde{u}$, $\tilde{u}'$, $\tilde{u}''$ are the vertices of P, taken in order starting from the end vertex $\tilde{w}$, opposite to w, then the sequence of degrees

$$(\deg w,\ \deg w',\ \deg u,\ \deg u',\ \deg u'')$$

is lexicographically not less than the sequence of degrees $(\deg \tilde{w},\ \deg \tilde{w}',\ \deg \tilde{u},\ \deg \tilde{u}',\ \deg \tilde{u}''$
Let us consider several cases:

1. Vertex u in T is adjacent to t paths of two vertices, where $t \geqslant 2$, and is not adjacent to any leaves. In this case tree T has the form shown in Fig. 16a, where $\operatorname{diam}(T') \geqslant d-3$. We have

$$i_M(T) \leqslant M(n-2,d) + 2^{t-1} \cdot \max_{d' \geqslant d-3} M(n-2t-1,d'). \tag{23}$$

1.1. If $2 \nmid (n-d)$, then from lemma 15 it follows that

$$\max_{d' \geqslant d-3} M(n-2t-1,d') \leqslant M(n-2t-1,d-3).$$

Then (23) implies

$$\begin{aligned} M(n,d) \ &-i_M(T) \geqslant M(n,d) - M(n-2,d) - 2^{t-1} \cdot M(n-2t-1,d-3) = \\ &= 2^{(n-d-1)/2}\psi_{d-2} - 2^{(n-d+1)}\psi_{d-5} - 2^{t-1}(\psi_{d-4} - \psi_{d-5}) \geqslant \\ &\geqslant 2^{(n-d-1)/2}\psi_{d-2} - 2^{(n-d+1)/2}\psi_{d-5} - 2^{(n-d-1)/2}(\psi_{d-4} - \psi_{d-5}) = 0, \end{aligned}$$

where the equality $i_M(T) = M(n,d)$ occurs only in the case $t = \frac{n-d+1}{2}$, that is, only if tree T has the form $\check{B}_{d,n}$.

1.2. If $2 \mid (n-d)$, then from lemma 15 it follows that

$$\max_{d' \geqslant d-3} M(n-2t-1, d') \leqslant M(n-2t-1, d-2).$$

Then two situations are possible.

1.2.1. $n \geqslant d+6$. Then

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(n,d) - M(n-2,d) - 2^{t-1} \cdot M(n-2t-1, d-2) = \\ &= (2^{(n-d-2)/2} - 2^{t-1})(\psi_{d-3} - \psi_{d-4}) \geqslant 0, \end{aligned}$$

where the equality $i_M(T) = M(n,d)$ is possible only if $t = \frac{n-d}{2}$ and $\operatorname{diam}(T') = d-2$. But then tree T has the form $\check{B}'_{d,n}$.

1.2.2. $n = d+4$. Then tree T has the form $\widehat{B}^*_{d,k}$ for $k \geqslant 3$. If T has the form $\widehat{B}^*_{d,3}$, then

$$M(n,d) - i_M(T) = 4\psi_{d-1} - 2(\psi_d + \psi_{d-5}) - \psi_{d-3} > 0.$$

If T has the form $\widehat{B}^*_{d,4}$, then

$$M(n,d) - i_M(T) = 2\psi_{d-1} - 4\psi_{d-4} > 0.$$

If T has the form $\widehat{B}^*_{d,k}$, $k \geqslant 5$, then for $8 \leqslant d \leqslant 10$ the theorem's statement is verified by enumeration, and for $d \geqslant 11$ from the induction hypothesis it follows that

$$M(n,d) - i_M(T) \geqslant M(n,d) - M(n-2,d-2) - M(n-3,d-3) = 0,$$

where $i_M(T) = M(n,d)$ only if T has the form $\widetilde{B}'_{4,n}$.

2. Vertex u in T is adjacent to t, $t \geqslant 2$, paths of two vertices, and exactly one leaf. In this case tree T has the form shown in Fig. 16b, where $\operatorname{diam}(T') \geqslant d-3$. We have

$$i_M(T) \leqslant M(n-2,d) + 2^{t-1} \cdot \max_{d' \geqslant d-3} M(n-2t-2, d'). \tag{24}$$

2.1. If $2 \nmid (n-d)$, then from lemma 15 it follows that

$$\max_{d' \geqslant d-3} M(n-2t-1, d') \leqslant M(n-2t-2, d-2).$$

Then (24) implies

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(n,d) - M(n-2,d) - 2^{t-1} \cdot M(n-2t-2, d-2) = \\ &= 2^{(n-d-1)/2}(\psi_{d-2} - \psi_{d-4}) - 2^{t-1}(\psi_{d-3} - \psi_{d-4}) \geqslant \\ &\geqslant 2^{(n-d-1)/2}(\psi_{d-2} - \psi_{d-4}) - 2^{(n-d-3)/2}(\psi_{d-3} - \psi_{d-4}) = \\ &= 2^{(n-d-3)/2}(2\psi_{d-2} - \psi_{d-1}) > 0. \end{aligned}$$

2.2. If $2 \mid (n-d)$, then from lemma 15 it follows that

$$\max_{d' \geqslant d-3} M(n-2t-2, d') \leqslant M(n-2t-2, d-3).$$

Then (24) implies

$$\begin{aligned} M(n,d) \ &-i_M(T) \geqslant M(n,d) - M(n-2,d) - 2^{t-1} \cdot M(n-2t-2, d-3) = \\ &= 2^{(n-d-2)/2}\psi_{d-1} - 2^{t-1}(\psi_{d-4} - \psi_{d-5}) - 2^{(n-d)/2}\psi_{d-5} \geqslant \\ &\geqslant 2^{(n-d-2)/2}\psi_{d-1} - 2^{(n-d-2)/2}(\psi_{d-4} - \psi_{d-5}) - 2^{(n-d)/2}\psi_{d-5} = 0, \end{aligned}$$

where for the equality $i_M(T) = M(n,d)$ it is necessary that $t = \frac{n-d}{2}$. But for $t = \frac{n-d}{2}$ we have

$$M(n,d) - i_M(T) = 2^{(n-d)/2}(\psi_{d-1} - \psi_{d-2}) - \psi_{d-3} \geqslant 4(\psi_{d-1} - \psi_{d-2}) - \psi_{d-3} > 0.$$

3. Vertex u in T is adjacent to one path of two vertices and one leaf. In this case tree T has the form shown in Fig. 16c, where $\operatorname{diam}(T') \geqslant d-3$. In this case, as in the previous ones, we apply the induction hypothesis and lemma 15:

3.1. If $2 \mid (n-d)$, then

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(n,d) - M(n-2,d-1) - M(n-4,d-3) = \\ &= (2^{(n-d)/2} - 1)(\psi_{d-4} - \psi_{d-5}) - \psi_{d-2} + \psi_{d-3} \geqslant \\ &\geqslant 3(\psi_{d-4} - \psi_{d-5}) - \psi_{d-2} + \psi_{d-3} > 0. \end{aligned}$$

3.2. If $2 \nmid (n-d)$, then

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(n,d) - M(n-2,d-1) - M(n-4,d-2) \geqslant \\ &\geqslant (2^{(n-d-1)/2} - 1)(\psi_{d-2} - \psi_{d-4}) + \psi_{d-1} - \psi_{d-3} - 1 > 0. \end{aligned}$$

4. Now suppose that vertex u is adjacent to one path of two vertices and is not adjacent to any leaves (i.e., $\deg u = 2$). Let us consider vertex u' adjacent to u and located at distance 3 from the end of the diametral path P. Four cases are possible:

4.1. Vertex u' is adjacent to at least one path of two vertices. Then $M(n,d) - - i_M(T) \geqslant D_3(n,d)$, where

$$D_3(n,d) = M(n,d) - M(n-2,d-1) - M(n-3,d-1).$$

4.1.1. If $n = d+3$, then $D_3(n,d) = 3\psi_{d-2} - \psi_{d-3} - \psi_d > 0$.

4.1.2. If $n = d+4$, then for $d \geqslant 12$ the relations

$$D_3(n,d) = 2\psi_{d-4} - \psi_{d-3} - \psi_{d-5} > 0$$

hold, and for $8 \leqslant d \leqslant 11$ the inequality $i_M(T) < M(n,d)$ is verified by enumeration.

