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Maximal independent sets in bipartite graphs with at least one cycle

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A maximal independent set is an independent set that is not a proper subset of any other independent set. Liu [J.Q. Liu, Maximal independent sets of bipartite graphs, J. Graph Theory, 17 (4) (1993) 495-507] determined the largest number of maximal independent sets among all n-vertex bipartite graphs. The corresponding extremal graphs are forests. It is natural and interesting for us to consider this problem on bipartite graphs with cycles. Let $\mathscr{B}_n$ (resp. $\mathscr{B}'_n$) be the set of all n-vertex bipartite graphs with at least one cycle for even (resp. odd) n. In this paper, the largest number of maximal independent sets of graphs in $\mathscr{B}_n$ (resp. $\mathscr{B}'_n$) is considered. Among $\mathscr{B}_n$ the disconnected graphs with the first-, second-, $\dots$, $\frac{n-2}{2}$-th largest number of maximal independent sets are characterized, while the connected graphs in $\mathscr{B}_n$ having the largest and the second largest number of maximal independent sets are determined. Among $\mathscr{B}'_n$ graphs having the largest number of maximal independent sets are identified.

Keywords: Maximal independent set, bipartite graph, cycle

1 Introduction

Given a graph $G = (V_G, E_G)$, a set $I \subseteq V_G$ is *independent* if there is no edge of G between any two vertices of I. A *maximal independent set* is an independent set that is not a proper subset of any other independent set. The dual of an independent set is a clique, in the sense that a clique corresponds to an independent set in the complement graph. The set of all maximal independent sets of a graph G is denoted by MI(G) and its cardinality by $\mathrm{mi}(G)$.

Around 1960, Erdős and Moser proposed the problem to determine the maximum value of $\mathrm{mi}(G)$ when G runs over all n-vertex graphs and to characterize the graphs attaining this maximum, both of which were answered by Moon and Moser [18]. It is interesting to see that the extremal graphs turn to have most components isomorphic to the complete graph K_3. On the other hand, the theory on maximal independent set has some applications in other research field. For example, in chemistry, a *Clar structure* is defined to be a maximal independent set of vertices of the Clar graph of the corresponding benzenoid hydrocarbons [5]. Clar structures recently are used as basis-set to compute resonance energies. The theory of maximal

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independent set is also applied to the areas of managements and networks. For the *compatibility graph* G, its vertices denote tasks, and an edge denotes a resource sharing constraint between the two tasks linked by it. A maximal independent set of a compatibility graph represents a maximal set of tasks that can be executed concurrently. Basagni [2] and Alzoubi et al. [21] pointed out the importance of a maximal independent set in the wireless network. Moscibroda and Watenhofer [19] obtained the well-known Maximal Independent Set problem when they modeled the unstructured radio network as a graph.

Along the line on the study of the maximal independent set in mathematical literature, mathematicians focused on determining the largest number of $\mathrm{mi}(G)$ in various interesting classes of graphs. Ying et al. [22] determined the maximum number of maximal independent sets in graphs of order n with at most r cycles and in connected graphs of order $n \geqslant 3r$ with at most r cycles. Ortiz [20] established a sharp upper bound for the number of maximal independent sets in caterpillar graphs. Arumugam et al. [1] studied the maximal independent set of graphs with minimum coloring. Duffus, Frankl and Rödl [4] studied maximal independent sets in graphs obtained from Boolean lattices. Jing and one of the present authors [16] studied the maximal independent set of graphs with cyclomatic number at most two. Jin and Li [8] determined the second largest number of maximal independent sets among all graphs of order n. Hua and Hou [6] determined the n-vertex graph having the third largest number of maximal independent sets. Jou and Lin [10, 13] settled the problem for trees and forests. Jin and Yan [9] settled the problem for the second and third largest number of maximal independent sets of trees.

This paper is motivated directly from [17], in which the author completely characterized the n-vertex bipartite graphs having the largest number of maximal independent sets. The corresponding extremal graphs are forests. Furthermore, for the bipartite graph of order n that contains cycles, the author in [17] determined the upper bound on the number of maximal independent sets for odd n. Unfortunately, the graphs which attain this value were not characterized. It is natural and interesting to determine the corresponding extremal graphs, which is settled in this paper. On the other hand, it is necessary and interesting to consider this problem on the n-vertex bipartite graphs with cycles for even n. In this paper, among the set of all disconnected bipartite graphs with even order, the extremal graphs which have the first-, second-, $\ldots$, $\frac{n-2}{2}$-th largest number of maximal independent sets are characterized respectively, while among the set of all connected bipartite graphs with even order, the extremal graphs having the largest and the second largest number of maximal independent sets are identified.

2 Preliminary

Given a simple graph $G = (V_G, E_G)$, the cardinality of V_G is called the *order* of G. And $G - v$ denotes the graph obtained from G by deleting vertex $v \in V_G$ (this notation is naturally extended if more than one vertex is deleted). For $v \in V_G$, let $N_G(v)$ (or $N(v)$ for short) denote the set of all the adjacent vertices of v in G and $d(v) = |N_G(v)|$. For convenience, let $N_G[v] = N_G(v) \cup \{v\}$. A *leaf* of G is a vertex of degree one, while an *isolated vertex* of G is a vertex of degree zero. For any two graphs G and H, let $G \uplus H$ denote the disjoint union of G and H, and for any nonnegative integer t, let tG stand for the disjoint union of t copies of G. For a connected graph H with maximum degree vertex x and a graph $G = G_1 \uplus G_2 \uplus \cdots \uplus G_k$ with u_i being a maximum degree vertex in $G_i, i = 1, 2, \ldots, k$. Define the graph $H * G$ to be the graph with vertex set $V_{H*G} = V_H \cup V_G$ and edge set $E_{H*G} = E_H \cup E_G \cup \{xu_i : i = 1, 2, \ldots, k\}$. An *odd* (resp. *even*) component is a component of odd (resp. even) order. Throughout the text we denote by $P_n,\ C_n,\ K_{1,n-1}$ and K_n the path, cycle, star and complete graph on n vertices, respectively. Undefined terminology and notation may be referred to [3].

Throughout this paper, for simplicity, r denotes $\sqrt{2}$.

We begin with some useful known results which are needed to prove our main results.

Lemma 1 ([7, 14]) *For any vertex v in a graph G, $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-v) + \mathrm{mi}(G - N_G[v])$. If v is a leaf adjacent to u, then $\mathrm{mi}(G) = \mathrm{mi}(G - N_G[v]) + \mathrm{mi}(G - N_G[u])$.*

Lemma 2 ([14]) *If G is the union of two disjoint graphs G_1 and G_2, then $\mathrm{mi}(G) = \mathrm{mi}(G_1) \cdot \mathrm{mi}(G_2)$.*

Lemma 3 ([13]) *If T is a tree with $n \geqslant 1$ vertices, then $\mathrm{mi}(T) \leqslant t_1(n)$, where*

$$t_1(n) = \begin{cases} r^{n-2}+1, & \text{if } n \text{ is even;} \\ r^{n-1}, & \text{if } n \text{ is odd.} \end{cases}$$

Furthermore, $\mathrm{mi}(T) = t_1(n)$ if and only if $T \in T_1(n)$, where

$$T_1(n) = \begin{cases} B(2, \frac{n-2}{2}) \ or\ B(4, \frac{n-4}{2}), & \text{if } n \text{ is even;} \\ B(1, \frac{n-1}{2}), & \text{if } n \text{ is odd,} \end{cases}$$

where $B(i,j)$ is the set of batons, which are the graphs obtained from a basic path P_i $(i \geqslant 1)$ by attaching $j \geqslant 0$ paths of length two to the endpoints of P_i in any possible ways.

Lemma 4 ([13]) *If F is a forest with $n \geqslant 1$ vertices, then $\mathrm{mi}(F) \leqslant f_1(n)$, where*

$$f_1(n) = \begin{cases} r^{n}, & \text{if } n \text{ is even;} \\ r^{n-1}, & \text{if } n \text{ is odd.} \end{cases}$$

Furthermore, $\mathrm{mi}(F) = f_1(n)$ if and only if $F \in F_1(n)$, where

$$F_1(n) = \begin{cases} \frac{n}{2}K_2, & \text{if } n \text{ is even;} \\ B(1, \frac{n-1-2s}{2}) \uplus sK_2 \ for\ some\ s\ with\ 0 \leqslant s \leqslant \frac{n-1}{2}, & \text{if } n \text{ is odd.} \end{cases}$$

Lemma 5 ([14]) *If F is a forest with $n \geqslant 4$ vertices having $F \notin F_1(n)$, then $\mathrm{mi}(F) \leqslant f_2(n)$, where*

$$f_2(n) = \begin{cases} 3r^{n-4}, & \text{if } n \geqslant 4 \text{ is even;} \\ 3, & \text{if } n = 5; \\ 7r^{n-7}, & \text{if } n \geqslant 7 \text{ is odd.} \end{cases}$$

Furthermore, $\mathrm{mi}(F) = f_2(n)$ if and only if $F \in F_2(n)$, where

$$F_2(n) = \begin{cases} P_4 \uplus \frac{n-4}{2}K_2, & \text{if } n \geqslant 4 \text{ is even;} \\ P_1 * P_4 \text{ or}, P_1 \uplus P_4, & \text{if } n = 5; \\ P_7 \uplus \frac{n-7}{2}K_2, & \text{if } n \geqslant 7 \text{ is odd.} \end{cases}$$

For $n \geqslant 2, 0 \leqslant k \leqslant \lfloor \frac{n}{2} \rfloor$, define

$$B_{n,k} = \begin{cases} 2P_4 \uplus \frac{n-8}{2}K_2 \text{ or}, T_1(n-2k) \uplus kK_2, & \text{if } n \text{ is even;} \\ T_1(n-2k) \uplus kK_2, & \text{if } n \text{ is odd.} \end{cases}$$

Then $\mathrm{mi}(B_{n,k}) = 2^k \cdot \mathrm{mi}(T_1(n-2k))$, or $9r^{n-8}$.