4.1.3. If $2 \nmid (n-d)$ and $n \geqslant d+5$, then

$$D_3(n,d) \geqslant (2^{(n-d-1)/2} - 1)(\psi_{d-2} - \psi_{d-3}) + \psi_{d-1} - \psi_{d-2} - 1 > 0.$$

4.1.4. If $2 \mid (n-d)$ and $n \geqslant d+6$, then

$$\begin{aligned} D_3(n,d) &= 2^{(n-d-2)/2}(2\psi_{d-4} - \psi_{d-2}) - \psi_{d-2} + \psi_{d-3} - 1 \geqslant \\ &\geqslant 4(2\psi_{d-4} - \psi_{d-2}) - \psi_{d-2} + \psi_{d-3} - 1 > 0. \end{aligned}$$

4.2. Vertex u' is not adjacent to any path of two vertices, but is adjacent to one leaf. In this case from statement 13 and the induction hypothesis it follows that $i_M(T) \leqslant 2M(n-3,d-2) < M(n,d)$.

4.3. The degree of vertex u' equals 2. In this case let us consider vertex u'' — adjacent to u' and located at distance 4 from the end of path P. Let us first consider the situation when u'' is not adjacent to any path of two vertices. If $d \notin \{9, 10\}$, or $2 \nmid (n-d)$, then the theorem's statement immediately follows from the induction hypothesis and the equality

$$M(n-2,d-2) + M(n-3,d-3) = M(n,d).$$

The cases $d = 9$, $2 \nmid n$ and $d = 10$, $2 \mid n$ need to be considered separately due to the "non-standard" behavior of function $M(n,d)$ for $d = 7$, $2 \nmid n$:

4.3.1. $d = 9$ and $2 \nmid n$. If tree $T \setminus \{w, w'\}$ is not isomorphic to tree $\widetilde{B}'_{7,n-2}$ and simultaneously tree $T \setminus \{w, w', u\}$ is not isomorphic to tree $\widetilde{B}'_{6,n-3,p}$, then from the induction hypothesis it follows that

$$i_M(T) \leqslant M(n-2,7) + M(n-3,6) - 2 < M(n,7).$$

If however tree $T \setminus \{w, w'\}$ is isomorphic to tree $\widetilde{B}'_{7,n-2}$, or tree $T \setminus \{w, w', u\}$ is isomorphic to tree $\widetilde{B}'_{6,n-3,p}$, then tree T falls under one of the already examined cases 1, 3, 4.2.

4.3.2 $d = 10$ and $2 \mid n$. If tree $T \setminus \{w, w'\}$ is not isomorphic to tree $\check{B}'_{d,n-2}$ and simultaneously tree $T \setminus \{w, w', u\}$ is not isomorphic to tree $\widetilde{B}'_{7,n-3}$, then from the induction hypothesis it follows that

$$i_M(T) \leqslant M(n-2,8) + M(n-3,7) - 2 < M(n,7).$$

If tree $T \setminus \{w, w'\}$ is isomorphic to tree $\check{B}'_{d,n-2}$, then T has the form $\widetilde{B}'_{7,n}$. If tree $T \setminus \{w, w', u\}$ is isomorphic to tree $\widetilde{B}'_{7,n-3}$, then tree T falls under one of the already examined cases 1, 3, 4.2.

4.4. It remains now only to consider the case when the degree of vertex u' equals 2, and vertex u'' is adjacent to at least one path of two vertices. Four subcases are possible:

4.4.1. Tree T has diameter 8. Then $n \geqslant 11$ and T has the form $\widehat{B}_{8,n}$ or $\widehat{B}'_{8,n}$. From the table below, it is evident that in both cases $i_M(T) < M(n,8)$.

T	$i_M(T)$	$M(n,8) - i_M(T)$
$\widehat{B}_{8,n}$	$9 \cdot 2^{(n-9)/2} + 3$	$2^{(n-9)/2} - 1$
$\widehat{B}'_{8,n}$	$9 \cdot 2^{(n-10)/2} + 4$	$5 \cdot 2^{(n-10)/2} - 4$

4.4.2. Tree T has diameter 9. Then $n \geqslant 14$ and T has the form $\widehat{B}_{9,n,p}$, $\widehat{B}'_{9,n,p}$ or $\widehat{B}''_{9,n,p}$. From the table below, it is evident that in all three cases $i_M(T) < M(n,9)$.

[This is an automated translation of the original manuscript from Russian into English]

T	$i_M(T)$	lower bound for $(M(n,9) - i_M(T))$
$\widehat{B}_{9,n,p}$	$9 \cdot 2^{(n-10)/2} + 3(2^p + 2^{(n-10-2p)/2}) + 1$	$7 \cdot 2^{(n-12)/2} - 5$
$\widehat{B}'_{9,n,p}$	$9 \cdot 2^{(n-11)/2} + 3 \cdot 2^p + 6 \cdot 2^{(n-11-2p)/2}$	$3 \cdot 2^{(n-9)/2} - 6$
$\widehat{B}''_{9,n,p}$	$9 \cdot 2^{(n-12)/2} + 6(2^p + 2^{(n-12-2p)/2})$	$2^{(n-4)/2} - 10$

4.4.3. $d \geqslant 10$ and T has the form shown in Fig. 16d. Then, if $2 \mid (n-d)$ and $n \geqslant d+6$, then

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(n,d) - M(n-2,d) - 3 \cdot 2^{t-1} \cdot M(n-2t-5, d-4) = \\ &= 2^{(n-d-2)/2}(\psi_{d-1} - 3\psi_{d-6}) - 3 \cdot 2^{t-1}(\psi_{d-5} - \psi_{d-6}) \geqslant \\ &\geqslant 2^{(n-d-2)/2}(\psi_{d-1} - 3\psi_{d-6}) - 3 \cdot 2^{(n-d-4)/2}(\psi_{d-5} - \psi_{d-6}) = \\ &= 2^{(n-d-4)/2}(2\psi_{d-4} - \psi_{d-3}) > 0. \end{aligned}$$

If $n = d+4$, then $t = 1$ and

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(d+4,d) - M(d+2,d) - 3M(d-3,d-4) = \\ &= 4\psi_{d-1} - 2\psi_d - 2\psi_{d-3} > 0. \end{aligned}$$

If $2 \nmid (n-d)$, then

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(n,d) - M(n-2,d) - 3 \cdot 2^{t-1} \cdot M(n-2t-5, d-5) = \\ &= 2^{(n-d-1)/2}(\psi_{d-2} - 3\psi_{d-7}) - 3 \cdot 2^{t-1}(\psi_{d-6} - \psi_{d-7}) \geqslant \\ &\geqslant 2^{(n-d-1)/2}(\psi_{d-2} - 3\psi_{d-7}) - 3 \cdot 2^{(n-d-3)/2}(\psi_{d-6} - \psi_{d-7}) = \\ &= 2^{(n-d-3)/2}(2\psi_{d-2} - 3\psi_{d-4}) > 0. \end{aligned}$$