Lemma 6 ([17]) *The maximum number of maximal independent sets among all bipartite graphs of order n is $2^{\lfloor \frac{n}{2} \rfloor}$, and the only bipartite graphs of order n which have this many maximal independent sets are $F_1(n)$.*

Lemma 7 ([17]) *If G is an acyclic graph of order n and $G \ncong B_{n,k}$, then $\mathrm{mi}(G) < t_1(n)$.*

Lemma 8 *If $n \geqslant 6$, then $\mathrm{mi}(C_n) = \mathrm{mi}(C_{n-2}) + \mathrm{mi}(C_{n-3})$. Furthermore, one has*

$$\mathrm{mi}(C_n) < \begin{cases} r^{n-1}, & \text{if } n \geqslant 7 \text{ is odd;} \\ r^{n-2}, & \text{if } n \geqslant 12 \text{ is even.} \end{cases}$$

Proof: The first part is due to [13]; we show the second part by induction on n. It is routine to check that

$$\mathrm{mi}(C_7) = 7 < r^6, \quad \mathrm{mi}(C_9) = 12 < r^8, \quad \mathrm{mi}(C_{11}) = 22 < r^{10},$$
$$\mathrm{mi}(C_{12}) = 29 < r^{10}, \quad \mathrm{mi}(C_{13}) = 39 < r^{12}, \quad \mathrm{mi}(C_{14}) = 51 < r^{12}.$$

Assume the result holds for $n \leqslant k$. Now consider $n = k+1 \geqslant 15$. By induction hypothesis, we obtain

$$\mathrm{mi}(C_n) = \mathrm{mi}(C_{n-2}) + \mathrm{mi}(C_{n-3}) < \begin{cases} r^{n-2-1} + r^{n-3-2} = 3r^{n-5} < r^{n-1}, & \text{if } n \text{ is odd;} \\ r^{n-2-2} + r^{n-3-1} = r^{n-2}, & \text{if } n \text{ is even.} \end{cases}$$

This completes the proof. □

3 Sharp bounds and extremal graphs

Let $\mathscr{B}_n$ (resp. $\mathscr{B}'_n$) be the set of all n-vertex bipartite graphs with at least one cycle for even (resp. odd) n. In this section, among $\mathscr{B}_n$ the disconnected graphs with the first-, second-, ..., $\frac{n-2}{2}$-th largest number of maximal independent sets are characterized, while the connected graphs in $\mathscr{B}_n$ having the largest and the second largest number of maximal independent sets are determined; among $\mathscr{B}'_n$ the graphs having the largest number of maximal independent sets are identified.

For even n and $3 \leqslant k \leqslant \frac{n}{2}$, define $D_{n,k} = B_{2k} \uplus (\frac{n}{2} - k)K_2$, where B_{2k} is depicted in Fig. 1. Then $\mathrm{mi}(D_{n,k}) = 2^{\frac{n}{2}-k} \cdot \mathrm{mi}(B_{2k}) = 2^{\frac{n}{2}-k}(2^{k-1}+1) \leqslant r^{n-2} + r^{n-6}$.

Theorem 1 *For graphs $D_{n,3}, D_{n,4}, \dots, D_{n,\frac{n}{2}}, C_8 \uplus \frac{n-8}{2}K_2, C_{10} \uplus \frac{n-10}{2}K_2, (C_8 * K_2) \uplus \frac{n-10}{2}K_2$, one has*

$$\begin{aligned} \mathrm{mi}(D_{n,3}) &= \mathrm{mi}(C_8 \uplus \frac{n-8}{2}K_2) > \mathrm{mi}(D_{n,4}) > \mathrm{mi}(D_{n,5}) = \mathrm{mi}(C_{10} \uplus \frac{n-10}{2}K_2) \\ &= \mathrm{mi}((C_8 * K_2) \uplus \frac{n-10}{2}K_2) > \mathrm{mi}(D_{n,6}) > \mathrm{mi}(D_{n,7}) > \cdots > \mathrm{mi}(D_{n,\frac{n}{2}}) = r^{n-2} + 1. \end{aligned}$$

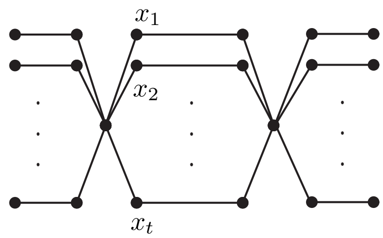

Fig. 1: Graph B_{2k}, where $k \geqslant 3$ and $t \geqslant 2$.

Proof: By direct computing, we have

$$\begin{aligned} \mathrm{mi}(D_{n,t}) &= 2^{\frac{n-2t}{2}} \cdot \mathrm{mi}(B_{2t}) = 2^{\frac{n-2}{2}} + 2^{\frac{n-2t}{2}}, \qquad t = 3, 4, \ldots, \frac{n}{2}, &(1)\\ \mathrm{mi}(C_8 \uplus \frac{n-8}{2} K_2) &= 10 \cdot 2^{\frac{n-8}{2}}, &(2)\\ \mathrm{mi}(C_{10} \uplus \frac{n-10}{2} K_2) &= 17 \cdot 2^{\frac{n-10}{2}}, &(3)\\ \mathrm{mi}((C_8 * K_2) \uplus \frac{n-10}{2} K_2) &= 17 \cdot 2^{\frac{n-10}{2}}. &(4)\end{aligned}$$

By (1), it is easy to see that $\mathrm{mi}(D_{n,t}) < \mathrm{mi}(D_{n,t-1})$ for $4 \leqslant t \leqslant \frac{n}{2}$. Combining with (2)-(4), our results follow immediately. □

Let $H_0(6), H_0(8), H_0(10), H_1(n), H_2(n), H_3(n)$ and $O_1(n)$ be the graphs depicted in Fig. 2.

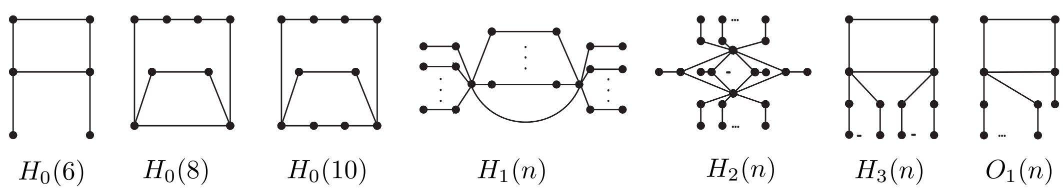

Fig. 2: The extremal graphs

Theorem 2 *Consider an n-vertex bipartite graph G containing cycles with $n \geqslant 5$.*

(i) *If $G \in \mathscr{B}_n \setminus \{D_{n,3}, D_{n,4}, \ldots, D_{n,\frac{n}{2}}, C_8 \uplus \frac{n-8}{2}K_2, C_{10} \uplus \frac{n-10}{2}K_2, (C_8 * K_2) \uplus \frac{n-10}{2}K_2\}$, then*

$$\mathrm{mi}(G) \leqslant r^{n-2}. \tag{5}$$

If G is connected, the equality holds in (5) *if and only if $G \cong H_0(n), H_1(n), H_2(n)$, or $H_3(n)$ for $n = 6, 8, 10$; and $G \cong H_1(n), H_2(n)$, or $H_3(n)$ for $n \geqslant 12$.*

If G is disconnected, the equality holds in (5) *if and only if $G \cong C_4 \uplus \frac{n-4}{2}K_2, H_0(6) \uplus \frac{n-6}{2}K_2, H_0(8) \uplus \frac{n-8}{2}K_2, H_0(10) \uplus \frac{n-10}{2}K_2, H_1(n-2k) \uplus kK_2, H_2(n-2k) \uplus kK_2$, or $H_3(n-2k) \uplus kK_2$.*

(ii) *If $G \in \mathscr{B}'_n$, then*

$$\mathrm{mi}(G) \leqslant 3r^{n-5}. \tag{6}$$

The equality holds in (6) *if and only if $G \cong C_6 * K_1$, or $O_1(n)$ for connected G and $G \cong O_1(n-2k) \uplus kK_2$, or $(C_6 * K_1) \uplus \frac{n-7}{2}K_2$ for disconnected G.*

Proof: We put the proofs of (i) and (ii) together as below. Choose G in $\mathscr{B}_n \setminus \{D_{n,3}, D_{n,4}, \ldots, D_{n,\frac{n}{2}}, C_8 \uplus \frac{n-8}{2}K_2, C_{10} \uplus \frac{n-10}{2}K_2, (C_8 * K_2) \uplus \frac{n-10}{2}K_2\}$ (resp. $\mathscr{B}'_n$) such that $\mathrm{mi}(G)$ is as large as possible. We proceed by induction on n.