4.4.4. $d \geqslant 10$ and T has the form shown in Fig. 16e. Then, if $2 \mid (n-d)$ and $n \geqslant d+6$, then

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(n,d) - M(n-2,d) - 3 \cdot 2^{t-1} \cdot M(n-2t-6, d-5) = \\ &= 2^{(n-d-2)/2}(\psi_{d-1} - 3\psi_{d-7}) - 3 \cdot 2^{t-1}(\psi_{d-6} - \psi_{d-7}) \geqslant \\ &\geqslant 2^{(n-d-2)/2}(\psi_{d-1} - 3\psi_{d-7}) - 3 \cdot 2^{(n-d-4)/2}(\psi_{d-6} - \psi_{d-7}) = \\ &= 2^{(n-d-4)/2}(2\psi_{d-3} - \psi_{d-4}) > 0. \end{aligned}$$

If $n = d+4$, then $t = 1$ and

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(d+4,d) - M(d+2,d) - 3M(d-4,d-5) = \\ &= \psi_{d-1} + 2\psi_{d-3} - 2\psi_{d-2} > 0. \end{aligned}$$

If $2 \nmid (n-d)$, then

$$\begin{aligned} M(n,d) - i_M(T) &\geqslant M(n,d) - M(n-2,d) - 3 \cdot 2^{t-1} \cdot M(n-2t-6, d-4) = \\ &= 2^{(n-d-3)/2}(2\psi_{d-2} - 3\psi_{d-6}) - 3 \cdot 2^{t-1}(\psi_{d-5} - \psi_{d-6}) \geqslant \\ &\geqslant 2^{(n-d-3)/2}(2\psi_{d-2} - 3\psi_{d-6}) - 3 \cdot 2^{(n-d-5)/2}(\psi_{d-5} - \psi_{d-6}) = \\ &= 2^{(n-d-5)/2}(4\psi_{d-2} - 3\psi_{d-3}) > 0. \end{aligned}$$

The theorem is proved. □

Chapter 3. Estimates of the Number of Independent Sets in Graphs with Fixed Independence Number

We study the relationships between the size of a maximum independent set and the number of independent sets in various classes of graphs.

3.1 Upper Bound on the Number of Independent Sets in the Class of All Graphs with a Given Independence Number

Let $n, \alpha \in \mathbb{N}$, $\alpha \leqslant n$. Let $i(n,\alpha)$ denote the maximum number of independent sets among all graphs on n vertices with independence number α:

$$i(n,\alpha) = \max_{\substack{n(G)=n,\\ \alpha(G)=\alpha}} i(G). \tag{25}$$

Recall that $UK_{n,\alpha}$ denotes the union of $(\alpha\cdot(\lfloor n/\alpha\rfloor+1)-n)$ cliques of size $\lfloor n/\alpha\rfloor$ and $(n-\alpha\cdot\lfloor n/\alpha\rfloor)$ cliques of size $\lceil n/\alpha\rceil$.

Let us prove several auxiliary statements.

Proposition 17. *For $\alpha < n$, the following inequalities hold:*

1. $i(n,\alpha) < i(n,\alpha+1)$,
2. $i(n-1,\alpha) < i(n,\alpha)$.

Proof.

1. Let G be a graph such that $n(G) = n, \alpha(G) = \alpha$ and $i(G) = i(n,\alpha)$. Then G has the following property: any graph G' obtained from G by removing one edge has parameters $n(G') = n$, $\alpha(G') = \alpha+1$. We have

$$i(n,\alpha+1) \geqslant i(G') > i(G) = i(n,\alpha).$$

2. Let G be a graph such that $n(G) = n-1, \alpha(G) = \alpha$ and $i(G) = i(n-1, \alpha)$. By adding to G a vertex $v \notin V(G)$ and all edges $\{v\} \times V(G)$, we obtain a graph G' such that $n(G') = n$, $\alpha(G') = \alpha$. We get

$$i(n, \alpha) \geqslant i(G') > i(G) = i(n-1, \alpha).$$

□

For $n, \alpha \in \mathbb{N}$ let

$$m(n, \alpha) = (\lceil n/\alpha \rceil + 1)^{n - \alpha \cdot \lfloor n/\alpha \rfloor} \cdot (\lfloor n/\alpha \rfloor + 1)^{\alpha \cdot (\lfloor n/\alpha \rfloor + 1) - n}.$$

One can easily verify that $i(UK_{n,\alpha}) = m(n, \alpha)$.

Proposition 18. *For $1 < \alpha < n$, the following inequalities hold*

$$2^{\alpha-1} \leqslant m(n - \lceil n/\alpha \rceil, \alpha - 1) = m(n, \alpha) - m(n-1, \alpha).$$

Proof. The inequality $m(n - \lceil n/\alpha \rceil, \alpha - 1) \geqslant 2^{\alpha-1}$ follows from the fact that $m(n - \lceil n/\alpha \rceil, \alpha - 1)$ is a product of $\alpha - 1$ factors, each of which is not less than 2. Let us prove the equality

$$m(n - \lceil n/\alpha \rceil, \alpha - 1) = m(n, \alpha) - m(n-1, \alpha).$$

Consider first the case when $n = \alpha \cdot t$, $t \in \mathbb{N}$. We have

$$\begin{aligned} m(n - \lceil n/\alpha \rceil, \alpha - 1) &= m(n - t, \alpha - 1) = (t+1)^{\alpha-1} = \\ &= (t+1)^{\alpha} - (t+1)^{\alpha-1} t = \\ &= m(n, \alpha) - m(n-1, \alpha). \end{aligned}$$

Now let $n = \alpha \cdot t + s$, where $t, s \in \mathbb{N}$ and $1 \leqslant s < \alpha$. Then

$$\begin{aligned} m(n - \lceil n/\alpha \rceil, \alpha - 1) &= m(n - t - 1, \alpha - 1) = (t+2)^{s-1}(t+1)^{\alpha-s} = \\ &= (t+2)^{s}(t+1)^{\alpha-s} - (t+2)^{s-1}(t+1)^{\alpha-s+1} = \\ &= m(n, \alpha) - m(n-1, \alpha). \end{aligned}$$

□

Theorem 18. *For any n, α, the following equality holds*

$$i(n,\alpha) = m(n,\alpha), \tag{26}$$

and the maximum in (25) is achieved on graphs isomorphic to $UK_{n,\alpha}$, and only on them.[2]

Proof. The proof is by induction on n. If $n = 1$, then the statement of the theorem holds. Let $n > 1$ and assume the theorem holds for all $n' < n$. In the case when $\alpha = 1$ or $\alpha = n$, the statement of the theorem holds. From now on, we assume $1 < \alpha < n$. Note immediately that $i(n,\alpha) \geqslant m(n,\alpha)$, since $i(UK_{n,\alpha}) = m(n,\alpha)$. Let G be a graph for which $n(G) = n$, $\alpha(G) = \alpha$, $i(G) = i(n,\alpha)$. Consider two cases.

Suppose that the maximum degree of vertices in G does not exceed $(\lceil n/\alpha \rceil - 2)$. Any set of vertices $\{v_1, \ldots, v_t\} \subseteq V(G)$ satisfying the conditions

$$v_j \in V(G) \setminus (\bigcup_{j'<j} (\{v_{j'}\} \cup \partial v_{j'}))$$

will be independent. The size of the largest such set will be not less than $\frac{n}{\lceil n/\alpha \rceil - 1} > \alpha$, which contradicts the equality $\alpha(G) = \alpha$.