For $5 \leqslant n \leqslant 6$, it is straightforward to check that our results hold. Assume that our results hold for $n \leqslant k$. Now consider $n = k+1 \geqslant 7$.

First we consider that G is disconnected. Denote

$$G = G_{o_1} \uplus G_{o_2} \uplus \cdots \uplus G_{o_{l_1}} \uplus G_{e_1} \uplus G_{e_2} \uplus \cdots \uplus G_{e_{l_2}},$$

where G_{o_i} is an odd component for $1 \leqslant i \leqslant l_1$ and G_{e_j} is an even component for $1 \leqslant j \leqslant l_2$.

Case 1. n is even. In this case, we have that l_1 is also even. If $l_1 \geqslant 2$, then

$$\begin{aligned}
\mathrm{mi}(G) &= \prod_{i=1}^{l_1} \mathrm{mi}(G_{o_i}) \cdot \prod_{j=1}^{l_2} \mathrm{mi}(G_{e_j}) && \text{(by Lemma 2)} \\
&\leqslant \prod_{i=1}^{l_1} r^{|V_{G_{o_i}}|-1} \cdot \prod_{j=1}^{l_2} r^{|V_{G_{e_j}}|} && \text{(by Lemma 6)} \qquad (7)\\
&= r^{n-l_1} \\
&\leqslant r^{n-2}. && (8)
\end{aligned}$$

The equality in (7) holds if and only if $G_{o_i} \cong F_1(|V_{G_{o_i}}|)$ for $1 \leqslant i \leqslant l_1$, $G_{e_j} \cong F_1(|V_{G_{e_j}}|)$ for $1 \leqslant j \leqslant l_2$; while the equality in (8) holds if and only if $l_1 = 2$, which implies that $G \cong F_1(|V_{G_{o_1}}|) \uplus F_1(|V_{G_{o_2}}|) \uplus \frac{n-|V_{G_{o_1}}|-|V_{G_{o_2}}|}{2}K_2$. Obviously, G does not contain cycles, so $\mathrm{mi}(G) < r^{n-2}$.

Therefore we consider that $l_1 = 0$, that is to say, each component contained in G is an even component. Without loss of generality, assume that $|V_{G_{e_1}}| \geqslant |V_{G_{e_2}}| \geqslant \cdots \geqslant |V_{G_{e_{l_2}}}|$. Note that G contains cycles, hence $|V_{G_{e_1}}| \geqslant 4$.

If $|V_{G_{e_1}}| = 4$, then there exists a $p \in \{1, 2, \ldots, l_2\}$ such that $|V_{G_{e_1}}| = |V_{G_{e_2}}| = |V_{G_{e_3}}| = \cdots = |V_{G_{e_p}}| = 4$. As G contains cycles, there at least one $i \in \{1, 2, \ldots, p\}$ such that $G_{e_i} \cong C_4$. We obtain that

$$\begin{aligned}
\mathrm{mi}(G) &= \mathrm{mi}(G_{e_i}) \cdot \prod_{1 \leqslant j \neq i \leqslant p} \mathrm{mi}(G_{e_j}) \cdot \prod_{k=p+1}^{l_2} \mathrm{mi}(G_{e_k}) && \text{(by Lemma 2)} \\
&\leqslant 2 \cdot 3^{p-1} \cdot r^{n-4p} && \text{(by Lemmas 3 and 6)} \qquad (9)\\
&= r^{n-2} \cdot (\frac{3}{4})^{p-1} \\
&\leqslant r^{n-2}. && (10)
\end{aligned}$$

The equality in (9) holds if and only if $G_{e_i} \cong C_4$, $G_{e_j} \cong P_4$ for $1 \leqslant j \neq i \leqslant p$, $G - (G_{e_1} \uplus G_{e_2} \uplus \cdots \uplus G_{e_p}) \cong F_1(n-4p) = \frac{n-4p}{2}K_2$; while the equality in (10) holds if and only if $p = 1$, which implies that $G \cong C_4 \uplus \frac{n-4}{2}K_2$, our result holds.

If $|V_{G_{e_1}}| \geqslant 6$, then we consider the following two possible subcases.

• $|V_{G_{e_2}}| = 2$. In this subcase, we have $G - G_{e_1} \cong \frac{n-|V_{G_{e_1}}|}{2}K_2$. Note that $G \ncong D_{n,|V_{G_{e_1}}|/2}, C_8 \uplus \frac{n-8}{2}K_2, C_{10} \uplus \frac{n-10}{2}K_2$ and $(C_8 * K_2) \uplus \frac{n-10}{2}K_2$, hence $G_{e_1} \ncong B_{|V_{G_{e_1}}|}, C_8, C_{10}$ and $C_8 * K_2$. By induction hypothesis and Lemma 2, we have

$$\begin{aligned} \mathrm{mi}(G) &= \mathrm{mi}(G_{e_1}) \cdot \mathrm{mi}(G - G_{e_1}) \\ &\leqslant r^{|V_{G_{e_1}}|-2} \cdot r^{n-|V_{G_{e_1}}|} \\ &= r^{n-2}. \end{aligned} \tag{11}$$

The equality in (11) holds if and only if $G_{e_1} \cong H_0(6)$, $H_0(8)$, $H_0(10)$, $H_1(|V_{G_{e_1}}|)$, $H_2(|V_{G_{e_1}}|)$, or $H_3(|V_{G_{e_1}}|)$. Together with $G - G_{e_1} \cong \frac{n-|V_{G_{e_1}}|}{2}K_2$, our result follows immediately.

• $|V_{G_{e_2}}| \geqslant 4$. In this subcase, we have

$$\begin{aligned} \mathrm{mi}(G) &= \mathrm{mi}(G_{e_1}) \cdot \mathrm{mi}(G_{e_2}) \cdot \prod_{j=3}^{l_2} \mathrm{mi}(G_{e_j}) \qquad \text{(by Lemma 2)} \\ &\leqslant (r^{|V_{G_{e_1}}|-2}+1) \cdot (r^{|V_{G_{e_2}}|-2}+1) \cdot r^{n-|V_{G_{e_1}}|-|V_{G_{e_2}}|} \quad \text{(by Lemmas 3, 6 and Theorem 1)} \\ &= r^{n-4} + r^{n-|V_{G_{e_2}}|-2} + r^{n-|V_{G_{e_1}}|-2} + r^{n-|V_{G_{e_1}}|-|V_{G_{e_2}}|} \\ &\leqslant r^{n-4} + r^{n-6} + r^{n-8} + r^{n-10} \\ &< r^{n-2}. \end{aligned}$$

Case 2. n is odd. In this case, l_1 is also odd. If $l_1 \geqslant 3$, by Lemmas 2 and 6 , we get

$$\mathrm{mi}(G) = \prod_{i=1}^{l_1} \mathrm{mi}(G_{o_i}) \cdot \prod_{j=1}^{l_2} \mathrm{mi}(G_{e_j}) \leqslant \prod_{i=1}^{l_1} r^{|V_{G_{o_i}}|-1} \cdot \prod_{j=1}^{l_2} r^{|V_{G_{e_j}}|} = r^{n-l_1} \leqslant r^{n-3} < 3r^{n-5}.$$

Hence, we consider that $l_1 = 1$ in what follows.

If G_{o_1} contains cycles, by induction hypothesis and Lemmas 2 and 6 , we obtain that

$$\mathrm{mi}(G) = \mathrm{mi}(G_{o_1}) \cdot \mathrm{mi}(G - G_{o_1}) \leqslant 3r^{|V_{G_{o_1}}|-5} \cdot r^{n-|V_{G_{o_1}}|} = 3r^{n-5},$$

the equality holds if and only if $G_{o_1} \cong O_1(|V_{G_{o_1}}|)$ or $C_6 * K_1$ and $G - G_{o_1} = \frac{n-|V_{G_{o_1}}|}{2}K_2$, which implies that $G \cong O_1(|V_{G_{o_1}}|) \uplus \frac{n-|V_{G_{o_1}}|}{2}K_2$ or $(C_6 * K_1) \uplus \frac{n-7}{2}K_2$, the result holds.

If G_{o_1} does not contain cycles, then there exists at least one even component G_{e_j} containing cycles with $|V_{G_{e_j}}| \geqslant 4$. If $|V_{G_{e_j}}| = 4$, then $G_{e_j} \cong C_4$. We obtain that

$$\begin{aligned} \mathrm{mi}(G) &= \mathrm{mi}(G_{o_1}) \cdot \mathrm{mi}(G_{e_j}) \cdot \prod_{1 \leqslant i \neq j \leqslant l_2} \mathrm{mi}(G_{e_i}) && \text{(by Lemma 2)} \\ &\leqslant r^{|V_{G_{o_1}}|-1} \cdot 2 \cdot r^{n-4-|V_{G_{o_1}}|} && \text{(by Lemmas 3 and 6)} \\ &< 3r^{n-5}, \end{aligned}$$

the result holds. If $|V_{G_{e_j}}| \geqslant 6$, we obtain that

$$\begin{aligned} \mathrm{mi}(G) &= \mathrm{mi}(G_{o_1}) \cdot \mathrm{mi}(G_{e_j}) \cdot \prod_{1 \leqslant i \neq j \leqslant l_2} \mathrm{mi}(G_{e_i}) && \text{(by Lemma 2)} \\ &\leqslant r^{|V_{G_{o_1}}|-1} \cdot (r^{|V_{G_{e_j}}|-2} + 1) \cdot r^{n-|V_{G_{o_1}}|-|V_{G_{e_j}}|} && \text{(by Lemmas 3, 6 and Theorem 1)} \\ &= r^{n-3} + r^{n-|V_{G_{e_j}}|-1} \\ &\leqslant r^{n-3} + r^{n-7} \\ &< 3r^{n-5}. \end{aligned}$$

The result holds.

Now we consider that G is connected. It suffices to consider the following two possible cases.

Case 1. G has a vertex v of degree $\geqslant 4$ such that $G - v$ has cycles.

Subcase 1.1. n is even. In this subcase, we have

$$\begin{aligned} \mathrm{mi}(G) &\leqslant \mathrm{mi}(G-v) + \mathrm{mi}(G - N_G[v]) && \text{(by Lemma 1)} \\ &\leqslant 3r^{n-6} + r^{n-5-1} && \text{(by induction hypothesis and Lemma 6)} \\ &= r^{n-2}. \end{aligned} \tag{12}$$

The equality in (12) holds if and only if $G-v \cong O_1(k) \uplus \frac{n-k-1}{2}K_2$ or $(C_6 * K_1) \uplus \frac{n-8}{2}K_2$, $G - N_G[v] \cong F_1(n-5)$. But there is no such bipartite graph since $G - N_G[v]$ is obtained from $G - v$ by deleting four independent vertices, hence $\mathrm{mi}(G) < r^{n-2}$.

Subcase 1.2. n is odd.

In this subcase, we first consider that $G-v \cong D_{n-1,k}$. Then by Theorem 1, $\mathrm{mi}(G-v) \leqslant r^{n-3}+r^{n-7}$. If $d(v) = 4$, then $G - N_G[v]$ is either an acyclic bipartite graph which is not isomorphic to $B_{n-5,k}$ or a bipartite graph with cycles which is not isomorphic to $D_{n-5,k}$. Hence by induction hypothesis or Lemma 7, $\mathrm{mi}(G - N_G[v]) \leqslant r^{n-7}$, which gives

$$\begin{aligned} \mathrm{mi}(G) &\leqslant \mathrm{mi}(G-v) + \mathrm{mi}(G - N_G[v]) && \text{(by Lemma 1)} \\ &\leqslant r^{n-3} + r^{n-7} + r^{n-7} \\ &= 3r^{n-5}. \end{aligned} \tag{13}$$

The equality in (13) holds if and only if $G-v \cong C_6 \uplus \frac{n-7}{2}K_2$ and $G-N_G[v] \cong H_0(6) \uplus \frac{n-11}{2}K_2,\ H_0(8) \uplus \frac{n-13}{2}K_2, H_0(10) \uplus \frac{n-15}{2}K_2, H_1(k) \uplus \frac{n-k-5}{2}K_2,\ H_2(k) \uplus \frac{n-k-5}{2}K_2$, or $H_3(k) \uplus \frac{n-k-5}{2}K_2$. Note that

$G-v\cong C_6\uplus\frac{n-7}{2}K_2$, hence $G-N_G[v]$ is a subgraph of $P_5\uplus\frac{n-7}{2}K_1$. It is easy to see that $G-N_G[v]$ contains no cycles, a contradiction.

Now we consider that $G-v\ncong D_{n-1,k}$. In order to use the induction hypothesis, we should show that $G-v\ncong C_8\uplus\frac{n-9}{2}K_2$, $C_{10}\uplus\frac{n-11}{2}K_2$, and $(C_8*K_2)\uplus\frac{n-11}{2}K_2$ first. In fact, if $G-v\cong C_8\uplus\frac{n-9}{2}K_2$, then $1\leqslant|N_G(v)\cap N_{C_8}(v)|\leqslant 4$.

If $|N_G(v)\cap N_{C_8}(v)|=1$, then $n\geqslant 15$ and $G-N_G[v]\cong P_7\uplus\frac{n-9}{2}K_1$. By Lemma 1, we get $\mathrm{mi}(G)\leqslant\mathrm{mi}(G-v)+\mathrm{mi}(G-N_G[v])=5r^{n-7}+7<3r^{n-5}$.

If $|N_G(v)\cap N_{C_8}(v)|=2$, then $n\geqslant 13$ and $G-N_G[v]\cong P_5\uplus\frac{n-7}{2}K_1$, or $2P_3\uplus\frac{n-9}{2}K_1$. By Lemma 1, we get $\mathrm{mi}(G)\leqslant\mathrm{mi}(G-v)+\mathrm{mi}(G-N_G[v])=5r^{n-7}+4<3r^{n-5}$.

If $|N_G(v)\cap N_{C_8}(v)|=3$, then $n\geqslant 11$ and $G-N_G[v]\cong P_3\uplus\frac{n-5}{2}K_1$. By Lemma 1, we get $\mathrm{mi}(G)\leqslant\mathrm{mi}(G-v)+\mathrm{mi}(G-N_G[v])=5r^{n-7}+2<3r^{n-5}$.

If $|N_G(v)\cap N_{C_8}(v)|=4$, then $n\geqslant 9$ and $G-N_G[v]\cong\frac{n-1}{2}K_1$. By Lemma 1, we get $\mathrm{mi}(G)\leqslant\mathrm{mi}(G-v)+\mathrm{mi}(G-N_G[v])=5r^{n-7}+1<3r^{n-5}$.

By a similar discussion as above, we may show that $G-v\ncong C_{10}\uplus\frac{n-11}{2}K_2,\ (C_8*K_2)\uplus\frac{n-11}{2}K_2$. Therefore, we have

$$G-v\ncong D_{n-1,k},\ C_8\uplus\frac{n-9}{2}K_2,\ C_{10}\uplus\frac{n-11}{2}K_2 \text{ and } (C_8*K_2)\uplus\frac{n-11}{2}K_2.$$

By induction hypothesis, we have $\mathrm{mi}(G-v)\leqslant r^{n-3}$. Thus,

$$\begin{aligned}\mathrm{mi}(G) &\leqslant \mathrm{mi}(G-v)+\mathrm{mi}(G-N_G[v]) && \text{(by Lemma 1)}\\ &\leqslant r^{n-3}+r^{n-5} && \text{(by Lemma 6)}\\ &= 3r^{n-5}.\end{aligned}\tag{14}$$

The equality in (14) holds if and only if $G-v\cong H_0(6)\uplus\frac{n-7}{2}K_2,\ H_0(8)\uplus\frac{n-9}{2}K_2,\ H_0(10)\uplus\frac{n-11}{2}K_2,\ H_1(k)\uplus\frac{n-k-1}{2}K_2,\ H_2(k)\uplus\frac{n-k-1}{2}K_2$, or $H_3(k)\uplus\frac{n-k-1}{2}K_2$ and $G-N_G[v]\cong F_1(n-5)$. Since G is connected and $G-N_G[v]$ has no isolated vertex, $G-v$ contains no K_2 as a component, i.e., $G-v\cong H_0(6),\ H_0(8),\ H_0(10),\ H_1(n-1),\ H_2(n-1)$, or $H_3(n-1)$. However, $G-N_G[v]$ is obtained from $G-v$ by deleting four independent vertices which is impossible. Hence $\mathrm{mi}(G)<3r^{n-5}$.

Case 2. Every vertex of degree $\geqslant 4$ is in all cycles of G.

First we consider $\delta(G)=1$. Choose an edge $uv\in E_G$ with $d(v)=1$. Let $G_1=G-\{u,v\}$ and $G_2=G-N[u]$. We distinguish the following two possible subcases to show our results.