Now let the maximum degree of vertices in G be d, $d \geqslant \lceil n/\alpha \rceil - 1$. Let us decompose G with respect to an arbitrary vertex v of degree d:

$$i(G) = i(G \setminus \{v\}) + i(G \setminus (\{v\} \cup \partial v)).$$

Since $\alpha(G \setminus v) \leqslant \alpha$, and

$$\alpha(G \setminus (v \cup \partial v)) \leqslant \min\{\alpha - 1, n - d - 1\},$$

then, using statement 17, taking into account the induction hypothesis we have

$$\begin{aligned} i(G) &\leqslant i(n-1,\alpha) + i(n-d-1, \min\{\alpha-1, n-d-1\}) \leqslant \\ &\leqslant m(n-1,\alpha) + m(n-d-1, \min\{\alpha-1, n-d-1\}). \end{aligned}$$

[2]This theorem is a special case of one of Erdős's theorems. See footnote on p. 11.

Let us first consider the case when $d > n - \alpha$. Then, using statement 18, we obtain

$$\begin{aligned} i(G) &\leqslant m(n-1,\alpha) + m(n-d-1, n-d-1) = \\ &= m(n-1,\alpha) + 2^{n-d-1} \leqslant \\ &\leqslant m(n-1,\alpha) + 2^{\alpha-2} < \\ &< m(n,\alpha), \end{aligned}$$

which contradicts the choice of G. Now let $d \leqslant n - \alpha$. Taking into account the inequality $d \geqslant \lceil n/\alpha \rceil - 1$, using statement 18, we obtain

$$\begin{aligned} i(G) &\leqslant m(n-1,\alpha) + m(n-d-1, \alpha-1) \leqslant \\ &\leqslant m(n-1,\alpha) + m(n - \lceil n/\alpha \rceil, \alpha - 1) = \\ &= m(n,\alpha). \end{aligned} \tag{27}$$

From (27) and the induction hypothesis, it follows that to achieve equality $i(G) = m(n,\alpha)$, it is necessary that the graph $G \setminus \{v\}$ be isomorphic to $UK_{n-1,\alpha}$, the graph $G \setminus (\{v\} \cup \partial v)$ be isomorphic to $UK_{n-\lceil n/\alpha \rceil, \alpha-1}$, and the maximum degree of vertices in G be equal to $(\lceil n/\alpha \rceil - 1)$. But this is possible only when $G \simeq UK_{n,\alpha}$. The theorem is proved. □

Corollary. *Among all forests on n vertices with independence number α, only the union of a matching on $2(n-\alpha)$ vertices and $2\alpha - n$ isolated vertices has the maximum number of independent sets.*

Remark. *For a sequence of parameter pairs (n_k, α_k) such that $n_k = k^2 + 2k$ and $\alpha_k = k^2$, the ratio of the right-hand sides of (2) and (26) equals*

$$\frac{(2+2/k)^{k^2}}{2^{k^2} \cdot (3/2)^{2k}} = \left(\frac{4}{9}(1+1/k)^k\right)^k > c^k,$$

where $c > 1$. At the same time, the logarithms of the right-hand sides of (2) and (26) are asymptotically equal.

3.2 Upper Bounds on the Number of Independent Sets in Forests with Given Independence Number

Let $T_{n,\alpha}$ denote the tree obtained from the star $K_{1,\alpha}$ by subdividing $(n-\alpha-1)$ edges. One can easily verify that $\alpha(T_{n,\alpha}) = \alpha$ and

$$i(T_{n,\alpha}) = 2^{n-\alpha+1} + 3^{n-\alpha+1}2^{2\alpha-n+1}.$$

Theorem 19. *For any n, α $(n \geqslant 2)$, among all trees on n vertices with independence number α, only trees isomorphic to $T_{n,\alpha}$ have the maximum number of independent sets.*

Proof. We shall prove this by induction on n. For $n \in \{2, 3\}$, the statement of the theorem holds. Let $n \geqslant 4$ and assume the theorem holds for smaller values of n. Let G be a tree such that $n(G) = n$, $\alpha(G) = \alpha$, and $i(G) \geqslant i(G')$ for any tree G' with parameters $n(G') = n$, $\alpha(G') = \alpha$. Let the diameter of graph G be d. Let v, v' be pendant vertices in G at distance d from each other, and let w be the only neighbor of v in G.

1. Let w have degree 2. In this case, the graph $G \setminus \{v, w\}$ is a tree. Using the induction hypothesis taking into account $i(G \setminus \{v, w\}) \leqslant \alpha - 1$, as well as the monotonicity of $i(T_{n,\alpha})$ with respect to α for fixed n, we obtain

$$\begin{aligned} i(G) &= i(G \setminus \{v\}) + i(G \setminus \{v, w\}) \leqslant \\ &\leqslant (2^{n-\alpha-2} + 3^{n-\alpha-2} \cdot 2^{2\alpha-n+2}) + (2^{n-\alpha-2} + 3^{n-\alpha-2} \cdot 2^{2\alpha-n+1}) = \\ &= 2^{n-\alpha-1} + 3^{n-\alpha-1} \cdot 2^{2\alpha-n+1}. \end{aligned}$$

   Moreover, from the induction hypothesis it follows that for equality $i(G) = 2^{n-\alpha-1}+3^{n-\alpha-}$ to hold, it is necessary that graphs $G\setminus\{v\}$ and $G\setminus\{v, w\}$ be isomorphic to $T_{n-1,\alpha}$ and $T_{n-2,\alpha-1}$ respectively. This is possible only when $G \simeq T_{n,\alpha}$.

2. Let $\deg w \geqslant 3$. Let us show that in this case vertex w is adjacent to at least one more pendant vertex besides v. Assume the contrary, in which case there exist vertices w_1, $w_2 \in \partial w \setminus \{v\}$ for which $\deg w_1 \geqslant 2, \deg w_2 \geqslant 2$. At least one of vertices w_1, w_2 does not lie on the path from v' to v, let it be w_1. Let

$v'' \in \partial w_1 \setminus \{w\}$. The distance between vertices v' and v'' will be not less than $(d+1)$, which contradicts the definition of d. Thus, among the neighbors of vertex w there are at least two pendant vertices. From this it follows that vertex w does not belong to any maximum independent set in G, while vertex v belongs to all such sets. Consequently, $\alpha(G \setminus \{v\}) = \alpha - 1$. We have

$$\begin{aligned} i(G) &= i(G \setminus \{v\}) + i(G \setminus \{v, w\}) \leqslant \\ &\leqslant (2^{n-\alpha-1} + 3^{n-\alpha-1} \cdot 2^{2\alpha-n}) + i(n-2, \alpha-1) = \\ &= (2^{n-\alpha-1} + 3^{n-\alpha-1} \cdot 2^{2\alpha-n}) + 3^{n-\alpha-1} \cdot 2^{2\alpha-n} = \\ &= 2^{n-\alpha-1} + 3^{n-\alpha-1} \cdot 2^{2\alpha-n+1}. \end{aligned}$$

From the induction hypothesis and corollary to theorem 18 it follows that for equality $i(G) = 2^{n-\alpha-1} + 3^{n-\alpha-1} \cdot 2^{2\alpha-n+1}$ to hold, it is necessary that graph $G \setminus \{v\}$ be isomorphic to $T_{n-1,\alpha-1}$, and graph $G \setminus \{v, w\}$ be a union of a matching and isolated vertices. This is possible only when $G \simeq T_{n,\alpha}$.

□

Let $F_{n,\alpha}$ denote the union of a matching on $2(n-\alpha-1)$ vertices and a star $K_{1,2\alpha-n+1}$.