Subcase 2.1. n is odd.

If $d(u)=2$, then G_1 is a connected graph with cycles and $G_2\ncong\frac{n-3}{2}K_2$. By induction hypothesis and Lemma 5 and Theorem 1, we have $\mathrm{mi}(G_1)\leqslant 3r^{n-7}$ and $\mathrm{mi}(G_2)\leqslant\max\{3r^{n-7},r^{n-5}+r^{n-9}\}=3r^{n-7}$. By Lemma 1, we get

$$\mathrm{mi}(G)=\mathrm{mi}(G_1)+\mathrm{mi}(G_2)\leqslant 3r^{n-7}+3r^{n-7}=3r^{n-5},$$

the equality holds if and only if $G_1\cong O_1(n-2)$ or C_6*K_1, $G_2\cong P_4\uplus\frac{n-7}{2}K_2$, i.e., $G\cong O_1(n)$.

If $d(u)\geqslant 3$, by Lemmas 1 and 6 , we obtain that

$$\mathrm{mi}(G)=\mathrm{mi}(G_1)+\mathrm{mi}(G_2)\leqslant r^{n-2-1}+r^{n-4-1}=3r^{n-5},$$

the equality holds if and only if $G_1 \cong F_1(n-2)$, $G_2 \cong F_1(n-4)$ or $F_1(n-5)$. If $G_2 \cong F_1(n-4)$, we have $d(u) = 3$. In this situation, we get $G \cong C_6 * K_1$. If $G_2 \cong F_1(n-5)$, we have $d(u) = 4$. G_2 is obtained from G_1 by deleting three independent vertices which is impossible.

Subcase 2.2. n is even.

• $d(u) = 2$. In this subcase, we know that G_1 is a connected graph with cycles. Note that $G \ncong C_8 * K_2$, hence $G_1 \ncong C_8$. By Theorem 1, we have $\mathrm{mi}(G_1) \leqslant r^{n-4} + 1$. On the other hand, notice that $G \ncong D_{n,k}$, hence if $G_2 \cong B_{n-3,k}$, we obtain that $G \cong H_1(n),\ H_2(n)$, or $\ H_3(n)$, our result holds. If $G_2 \ncong B_{n-3,k}$, by induction hypothesis or Lemma 7, we have $\mathrm{mi}(G_2) \leqslant \max\{r^{n-4}-1, 3r^{n-8}\} = r^{n-4}-1$. Combining with Lemma 1, we have

$$\mathrm{mi}(G) = \mathrm{mi}(G_1) + \mathrm{mi}(G_2) \leqslant r^{n-4} + 1 + r^{n-4} - 1 = r^{n-2},$$

the equality holds if and only if $G_1 \cong B_{n-2}, C_{10}$ or $C_8 * K_2$ and $\mathrm{mi}(G_2) = r^{n-4} - 1$, but there is no such bipartite graph.

• $d(u) = 3$. If G_1 is disconnected, then G_1 must have cycles and $G_2 \ncong \frac{n-4}{2}K_2$ since G have cycles. Thus, by Lemma 5 and Theorem 1, we get $\mathrm{mi}(G_1) \leqslant r^{n-4}+r^{n-8} = 5r^{n-8}$ and $\mathrm{mi}(G_2) \leqslant \max\{3r^{n-8}, r^{n-6}+r^{n-10}\} = 3r^{n-8}$. By Lemma 1, we have

$$\mathrm{mi}(G) = \mathrm{mi}(G_1) + \mathrm{mi}(G_2) \leqslant 5r^{n-8} + 3r^{n-8} = r^{n-2},$$

the equality holds if and only if $G_1 \cong C_6 \uplus \frac{n-8}{2}K_2$ and $G_2 \cong P_4 \uplus \frac{n-8}{2}K_2$, but there is no such bipartite graph. If G_1 is connected and $G_2 \cong \frac{n-4}{2}K_2$, then we have $G \cong H_2(n)$ and $\mathrm{mi}(G) = r^{n-2}$, the result holds. If G_1 is connected and $G_2 \ncong \frac{n-4}{2}K_2$, then for $n = 6$, we get $G_2 = 2K_1$ and $G \cong H_0(6)$, the result holds. We assume $n \geqslant 8$. Obviously, $G_1 \ncong C_8$ since $G \ncong C_8 * K_2$. By Lemmas 3, 5 and Theorem 1, we have $\mathrm{mi}(G_1) \leqslant r^{n-4} + 1$, $\mathrm{mi}(G_2) \leqslant \max\{3r^{n-8}, r^{n-6} + r^{n-10}\} = 3r^{n-8}$. Thus,

$$\begin{aligned}
\mathrm{mi}(G) &= \mathrm{mi}(G_1) + \mathrm{mi}(G_2) \qquad \text{(by Lemma 1)} \\
&\leqslant r^{n-4} + 1 + 3r^{n-8} \qquad (15) \\
&= 7r^{n-8} + 1 \\
&\leqslant r^{n-2}. \qquad (16)
\end{aligned}$$

The equality in (15) holds if and only if $G_1 \cong T_1(n-2)$, or B_{n-2}, $G_2 \cong P_4 \uplus \frac{n-8}{2}K_2$; while the equality in (16) holds if and only if $n = 8$, i.e., $G_1 \cong P_4 * K_2$, C_6 or P_6 and $G_2 \cong P_4$, but there is no such bipartite graph.

• $d(u) \geqslant 4$. Note that G contains cycles, it is easy to see that $G_1 \ncong \frac{n-2}{2}K_2$. By Lemmas 5, 6 and Theorem 1, we get $\mathrm{mi}(G_1) \leqslant \max\{3r^{n-6}, r^{n-4} + r^{n-8}\} = 3r^{n-6}$ and $\mathrm{mi}(G_2) \leqslant r^{n-6}$. By Lemma 1,

$$\mathrm{mi}(G) = \mathrm{mi}(G_1) + \mathrm{mi}(G_2) \leqslant 3r^{n-6} + r^{n-5-1} = r^{n-2},$$

the equality holds if and only if $G_1 \cong P_4 \uplus \frac{n-6}{2}K_2$, $G_2 \cong F_1(n-5)$ or $F_1(n-6)$. Note that G_2 is obtained from G_1 by deleting three or four independent vertices, hence there is no such bipartite graph of order n. Hence $\mathrm{mi}(G) < r^{n-2}$.

Now we consider $\delta(G) \geqslant 2$. In this subcase, we used the following two facts (for their proofs one may be referred to the Appendix).

Fact 1 *Suppose $n \geqslant 7$ is odd and each vertex of degree $\geqslant 4$ is in all cycles of G, then $\mathrm{mi}(G) < 3r^{n-5}$.*

Fact 2 *Suppose $n \geqslant 6$ is even and each vertex of degree $\geqslant 4$ is in all cycles of G, then $\mathrm{mi}(G) \leqslant r^{n-2}$. The equality holds if and only if $G \cong H_1(n)$.*

Obviously, in this case, if $\delta(G) \geqslant 2$, Theorem 2 holds directly from Facts 1 and 2. □

4 Concluding remark

In view of Theorems 1 and 2(i), the disconnected graphs among $\mathscr{B}_n$ with the first-, second-, ..., $\frac{n-2}{2}$-th largest number of maximal independent sets are characterized, while the connected graphs in $\mathscr{B}_n$ having the largest and the second largest number of maximal independent sets are determined; whereas in view of Theorem 2(ii), graphs among $\mathscr{B}'_n$ having the largest number of maximal independent sets are identified.

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Appendix

In the appendix, we present the proofs for Facts 1 and 2.

Proof of Fact 1: We first assume that G has a vertex v of degree 3 such that $G-v$ has cycles. Note that G contains no odd cycles and $\delta(G) \geqslant 2$, hence $G-v$ (resp. $G-N_G[v]$) does not contain K_2 as a component.

• $G-v \ncong D_{n-1,k}$. Then we are to show that $G-v \ncong C_8 \uplus \frac{n-9}{2}K_2$, $C_{10} \uplus \frac{n-11}{2}K_2$ and $(C_8 * K_2) \uplus \frac{n-11}{2}K_2$ by contradiction.

If $G-v \cong C_8 \uplus \frac{n-9}{2}K_2$, i.e., $G-v \cong C_8$. Notice that $d(v)=3$, we have $G-N_G[v] \cong 2K_1 \uplus P_3$. So we obtain that the graph G is depicted in Fig. 3(a). By Lemma 1, we get $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-u)+\mathrm{mi}(G-N[u]) = 7+4 = 11 < 3r^4 = 12$.

If $G-v \cong C_{10} \uplus \frac{n-11}{2}K_2$, i.e., $G-v \cong C_{10}$. Note that $d(v)=3$, we have $G-N_G[v] \cong 2K_1 \uplus P_5$ or $K_1 \uplus 2P_3$. By Lemma 1, we get $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-v)+\mathrm{mi}(G-N_G[v]) = 17+4 = 21 < 3r^6 = 24$.

If $G-v \cong (C_8 * K_2) \uplus \frac{n-11}{2}K_2$, i.e., $G-v \cong C_8 * K_2$. Note that $d(v)=3$, we have $G-N_G[v] \cong 2K_1 \uplus P_5,\ K_1 \uplus 2P_3$, $K_1 \uplus (K_1 * (K_2 \uplus P_3))$ or $P_3 \uplus K_{1,3}$. By Lemma 1, we get $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-v)+\mathrm{mi}(G-N_G[v]) = 17+4 = 21 < 3r^6 = 24$.

Hence, we have

$$G-v \ncong D_{n-1,k},\ C_8 \uplus \frac{n-9}{2}K_2, C_{10} \uplus \frac{n-11}{2}K_2 \text{ and } (C_8 * K_2) \uplus \frac{n-11}{2}K_2.$$

By induction hypothesis, $\mathrm{mi}(G-v) \leqslant r^{n-3}$. In view of Lemmas 1 and 6, we have

$$\begin{aligned}\mathrm{mi}(G) &\leqslant \mathrm{mi}(G-v)+\mathrm{mi}(G-N_G[v]) \\ &\leqslant r^{n-3}+r^{n-4-1} \\ &= 3r^{n-5}.\end{aligned} \tag{A.1}$$

The equality in (A.1) holds if and only if $G-v \cong H_0(n-1),\ H_1(n-1),\ H_2(n-1)$, or $H_3(n-1)$ for $n=7,9,11$ and $G-v \cong H_1(n-1),\ H_2(n-1)$, or $H_3(n-1)$ for $n \geqslant 13$, $G-N_G[v] \cong F_1(n-4)$, i.e., $G-N_G[v] \cong T_1(n-4)$. Note that $G-N_G[v]$ is obtained from $G-v$ by deleting three independent disjoint vertices, but there is no such bipartite graph of order n. Hence $\mathrm{mi}(G) < 3r^{n-5}$.

• $G - v \cong D_{n-1,k}$, i.e., $G - v \cong B_{n-1}$. In this case, we have $\mathrm{mi}(G - v) = r^{n-3} + 1$. Furthermore, $G - N_G[v]$ is either an acyclic graph which is not isomorphic to $B_{n-4,k}$ or a bipartite graph containing cycles. It follows from induction hypothesis or Lemma 7 that $\mathrm{mi}(G - N_G[v]) \leqslant \max\{r^{n-4-1} - 1, 3r^{n-4-5}\} = r^{n-5} - 1$. Together with Lemma 1, we have

$$\begin{aligned}\mathrm{mi}(G) &\leqslant \mathrm{mi}(G - v) + \mathrm{mi}(G - N_G[v]) \\ &\leqslant r^{n-3} + 1 + r^{n-5} - 1 \\ &= 3r^{n-5}.\end{aligned} \tag{A.2}$$

The equality in (A.2) holds if and only if $G - v \cong B_{n-1}$, $\mathrm{mi}(G - N_G[v]) = r^{n-5} - 1$. Note that G is a bipartite graph with $\delta(G) \geqslant 2$, hence $G - v$ must be the graph as depicted in Fig. 3(b). $G - N_G[v]$ is obtained from $G - v$ by deleting three independent vertices. Elementary calculation yields $\mathrm{mi}(G - N_G[v]) < r^{n-5} - 1$. Hence, $\mathrm{mi}(G) < 3r^{n-5}$.

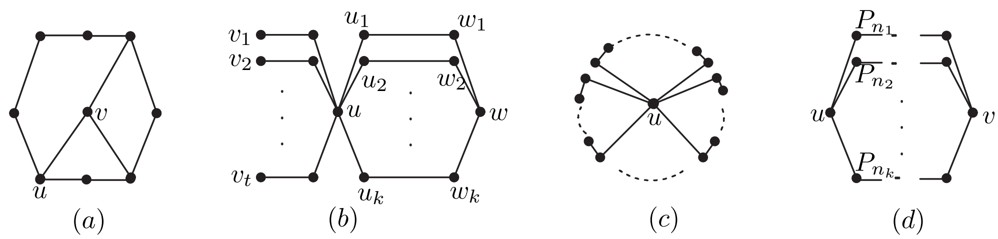


Fig. 3: Graphs used in the proof of Fact 1.

Now, we consider the case that each vertex of degree $\geqslant 3$ is in all cycles of G. Then G must be a graph with the structures as depicted in Figs. 3(c) or 3(d). Assume that the vertex u is in all cycles of G, then $d(u) \geqslant 3$. Note that n is odd and $\delta(G) \geqslant 2$, hence $G - u \ncong B_{n-1,k}$ and $G - u$ contains no cycles. By Lemma 7, we get $\mathrm{mi}(G - u) \leqslant r^{n-3}$. Thus, we have

$$\begin{aligned}\mathrm{mi}(G) &\leqslant \mathrm{mi}(G - u) + \mathrm{mi}(G - N[u]) \qquad \text{(by Lemma 1)} \\ &\leqslant r^{n-3} + r^{n-4-1} \qquad \text{(by Lemma 6)} \\ &= 3r^{n-5}.\end{aligned} \tag{A.3}$$

The equality in (A.3) holds if and only if $\mathrm{mi}(G - u) = r^{n-3}$, $G - N[u] \cong F_1(n-4)$ or $F_1(n-5)$, i.e., $G - N[u] \cong T_1(n-4)$ or $T_1(n-5)$. Notice that $\delta(G) \geqslant 2$ and u is in all cycles of G, it is straightforward to check that $n \in \{7, 9, 11\}$ and $G - N[u] \ncong T_1(n-5)$. So we get that G is a graph of the structure in Fig. 3(d). That is to say, G has exactly two vertices of degree $\geqslant 3$, say u and v. It follows that $d(u) = d(v) = d$ and $G - \{u, v\} = P_{n_1} \uplus \cdots \uplus P_{n_k}$ with $n_1 \geqslant n_2 \geqslant \cdots \geqslant n_k$. If $n = 7$, then $n_1 = 3$, $n_2 = 1$, $n_3 = 1$. By elementary calculation, $\mathrm{mi}(G) = 5 < 6$. If $n = 9$, then $n_1 = 5$, $n_2 = 1$, $n_3 = 1$. By Lemma 1, $\mathrm{mi}(G) \leqslant \mathrm{mi}(G - u) + \mathrm{mi}(G - N[u]) = 4 + 7 = 11 < 12$. If $n = 11$, then $n_1 = n_2 = n_3 = 3$. By Lemma 1, $\mathrm{mi}(G) \leqslant \mathrm{mi}(G - u) + \mathrm{mi}(G - N[u]) = 13 + 8 = 21 < 24$. Hence, we obtain $\mathrm{mi}(G) < 3r^{n-5}$. Thus, Fact 1 holds. □

Further on we need the following lemma to prove Fact 2.

Lemma A *Suppose $n \geqslant 6$ is even. If G has a path $P_5 = u_1u_2u_3u_4u_5$ such that $d(u_3) = 2$, $G - \{u_1, u_2, u_3, u_4, u_5\}$ has cycles and $G - \{u_2, u_3, u_4, u_5\} \ncong D_{n-4,k}, C_8 \uplus \frac{n-12}{2}K_2, C_{10} \uplus \frac{n-14}{2}K_2$ and $(C_8 * K_2) \uplus \frac{n-14}{2}K_2$, then $\mathrm{mi}(G) < r^{n-2}$.*

Proof: From the assumption it follows that $G_1 := G - \{u_1, u_2, u_3\}$, $G_2 := G - \{u_2, u_3, u_4\}$ and $G_3 := G - \{u_2, u_3, u_4, u_5\}$, respectively, has cycles and $G_3 \ncong D_{n-4,k}, C_8 \uplus \frac{n-12}{2}K_2, C_{10} \uplus \frac{n-14}{2}K_2$ and $(C_8 * K_2) \uplus \frac{n-14}{2}K_2$. Hence, by Lemma 1 we obtain

$$\begin{aligned}\mathrm{mi}(G) &\leqslant \mathrm{mi}(G - u_2 - u_4) + \mathrm{mi}(G - u_2 - u_4 - N(u_4)) + \mathrm{mi}(G - N[u_2]) \\ &= \mathrm{mi}(G_2) + \mathrm{mi}(G_3) + \mathrm{mi}(G_1) \\ &\leqslant 3r^{n-3-5} + r^{n-4-2} + 3r^{n-3-5} \qquad \text{(by induction hypothesis)} \\ &= r^{n-2}.\end{aligned} \tag{A.4}$$