Theorem 20. *Among all forests on n vertices without isolated vertices with independence number α, the maximum number of independent sets is achieved only on forests isomorphic to $F_{n,\alpha}$.*

Proof. We shall prove this by induction on n. For $n \in \{2, 3\}$, the statement of the theorem holds. The theorem is also obviously true when $\alpha = n - 1$. From now on we assume $\alpha < n - 1$. Let F be a forest without isolated vertices such that $n(F) = n$, $\alpha(F) = \alpha$ and $i(F) \geqslant i(F')$ for any forest F' without isolated vertices with the same number of vertices and independence number. From theorem 19 and inequality $i(T_{n,\alpha}) < i(F_{n,\alpha})$ for $\alpha < n - 1$ it follows that F cannot be a tree. Consequently, there exist induced subgraphs F_1, F_2 such that $V(F_1) \cap V(F_2) = \varnothing$ and $F = F_1 \cup F_2$. We have

$$i(F) = i(F_1)i(F_2); \quad n(F) = n(F_1) + n(F_2); \quad \alpha(F) = \alpha(F_1) + \alpha(F_2),$$

from which it follows that if at least one of the graphs F_1, F_2 is not isomorphic to $F_{n',\alpha'}$ for some n', α', then $i(F) < i(F_{n,\alpha})$. If both graphs F_1, F_2 contain stars on t_1 and t_2 vertices respectively ($t_1, t_2 \geqslant 3$), then by replacing these stars in F with one star K_{1,t_1+t_2-3} and an edge, we obtain a graph F' such that $n(F') = n, \alpha(F') = \alpha, i(F') > i($ — a contradiction. If one of the graphs F_1, F_2 is a matching, then $F \simeq F_{n,\alpha}$, which was to be proved. □

3.3 Relationships Between Independence Number and Number of Independent Sets in Regular Graphs

Let $\mathcal{G}(n,k)$ denote the class of all k-regular graphs on n vertices. N. Alon's conjecture (see Introduction) states that the maximum number of independent sets in class $\mathcal{G}(n,k)$ for $2k \mid n$ is achieved on $G_A(n,k)$ — the union of $\frac{n}{2k}$ disjoint complete bipartite graphs. Alon's graph $G_A(n,k)$ has the maximum possible independence number for a regular graph, $\frac{n}{2}$, with

$$i(G_A(n,k)) = 2^{\frac{n}{2}(1+\theta(k^{-1}))}.$$

A question arises: how much does one need to restrict the independence number of graph G from class $\mathcal{G}(n,k)$ to achieve the inequality $i(G) \leqslant 2^{\frac{n}{2}}$? A partial answer to this question is given by theorem 22 below.

Lemma 18. *For any natural number k, $k \geqslant 3$, there exists a k-regular graph G_k for which the following inequalities hold*

$$\alpha(G_k) < \frac{|V(G_k)|}{2}\left(1 - \Omega(k^{-1})\right), \tag{28}$$

$$\log_2(i(G_k)) > \frac{|V(G_k)|}{2}\left(1 + \Omega(k^{-1})\right). \tag{29}$$

Proof. Let us consider graphs G_k of the following form:

- If k is even, then

$$
\begin{aligned}
V(G_k) \;=\;& \{u_i \mid i = \overline{1,\, k}\,\} \cup \\
& \cup \{v_i^j \mid i = \overline{1,\, k},\; j = \overline{1,\, k-2}\,\} \cup \\
& \cup \{w_l^j \mid l = \overline{1,\, k-2},\; j = \overline{1,\, k-2}\,\};
\end{aligned}
$$

$$
\begin{aligned}
E(G_k) \;=\;& \{\,\{u_i, u_{i+1}\} \mid i = \overline{1,\, k-1}\,\} \cup \{\,\{u_k, u_1\}\,\} \cup \\
& \cup \{\,\{u_i, v_i^j\} \mid i = \overline{1,\, k},\; j = \overline{1,\, k-2}\,\} \cup \\
& \cup \{\,\{v_i^j, w_l^j\} \mid i = \overline{1,\, k},\; l = \overline{1,\, k-2},\; j = \overline{1,\, k-2}\,\} \cup \\
& \cup \{\,\{v_i^j, v_i^{j+1}\} \mid i = \overline{1,\, k},\; j = 1,\, 3,\, \ldots,\, k-3\}.
\end{aligned}
$$

- If k is odd, then

$$
\begin{aligned}
V(G_k) \;=\;& \{u_i \mid i = \overline{1,\, k}\,\} \cup \\
& \cup \{v_i^j \mid i = \overline{1,\, k},\; j = \overline{1,\, k-2}\,\} \cup \\
& \cup \{w_l^j \mid l = \overline{1,\, k-2},\; j = \overline{1,\, k-3}\,\} \cup \\
& \cup \{w_l^{k-2} \mid l = \overline{1,\, k-1}\};
\end{aligned}
$$

$$
\begin{aligned}
E(G_k) \;=\;& \{\,\{u_i, u_{i+1}\} \mid i = \overline{1,\, k-1}\,\} \cup \{\,\{u_k, u_1\}\,\} \cup \\
& \cup \{\,\{u_i, v_i^j\} \mid i = \overline{1,\, k},\; j = \overline{1,\, k-2}\,\} \cup \\
& \cup \{\,\{v_i^j, w_l^j\} \mid i = \overline{1,\, k},\; l = \overline{1,\, k-2},\; j = \overline{1,\, k-3}\,\} \cup \\
& \cup \{\,\{v_i^{k-2}, w_l^{k-2}\} \mid i = \overline{1,\, k},\; l = \overline{1,\, k-1}\,\} \cup \\
& \cup \{\,\{v_i^j, v_i^{j+1}\} \mid i = \overline{1,\, k},\; j = 1,\, 3,\, \ldots,\, k-4\}.
\end{aligned}
$$

For any $k \geqslant 3$, graph G_k is k-regular. Examples of graphs G_3 and G_4 are shown in Fig. 17a and 17b respectively.

Fig. 18 shows how graph G_k is obtained as a union of simpler graphs (odd k case on top, even case below):

From now on we will only consider the case of even k; the reasoning for odd k is similar.

In this case G_k is a graph on $p = 2k^2 - 5k + 4$ vertices. Let us show that the inequality $\alpha(G_k) \leqslant \frac{p}{2}(1 - c'k^{-1})$ holds. Let A be an arbitrary independent set in graph G_k. There are two possible cases:

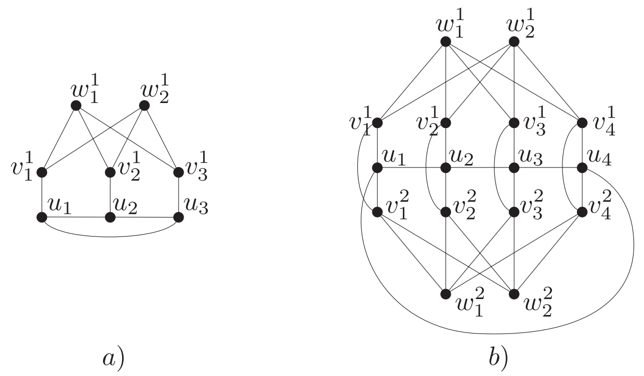

Figure 17. Graphs G_3 and G_4

i) Some vertex among $u_1, \ldots, u_k$ belongs to set A. Let it be vertex u_1. Then none of the vertices $v_1^1, \ldots, v_1^{k-2}$ belongs to set A. Moreover, in total from the set $\{u_1, \ldots, u_k\}$ at most $\left\lfloor \frac{k}{2} \right\rfloor$ vertices can belong to A. For each $j \in \{1, 3, \ldots, k-3\}$ from the set

$$\{v_i^j \mid i = \overline{1,\, k}\} \cup \{v_i^{j+1} \mid i = \overline{1,\, k}\} \cup \{w_l^j \mid l = \overline{1,\, k-2}\} \cup \{w_l^{j+1} \mid l = \overline{1,\, k-2}\}$$

at most $(k-1) + (k-2)$ vertices can belong to A. Therefore

$$|A| \leqslant \frac{k}{2} + \frac{k-2}{2}(2k-4) = k^2 - 3k + 3 = \frac{p}{2}(1 - \Omega(k^{-1})).$$

ii) None of the vertices $u_1, \ldots, u_k$ belongs to A. In this case

$$|A| \leqslant \frac{k-2}{2}(2k-2) = k^2 - 3k + 2.$$

This value is achieved when

$$A = \{v_i^j \mid i = \overline{1,\, k},\ j \equiv 1 \pmod 2\} \cup \{w_l^j \mid l = \overline{1,\, k-2},\ j \equiv 0 \pmod 2\}.$$