The equality in (A.4) holds if and only if $d(u_2) = d(u_4) = 2$, $G_1 = G_2 \cong (C_6 * K_1) \uplus \frac{n-10}{2}K_2$ or $O_1(k) \uplus \frac{n-k-3}{2}K_2$, and $G_3 \cong H_0(6) \uplus \frac{n-10}{2}K_2,\ H_0(8) \uplus \frac{n-12}{2}K_2,\ H_0(10) \uplus \frac{n-14}{2}K_2,\ H_1(k) \uplus \frac{n-k-4}{2}K_2,\ H_2(k) \uplus \frac{n-k-4}{2}K_2$, or $H_3(k) \uplus \frac{n-k-4}{2}K_2$. Since $\delta(G) \geqslant 2$, $G_1,\ G_2$ contains no K_2 as a component, i.e., $G_1 = G_2 \cong C_6 * K_1$ or $O_1(n-3)$. If $G_1 = G_2 \cong C_6 * K_1$, we get $G \cong H_0(10)$ or the graph depicted in Fig. $4(c)$. But this implies $G - \{u_1, u_2, u_3, u_4, u_5\}$ has no cycles, a contradiction. If $G_1 = G_2 \cong O_1(n-3)$, we get two such graphs which contain odd cycles, a contradiction. That is to say, the equality in (A.4) does not hold. Hence, $\mathrm{mi}(G) < r^{n-2}$, as desired. □

Proof of Fact 2: We say a vertex v is good if $d(v) = 3$ and $G - v$ has cycles. Since $\delta(G) \geqslant 2$ and G is bipartite, then $G - N_G[v] \ncong B_{n-4,k}$ for any good vertex v.

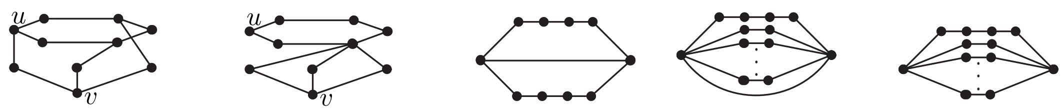
First we consider that G has good vertices by distinguishing the following two possible cases.

Case 1. For all good vertices v, $G - N_G[v] \cong D_{n-4,k}$.

For convenience, let $G_1 = G - N_G[v]$. Note that $\delta(G) \geqslant 2$ and G is bipartite, hence G_1 must be connected and $G_1 \cong B_{n-4}$. Furthermore, G_1 must be a graph with the structure shown in Fig. 3(b). Clearly, if $t \geqslant 1$, then $N(w) \cap N(v) = \emptyset$; if $t = 0$, then either $N(w) \cap N(v) = \emptyset$ or $N(u) \cap N(v) = \emptyset$. Hence, without loss of generality, assume $N(w) \cap N(v) = \emptyset$. Note that $d(v) = 3$ and $\delta(G) \geqslant 2$, hence $G - w$ has cycles. Thus, by the assumption that each vertex of degree$\geqslant 4$ is in all cycles of G, it follows that $2 \leqslant d(x) \leqslant 3$ for $x = w$ or $x \in N(v)$.

If $d(u) \leqslant 3$, note that $\delta(G) \geqslant 2$ and $G - N_G[v] \cong D_{n-4,k}$ for every good vertex v, G must be the graph shown in Figs. 4(a) or 4(b). For Fig. 4(a), $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-v) + \mathrm{mi}(G - N_G[v]) = 8 + 5 = 13 < 16$; For Fig. 4(b), $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-v) + \mathrm{mi}(G - N_G[v]) = 6 + 5 = 11 < 16$, they are not the extremal graphs.

If $d(u) \geqslant 4$, then G has at most one edge between $N(v)$ and $A = \{u_j : 1 \leqslant j \leqslant k\} \cup \{w_j : 1 \leqslant j \leqslant k\}$. Consequently, we have $d(w) = 2$. Otherwise, w is a good vertex of G, so in $G - N[w]$, there is at least one vertex $y \in N(u)$ such that $d(y) = 1$. Obviously, $G - N[w] \ncong D_{n-4,k}$, a contradiction. Similarly, we can conclude that each vertex in $N(v)$ has degree 2. Now, let $P_5 = u_1w_1ww_2u_2$. Obviously, $d(w) = 2$, $G - \{u_1, w_1, w, w_2, u_2\}$ has cycles and $G - \{w_1, w, w_2, u_2\} \ncong D_{n-4,k}, C_8 \uplus \frac{n-12}{2}K_2, C_{10} \uplus \frac{n-14}{2}K_2$ and $(C_8 * K_2) \uplus \frac{n-14}{2}K_2$. By Lemma A, we obtain that $\mathrm{mi}(G) < r^{n-2}$.



(a) (b) (c) (d) (f)

Fig. 4: Graphs used in the proof of Fact 2.

Case 2. There exists a good vertex v such that $G - N_G[v] \ncong D_{n-4,k}$.

In this case, we are to show that $G_1 := G - N_G[v] \ncong C_8 \uplus \frac{n-9}{2}K_2,\ C_{10} \uplus \frac{n-11}{2}K_2$ and $(C_8 * K_2) \uplus \frac{n-11}{2}K_2$. In fact, if $G_1 \cong C_8 \uplus \frac{n-9}{2}K_2$, then there exist eight such graphs, i.e., $G^1, G^2, \ldots, G^8$; if $G_1 \cong C_{10} \uplus \frac{n-11}{2}K_2$, then there exist thirteen such graphs, i.e., $G^9, G^{10}, \ldots, G^{21}$; if $G_1 \cong (C_8 * K_2) \uplus \frac{n-11}{2}K_2$, then there exist twenty-five such graphs, i.e., $G^{22}, G^{23}, \ldots, G^{46}$, where $G^1, G^2, \ldots, G^{46}$ are depicted in Fig. 5. By direct computation, we obtain $\mathrm{mi}(G) < r^{n-2}$. Hence, $G_1 \ncong C_8 \uplus \frac{n-9}{2}K_2,\ C_{10} \uplus \frac{n-11}{2}K_2$ and $(C_8 * K_2) \uplus \frac{n-11}{2}K_2$. By Lemma 7 (if G_1 is acyclic) or by induction hypothesis (if G_1 contains cycles), we obtain that $\mathrm{mi}(G_1) \leqslant r^{n-6}$. Thus, we obtain that

$$\begin{aligned} \mathrm{mi}(G) &\leqslant \mathrm{mi}(G-v) + \mathrm{mi}(G_1) && \text{(by Lemma 1)} \\ &\leqslant 3r^{n-6} + r^{n-6} && \text{(by induction hypothesis)} \\ &= r^{n-2}. \end{aligned} \tag{A.5}$$

The equality in (A.5) holds if and only if $G - v \cong (C_6 * K_1) \uplus \frac{n-8}{2}K_2$ or $O_1(k) \uplus \frac{n-1-k}{2}K_2$, $\mathrm{mi}(G_1) = r^{n-6}$. Note that $\delta(G) \geqslant 2$ and G contains no odd cycles, $G - v$ contains no K_2 as a component, hence $G - v \cong C_6 * K_1$ or $O_1(n-1)$. If $G - v \cong C_6 * K_1$, there are two such graphs. By a straightforward calculation, $\mathrm{mi}(G) = 6$ or $7 < r^6 = 8$. If $G - v \cong O_1(n-1)$, then $6 \leqslant n \leqslant 10$ since $d(v) = 3$ and $\delta(G) \geqslant 2$. For $n = 6$, there is one such graph. By a straightforward calculation, $\mathrm{mi}(G) = 3 < 4$. For $n = 8$, there are two such graphs. By a straightforward calculation, $\mathrm{mi}(G) = 7 < 8$. For $n = 10$, we get

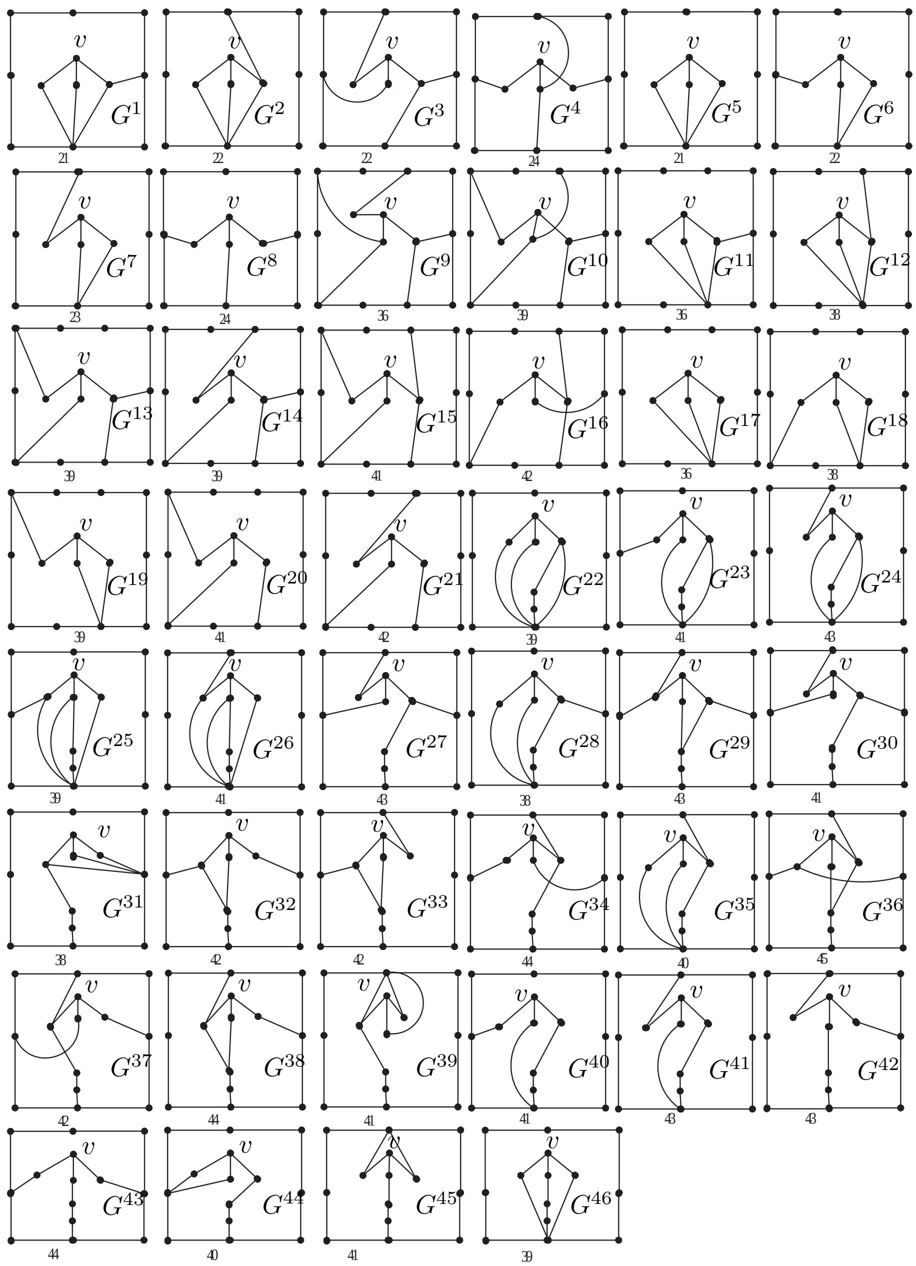


Fig. 5: Graphs $G^1, G^2, \ldots, G^{46}$ used in Case 2 of Fact 2, in which each number below the graph G^i is an upper bound of $\mathrm{mi}(G^i)$, $i = 1, 2, \ldots, 46$.

$G_1 \cong C_4 * 2K_1$. By Lemma 1, $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-v) + \mathrm{mi}(G_1) = 12 + 3 = 15 < 16$. Hence, $\mathrm{mi}(G) < r^{n-2}$. The result holds.

Now we consider that G has no good vertex, that is to say, each vertex of degree $\geqslant 3$ must be contained in all cycles of G. This implies that G must be the graph with structures shown in Figs. 3(c) or 3(d). By Lemma 8 and $G \ncong C_6, C_8$ and C_{10}, we assume that G is not a cycle. If G is a graph of the structure in Fig. 3(c), then G has only one vertex u of degree $\geqslant 3$. Since G is a bipartite graph of even order, then $d(u) \geqslant 6$ and $G - u$ consists of $k \geqslant 3$ disjoint paths of even length, say $P_{n_1}, P_{n_2}, \ldots, P_{n_k}$ (see Fig. 3(c)), where $k = \frac{d(u)}{2}$. By Lemmas 2 and 3, it follows that

$$\mathrm{mi}(G-u) = \prod_{j=1}^{k} \mathrm{mi}(P_{n_j}) \leqslant \prod_{j=1}^{k} r^{n_j - 1} \leqslant r^{n-4}$$

and so

$$\begin{aligned} \mathrm{mi}(G) &\leqslant \mathrm{mi}(G-u) + \mathrm{mi}(G - N_G[u]) && \text{(by Lemma 1)} \\ &\leqslant r^{n-4} + r^{n-8} && \text{(by Lemma 6)} \\ &= 5r^{n-8} < r^{n-2}. \end{aligned}$$

The result holds.

Suppose G is a graph of the structure in Fig. 3(d), then G has exactly two vertices degree $\geqslant 3$, say u, v. It follows that $d(u) = d(v) = d \geqslant 3$ and $G - \{u, v\}$ consists of k disjoint paths, say $P_{n_1}, P_{n_2}, \ldots, P_{n_k}$ with $n_1 \geqslant n_2 \geqslant \cdots \geqslant n_k$, where $k = d$ if u and v are not adjacent and $k = d - 1$ otherwise. Since G is a bipartite graph, either all n_j's are odd or all n_j's are even.

If all n_j's are odd, we have $k = d \geqslant 4$. By Lemmas 2 and 3, we get

$$\mathrm{mi}(G-u-v) = \prod_{j=1}^{k} \mathrm{mi}(P_{n_j}) \leqslant \prod_{j=1}^{k} r^{n_j - 1} \leqslant r^{n-6}.$$

This gives

$$\begin{aligned} \mathrm{mi}(G) &\leqslant \mathrm{mi}(G-u-v) + \mathrm{mi}(G-u-v-N_G(v)) + \mathrm{mi}(G - N_G[u]) && \text{(by applying Lemma 1 twice)} \\ &\leqslant r^{n-6} + r^{n-6} + r^{n-5-1} && \text{(by Lemma 6)} \\ &= 3r^{n-6} < r^{n-2}. \end{aligned}$$

Now we consider that all n_j's are even. Let $P_{n_1} = u_1 u_2 \ldots u_{n_1}$. By Lemma A, we assume $n_1 \leqslant 4$. If $n_1 = 4$, then both $L_1 = G - \{u_1, u_2, u_3\}$ and $L_2 = G - \{u_2, u_3, u_4\}$ have cycles and $L_3 = G - \{u_1, u_2, u_3, u_4, v_1\}$ is a tree. Furthermore, $L_3 \ncong T_1(n-4)$ unless G is one of the graphs shown in Figures 4(c), 4(d) and 4(f). If $L_3 \ncong T_1(n-4)$, by Lemma 1 we get

$$\begin{aligned} \mathrm{mi}(G) &\leqslant \mathrm{mi}(G-u_1-u_3) + \mathrm{mi}(G-u_1-u_3-N(u_1)) + \mathrm{mi}(G-N[u_3]) \\ &= \mathrm{mi}(L_1) + \mathrm{mi}(L_3) + \mathrm{mi}(L_2) \\ &\leqslant 3r^{n-8} + r^{n-6} + 3r^{n-8} && \text{(by induction hypothesis and Lemma 6)} \\ &= r^{n-2}. \end{aligned} \tag{A.6}$$

The equality in (A.6) holds if and only if $L_1 = L_2 \cong C_6 * K_1$ or $O_1(n-3)$, $L_3 \cong H_0(6) \uplus \frac{n-10}{2} K_2$, $H_0(8) \uplus \frac{n-12}{2} K_2$, $H_0(10) \uplus \frac{n-14}{2} K_2$, $H_1(k) \uplus \frac{n-k-4}{2} K_2$, $H_2(k) \uplus \frac{n-k-4}{2} K_2$, or $H_3(k) \uplus \frac{n-k-4}{2} K_2$. If $L_1 = L_2 \cong C_6 * K_1$, then $n = 10$ and $G \cong H_0(10)$. So $\mathrm{mi}(G) = \mathrm{mi}(H_0(10)) = 16$, hence we get the extremal graph $H_0(10)$. If $L_1 = L_2 \cong O_1(n-3)$, then $n = 8$ and $G \cong H_0(8)$. So $\mathrm{mi}(G) = \mathrm{mi}(H_0(8)) = 8$, hence we get the extremal graph $H_0(8)$. Our result holds.

If $L_3 \cong T_1(n-4)$, G is one of the graphs shown in Figs. 4(c), 4(d) and 4(f). By direct calculation, we have, for Fig. 4(c), $\mathrm{mi}(G) = 13 < 16$; for Fig. 4(d) ($n \geqslant 8$), $\mathrm{mi}(G) = 3r^{n-6} + 2 \leqslant r^{n-2}$, the equality holds if and only if $n = 8$, $G \cong H_0(8)$, hence we get extremal graph $H_0(8)$; for Fig. 4(f) ($n \geqslant 10$), $\mathrm{mi}(G) = 3r^{n-6} + 4 \leqslant r^{n-2}$, the equality holds if and only if $n = 10$, $G \cong H_0(10)$. Hence, we assume $n_1 \leqslant 2$, which implies $n_1 = n_2 = \cdots = n_k = 2$. Since $G \ncong B_n$, we conclude that v_1 must be adjacent to v_2. So $\mathrm{mi}(G) = r^{n-2}$ and $G \cong H_1(n)$.

This completes the proof. $\square$