As in the previous case, $|A| = \frac{p}{2}(1 - \Omega(k^{-1}))$, and thus inequality (28) holds.

Let us now estimate the lower bound for the number of independent sets in graph G_k. Note that $i(G) > (i(G'_k))^{(k-2)/2}$, where G'_k is a subgraph of graph G induced by the vertex set

$$\{v_i^j \mid i = \overline{1,k},\ j = 1,2\} \cup \{w_l^j \mid l = \overline{1,k-2},\ j = 1,2\}.$$

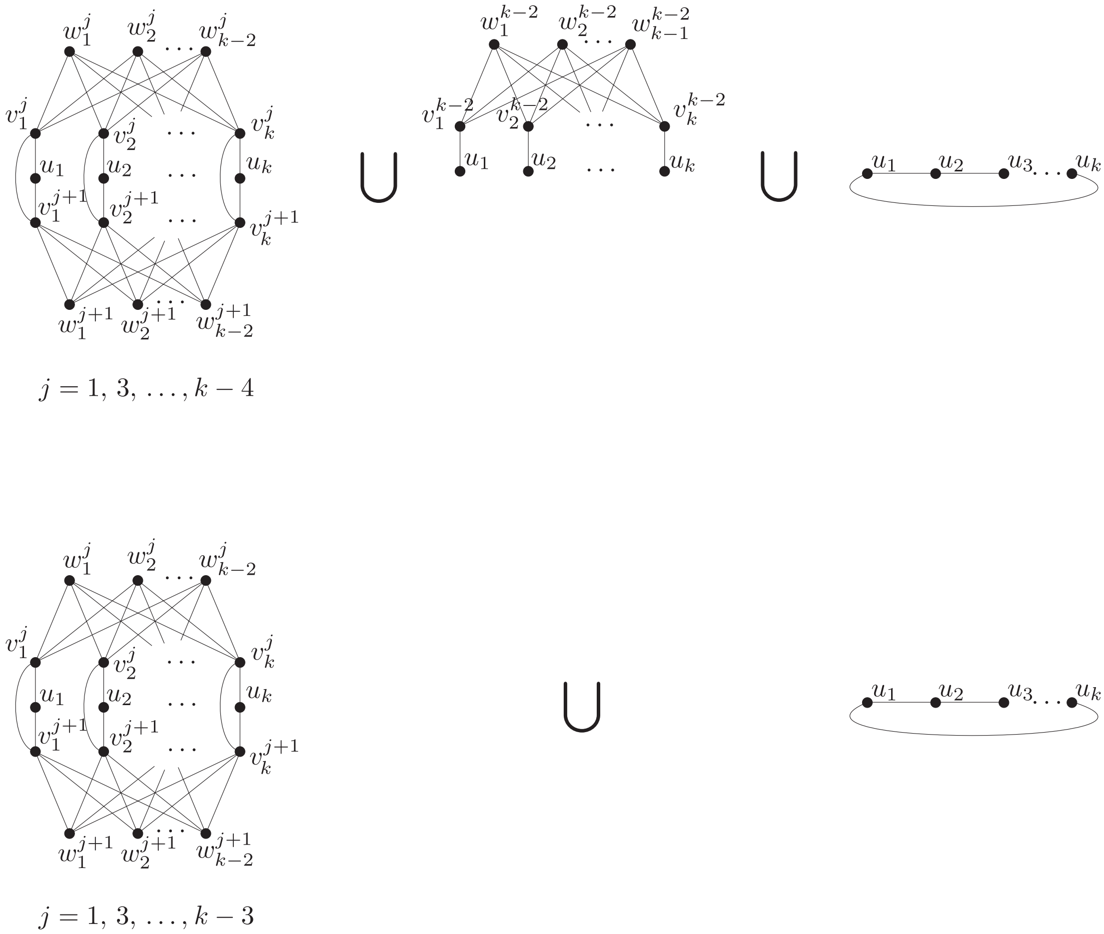

Figure 18. Structure of graph G_k

Graph G'_k is shown in Fig. 19.

The number $i(G'_k)$ can be written explicitly:

$$\begin{aligned} i(G'_k) &= (2^{k-2}-1)(2^k+2^{k-2}-1)+\sum_{j=0}^{k}\binom{k}{j}(2^{k-j}+2^{k-2}-1)= \\ &= \frac{9}{16}\cdot 2^{2k}+3^k-\frac{5}{2}\cdot 2^k+1>\frac{9}{16}\cdot 2^{2k}. \end{aligned}$$

Hence

$$\begin{aligned} \log_2(i(G)) &> (2k+\log_2(9/16))(k-2)/2= \\ &= k^2+k\log_2(3/16)-\log_2(9/16)=\frac{p}{2}(1+\Omega(k^{-1})). \end{aligned}$$

□

We will need the following theorem, proved in [18] using theorem 6:

Theorem 21 (A.A. Sapozhenko [18]). *Let graph G on n vertices be regular of degree*

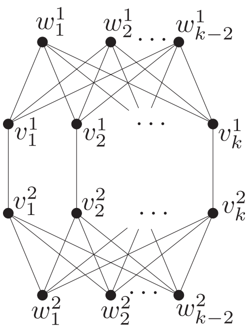

Figure 19. Graph G'_k

k, and let $\alpha(G) = \mu$. Then for any l, $1 \leqslant l \leqslant k$, the following inequality holds

$$i(G) \leqslant \left(\frac{nk}{\mu(2k-l)} + 1\right)^{\mu} \cdot (el)^{n/l},$$

where e is the base of the natural logarithm.

Theorem 22. *For arbitrarily large K and N there exists a k-regular graph G on n vertices such that $k > K$, $n > N$, and*

$$\begin{aligned} \alpha(G) &< \frac{n}{2}\left(1 - \Omega(k^{-1})\right), \\ \log_2(i(G)) &> \frac{n}{2}\left(1 + \Omega(k^{-1})\right). \end{aligned}$$

On the other hand, for any constant $\theta \in (0, 1/2)$ for any k-regular graph G on n vertices such that $\alpha(G) < \frac{n}{2}(1 - \Omega(k^{-\theta}))$, the following inequality holds

$$\log_2(i(G)) < \frac{n}{2}(1 - \Omega(k^{-\theta})).$$

Proof. Let us prove the first part of the theorem. Fix arbitrary natural numbers n and k such that $k \mid n$. Consider n/k graphs $G_{k,j}$, $j = \overline{1, n/k}$, each isomorphic to graph G_k, whose construction is described in lemma 18. Consider graph $G = \bigcup_{j=1}^{n/k} G_{k,j}$. Obviously, $G \in \mathcal{G}(n,k)$. From inequalities (28) and (29), and from equality $i(G) = \prod_{j=1}^{n/k} i(G_{k,j})$ it follows that

$$\begin{aligned} \alpha(G) &< \frac{n}{2}\left(1 - \Omega(k^{-1})\right), \\ \log_2(i(G)) &> \frac{n}{2}\left(1 + \Omega(k^{-1})\right), \end{aligned}$$

Now let us prove the second part of the theorem. From theorem 21, setting $l = \sqrt{k}$, for sufficiently large n and k for any graph $G \in \mathcal{G}(n,k)$ such that

$\alpha(G) < \frac{n}{2}(1-\varepsilon k^{-\theta})$, we obtain

$$
\begin{aligned}
i(G) \;&\leqslant \left(\frac{nk}{\frac{n}{2}(1-\varepsilon k^{-\theta})(2k-\sqrt{k})}+1\right)^{\frac{n}{2}(1-\varepsilon k^{-\theta})} \cdot (e\sqrt{k})^{nk^{-1/2}} = \\
&= 2^{\frac{n}{2}(1-\varepsilon k^{-\theta})} \cdot \left(\frac{k}{(1-\varepsilon k^{-\theta})(2k-\sqrt{k})}+\frac{1}{2}\right)^{\frac{n}{2}(1-\varepsilon k^{-\theta})} \cdot (e\sqrt{k})^{nk^{-1/2}} = \\
&= 2^{\frac{n}{2}(1-\varepsilon k^{-\theta})} \cdot \left(1+\frac{2\varepsilon k^{1-\theta}+\sqrt{k}-\varepsilon k^{1/2-\theta}}{2(1-\varepsilon k^{-\theta})(2k-\sqrt{k})}\right)^{\frac{n}{2}(1-\varepsilon k^{-\theta})} \cdot (e\sqrt{k})^{nk^{-1/2}} < \\
&< 2^{\frac{n}{2}(1-\varepsilon k^{-\theta})} \cdot \exp\left(\frac{n}{2}\cdot\frac{2\varepsilon k^{1-\theta}+\sqrt{k}-\varepsilon k^{1/2-\theta}}{4k-2\sqrt{k}}\right) \cdot (e\sqrt{k})^{nk^{-1/2}} = \\
&= 2^{\frac{n}{2}(1-\varepsilon k^{-\theta})} \cdot \exp\left(\frac{n}{2}\cdot\left(\frac{\varepsilon}{2}k^{-\theta}+O(k^{-1/2}\ln k)\right)\right) = \\
&= 2^{\frac{n}{2}\left(1-\left(\varepsilon-\frac{\varepsilon}{2\ln 2}\right)k^{-\theta}+O(k^{-1/2}\ln k)\right)} < 2^{\frac{n}{2}\left(1-\frac{\varepsilon}{4}k^{-\theta}+O(k^{-1/2}\ln k)\right)}.
\end{aligned}
$$

From this it follows that for any fixed $\theta \in (0,\, \frac{1}{2})$ we have $\log_2(i(G)) < \frac{n}{2}(1-\Omega(k^{-\theta}))$.

□

3.4 Number of Independent Sets in Quasi-Regular Bipartite Graphs

The *entropy* of a random variable X that takes values x_i with probabilities p_i is defined as $H(X) = -\sum\limits_i p_i \log_2 p_i$. The function of real argument $x \in [0,1]$ defined by the equality

$$H(x) = -x\log_2 x - (1-x)\log_2(1-x),$$

is called the *entropy function.*

Lemma 19 (J. Shearer [24])**.** *Let* $X = (X_1,\, X_2,\, \ldots,\, X_n)$ *be a vector random variable. Let* $\mathcal{A} = \{A_i\}_{i=1}^s$ *be a family of subsets of* $\{1,\, 2,\, \ldots,\, n\}$*. Let each number* i, $1 \leqslant i \leqslant n$ *appear in at least* k *sets* $A \in \mathcal{A}$*. For each* $A \in \mathcal{A}$ *define the vector r.v.* $X_A = (X_j \mid j \in A)$*. Then*

$$\sum_{A\in\mathcal{A}} H[X_A] \geqslant kH[X].$$

The main properties of entropy are given below (see, for example, [22, §14.6]).

Proposition 19. *For any r.v.* X_i

H1) $H[(X_1,\, X_2)] = H[X_1 \mid X_2] + H[X_2]$.

H2) $H[(X_1,\, X_2,\, \ldots,\, X_k)] \leqslant H[X_1] + H[X_2] + \ldots + H[X_k]$.

H3) *If r.v.* X_1 *is functionally dependent on* X_2*, then for any r.v.* X_3 *the inequality* $H[X_3 \mid X_2] \leqslant H[X_3 \mid X_1]$ *holds.*

H4) *If r.v.* X_1 *is functionally dependent on* X_2*, then* $H[(X_1,\, X_2)] = H[X_2]$*.*

H5) *If r.v.* X *takes* k *values, then* $H[X] \leqslant \log_2 k$*.*

The following theorem generalizes theorem 5 to quasi-regular bipartite graphs.

Theorem 23. *Let* G *be a bipartite graph with parts* A *and* B*. Let the degrees of vertices from* A *be bounded above by number* k_2*, and the degrees of vertices from* B *be bounded below by number* k_1*. Then*

$$i(G) \leqslant (2^{k_1} + 2^{k_2} - 1)^{\frac{|A|}{k_1}}.$$

Proof. Every independent set $I \in \mathcal{I}(G)$ will be identified with its vector indicator $(X_v \mid v \in A \cup B)$. Here X_v is the indicator of the event "vertex v is contained in the chosen independent set". Applying sequentially properties H1, H2, lemma 19, and property H3, we derive

$$\begin{aligned} \log_2 i(G) = H[I] \;&= H[X_A \mid X_B] + H[X_B] \leqslant \\ &\leqslant \sum_{v \in A} H[X_v \mid X_B] + \frac{1}{k_1} \sum_{v \in A} H[X_{N(v)}] \leqslant \\ &\leqslant \sum_{v \in A} \left(H[X_v \mid X_{N(v)}] + \frac{1}{k_1} H[X_{N(v)}] \right). \end{aligned} \tag{30}$$

Let us introduce for each vertex v a random variable Y_v — the indicator of event "$X_{N(v)} = \widetilde{0}$". Let $p_v = Pr[Y_v = 1]$. By property H3, from the definition of conditional entropy, we get

$$H[X_v \mid X_{N(v)}] \leqslant H[X_v \mid Y_v] \leqslant p_v. \tag{31}$$

By properties H4, H1, definition of conditional entropy and property H5,

$$\begin{aligned} H[X_{N(v)}] \;&= H[(X_{N(v)},\, Y_v)] = H[Y_v] + H[X_{N(v)} \mid Y_v] \leqslant \\ &\leqslant H(p_v) + (1 - p_v) \log_2(2^{k_2} - 1). \end{aligned} \tag{32}$$

Substituting (32) and (31) into (30), we arrive at the inequality:

$$
\begin{aligned}
\log_2 i(G) &\leqslant \sum_{v\in A}\Big(p_v + \frac{1}{k_1}\big(H(p_v) + (1-p_v)\log_2(2^{k_2}-1)\big)\Big) \leqslant \\
&\leqslant |A|\cdot \max_{p\in[0,1]}\Big(p + \frac{1}{k_1}\big(H(p) + (1-p)\log_2(2^{k_2}-1)\big)\Big) = \\
&= |A|\cdot \max_{p\in[0,1]}\Big(1-p + \frac{1}{k_1}\big(H(p) + p\log_2(2^{k_2}-1)\big)\Big) = \\
&= |A| + \frac{|A|}{k_1}\cdot \max_{p\in[0,1]}\left(H(p) + p\log_2\left(\frac{2^{k_2}-1}{2^{k_1}}\right)\right).
\end{aligned} \tag{33}
$$

Function $f(p) = H(p) + p\log_2\left(\frac{2^{k_2}-1}{2^{k_1}}\right)$ achieves its maximum at point

$$p_0 = \frac{2^{k_2}-1}{2^{k_1}+2^{k_2}-1},$$

and the maximum value equals $\log_2\left(\frac{2^{k_1}+2^{k_2}-1}{2^{k_1}}\right)$. From this and from (33) it follows that

$$\log_2 i(G) \leqslant |A| + \frac{|A|}{k_1}\log_2\left(\frac{2^{k_1}+2^{k_2}-1}{2^{k_1}}\right) = \frac{|A|}{k_1}\log_2(2^{k_1}+2^{k_2}-1),$$

which directly implies the statement of the theorem. □

The following statement, proved in a different way in [16], follows from lemma 1 and theorem 23.

Theorem 24 (A.A. Sapozhenko [16]). *Let G be a k-regular graph on n vertices. Then*

$$i(G) \leqslant 2^{\frac{n}{2}(1+O(\sqrt{(\log_2 k)/k}))}.$$

Appendix A. The Sturm sequence for $(x-1)(x^4+1)^4 - x^{16}$

$$
\begin{aligned}
f_0 = {} & x^{17} - 2x^{16} + 4x^{13} - 4x^{12} + 6x^9 - 6x^8 + 4x^5 - 4x^4 + x - 1, \\
f_1 = {} & x^{16} - \tfrac{32}{17}x^{15} + \tfrac{52}{17}x^{12} - \tfrac{48}{17}x^{11} + \tfrac{54}{17}x^8 - \tfrac{48}{17}x^7 + \tfrac{20}{17}x^4 - \tfrac{16}{17}x^3 + \tfrac{1}{17}, \\
f_2 = {} & x^{15} - \tfrac{17}{4}x^{13} + \tfrac{59}{16}x^{12} + \tfrac{3}{2}x^{11} - \tfrac{51}{4}x^9 + \tfrac{405}{32}x^8 + \tfrac{3}{2}x^7 - \tfrac{51}{4}x^5 + \tfrac{211}{16}x^4 + \tfrac{1}{2}x^3 - \tfrac{17}{4}x + \tfrac{287}{64}, \\
f_3 = {} & -x^{14} + \tfrac{11}{4}x^{13} - 2x^{12} - 3x^{10} + \tfrac{69}{8}x^9 - 6x^8 - 3x^6 + \tfrac{35}{4}x^5 - 6x^4 - x^2 + \tfrac{47}{16}x - 2, \\
f_4 = {} & -x^{13} + \tfrac{29}{21}x^{12} + \tfrac{8}{7}x^{11} - \tfrac{2}{7}x^{10} - \tfrac{53}{14}x^9 + \tfrac{41}{14}x^8 + \tfrac{8}{7}x^7 - \tfrac{8}{21}x^6 - \tfrac{85}{21}x^5 + \tfrac{53}{21}x^4 + \tfrac{8}{21}x^3 - \\
& -\tfrac{1}{7}x^2 - \tfrac{39}{28}x + \tfrac{65}{84}, \\
f_5 = {} & x^{12} - \tfrac{3264}{2209}x^{11} - \tfrac{696}{2209}x^{10} - \tfrac{906}{2209}x^9 + \tfrac{11055}{4418}x^8 - \tfrac{3432}{2209}x^7 - \tfrac{928}{2209}x^6 - \tfrac{1208}{2209}x^5 + \tfrac{5161}{2209}x^4 - \\
& -\tfrac{1172}{2209}x^3 - \tfrac{348}{2209}x^2 - \tfrac{453}{2209}x + \tfrac{6637}{8836}, \\
f_6 = {} & -x^{11} + \tfrac{879}{829}x^{10} + \tfrac{6405}{3316}x^9 - \tfrac{93919}{39792}x^8 - \tfrac{693}{829}x^7 + \tfrac{1172}{829}x^6 + \tfrac{2135}{829}x^5 - \tfrac{42969}{13264}x^4 - \tfrac{625}{2487}x^3 + \\
& +\tfrac{879}{1658}x^2 + \tfrac{6405}{6632}x - \tfrac{32779}{26528}, \\
f_7 = {} & -x^{10} + \tfrac{53407}{17532}x^9 - \tfrac{4399}{1948}x^8 - \tfrac{260}{1461}x^7 - \tfrac{4}{3}x^6 + \tfrac{24197}{5844}x^5 - \tfrac{51323}{17532}x^4 - \tfrac{130}{1461}x^3 - \tfrac{1}{2}x^2 + \\
& +\tfrac{18355}{11688}x - \tfrac{12611}{11688}, \\
f_8 = {} & x^9 - \tfrac{853668}{689617}x^8 - \tfrac{315456}{689617}x^7 + \tfrac{29220}{689617}x^6 + \tfrac{1008501}{689617}x^5 - \tfrac{987404}{689617}x^4 - \tfrac{157728}{689617}x^3 + \tfrac{17532}{689617}x^2 + \\
& +\tfrac{796431}{1379234}x - \tfrac{336342}{689617}, \\
f_9 = {} & x^8 - \tfrac{900527616}{621193153}x^7 - \tfrac{68293440}{621193153}x^6 - \tfrac{11922180}{88741879}x^5 + \tfrac{105438627}{88741879}x^4 - \tfrac{455780744}{621193153}x^3 - \tfrac{40976064}{621193153}x^2 - \\
& -\tfrac{7153308}{88741879}x + \tfrac{73281225}{177483758}, \\
f_{10} = {} & x^7 - \tfrac{145719580}{29489963}x^6 - \tfrac{882209825}{117959852}x^5 + \tfrac{11071460827}{471839408}x^4 + \tfrac{10728971}{58979926}x^3 - \tfrac{87431748}{29489963}x^2 - \\
& -\tfrac{529325895}{117959852}x + \tfrac{13409991623}{943678816}, \\
f_{11} = {} & -x^6 - \tfrac{56333223}{551533100}x^5 + \tfrac{3940569}{1198985}x^4 - \tfrac{357480}{5515331}x^3 - \tfrac{3}{5}x^2 - \tfrac{2468075}{44122648}x + \tfrac{551084501}{275766550}, \\
f_{12} = {} & x^5 - \tfrac{70388030335}{37930036817}x^4 + \tfrac{940679000}{37930036817}x^3 - \tfrac{55153310}{37930036817}x^2 + \tfrac{45527310825}{75860073634}x - \tfrac{85234936291}{75860073634}, \\
f_{13} = {} & x^4 + \tfrac{739310388352}{13435006309713}x^3 + \tfrac{112620848536}{13435006309713}x^2 + \tfrac{20883732410}{1492778478857}x + \tfrac{1868446901133}{2985556957714}, \\
f_{14} = {} & -x^3 - \tfrac{42628900319}{9038969207957}x^2 - \tfrac{312644395521}{36155876831828}x - \tfrac{85929196356567}{144623507327312}, \\
f_{15} = {} & x^2 + \tfrac{56493602552535}{48822373252}x - \tfrac{57985421050465}{48822373252}, \\
f_{16} = {} & x - \tfrac{310948912}{303217841}, \\
f_{17} = {} & 1.
\end{aligned}
$$

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