On the third largest number of maximal independent sets of graphs*

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Abstract: A maximal independent set is an independent set that is not a proper subset of any other independent set. In this paper, we determine the third largest number of maximal independent sets among all graphs of order $n \geqslant 3$ and identify the corresponding extremal graphs.

Keywords: Maximal independent set; Extremal graph

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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 clique corresponds to an independent set in the complement graph. The set of all maximal independent sets of a graph G is denoted by $\mathrm{MI}(G)$ and its cardinality by $\mathrm{mi}(G)$.

Given a simple graph $G = (V_G, E_G)$, the cardinality of V_G is called the *order* of G. $G - v$ 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 $d(v) = |N_G(v)|$, the degree of v in G. In particular, let $\Delta(G) = \max\{d(x)|x \in V_G\}$ and $\delta(G) = \min\{d(x)|x \in V_G\}$. For convenience, let $N_G[x] = \{x\} \cup N_G(x)$. A *leaf* of G is a vertex of degree one. 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 the 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 $E_{H*G} = E_H \cup E_G \cup \{xu_i : i = 1, 2, \ldots, k\}$. Throughout the text we denote by P_n, C_n, K_n and $K_{1,n-1}$ the path, cycle, complete graph and star on n vertices, respectively.

Further on we need the following lemmas.

Lemma 1.1 ([7]). *For any vertex v in a graph G, the followings hold.*

(i) $\mathrm{mi}(G) \leqslant \mathrm{mi}(G - v) + \mathrm{mi}(G - N_G[v])$;

(ii) *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 1.2 ([5]). *If $n \geqslant 6$, then* $\mathrm{mi}(C_n) = \mathrm{mi}(C_{n-2}) + \mathrm{mi}(C_{n-3})$.

Lemma 1.3 ([7]). *If $G = G_1 \uplus G_2$, then* $\mathrm{mi}(G) = \mathrm{mi}(G_1) \cdot \mathrm{mi}(G_2)$.

For $n \geqslant 2$, let $G(n), H(n)$ be two n-vertex graphs defined as

$$G(n) = \begin{cases} sK_3, & \text{if } n = 3s; \\ K_4 \uplus (s-1)K_3, \text{ or } 2K_2 \uplus (s-1)K_3, & \text{if } n = 3s+1; \\ K_2 \uplus sK_3, & \text{if } n = 3s+2 \end{cases}$$

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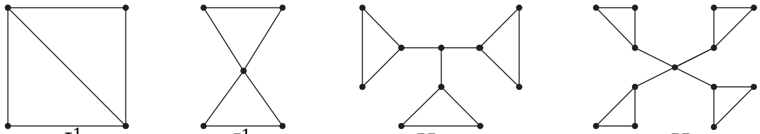

Figure 1: Graphs I_5^1, I_7^1, H_1 and H_2.

and

$$H(n)=\begin{cases} 2K_1, & \text{if } n=2;\\ P_3, \text{ or} K_2\uplus K_1, & \text{if } n=3;\\ I_5^1,\, P_4,\, K_3*K_1, \text{ or } K_3\uplus K_1, & \text{if } n=4;\\ C_5,\, K_5,\, K_3*K_2, \text{ or } I_7^1, & \text{if } n=5;\\ (K_3*K_3)\uplus(s-2)K_3,\ 3K_2\uplus(s-2)K_3, \text{or } K_4\uplus K_2\uplus(s-2)K_3, & \text{if } n=3s\geqslant 6;\\ (K_3*K_4)\uplus(s-2)K_3, & \text{if } n=3s+1\geqslant 7;\\ (K_3*K_3)\uplus K_2\uplus(s-2)K_3,\ 4K_2\uplus(s-2)K_3,\ 2K_4\uplus(s-2)K_3, \text{or } K_4\uplus 2K_2\uplus(s-2)K_3, & \text{if } n=3s+2\geqslant 8, \end{cases}$$

where I_5^1 and I_7^1 are depicted in Fig. 1. By Lemma 1.3, it is routine to check that

$$g(n):=\mathrm{mi}(G(n))=\begin{cases} 3^s, & \text{if } n=3s;\\ 4\cdot 3^{s-1}, & \text{if } n=3s+1;\\ 2\cdot 3^s, & \text{if } n=3s+2 \end{cases} \quad \text{and} \quad h(n):=\mathrm{mi}(H(n))=\begin{cases} 1, & \text{if } n=2;\\ 2, & \text{if } n=3;\\ 3, & \text{if } n=4;\\ 5, & \text{if } n=5;\\ \frac{11}{12}g(n), & \text{if } n=3s+1\geqslant 6;\\ \frac{8}{9}g(n), & \text{otherwise.} \end{cases}$$

Theorem 1.4 ([6])**.** *If G is a graph with $n\geqslant 2$ vertices, then $\mathrm{mi}(G)\leqslant g(n)$ with the equality holding if and only if $G\cong G(n)$.*

Theorem 1.5 ([3, 4])**.** *If G is a graph with n vertices and $G\ncong G(n)$, then $\mathrm{mi}(G)\leqslant h(n)$ with the equality holding if and only if $G\cong H(n)$.*

Further on, let $I(n), I'(n)$ be two n-vertex graphs ($n\geqslant 8$) defined, respectively, as

$$I(n)=\begin{cases} K_3*(K_3\uplus K_3)\uplus(s-3)K_3, \text{or } (K_4*K_3)\uplus K_2\uplus(s-3)K_3, & \text{if } n=3s;\\ K_4\uplus(K_3*K_3)\uplus(s-3)K_3,\ K_4\uplus 3K_2\uplus(s-3)K_3,\ 2K_4\uplus K_2\uplus(s-3)K_3, & \\ \ (K_3*K_3)\uplus 2K_2\uplus(s-3)K_3, \text{or } 5K_2\uplus(s-3)K_3, & \text{if } n=3s+1;\\ (K_4*K_4)\uplus(s-2)K_3,\ (K_3*K_2)\uplus(s-1)K_3,\ K_5\uplus(s-1)K_3,\ C_5\uplus(s-1)K_3, \text{or } I_7^1\uplus(s-1)K_3, & \text{if } n=3s+2 \end{cases}$$

and

$$I'(n)=\begin{cases} H_1\cup K_2\cup(s-4)K_3, & \text{if } n=3s;\\ H_2\cup(s-4)K_3, & \text{if } n=3s+1;\\ H_1\cup 2K_2\cup(s-4)K_3, & \text{if } n=3s+2, \end{cases}$$

where I_7^1, H_1 and H_2 are depicted in Fig. 1.

Set $i(n)=\mathrm{mi}(I(n))$ and $i'(n)=\mathrm{mi}(I'(n))$. By Lemma 1.3, it is easy to obtain that

$$i(n)=\begin{cases} \frac{22}{27}g(n), & \text{if } n=3s;\\ \frac{8}{9}g(n), & \text{if } n=3s+1;\\ \frac{5}{6}g(n), & \text{if } n=3s+2 \end{cases} \quad \text{and} \quad i'(n)=\begin{cases} \frac{3}{4}g(n), & \text{if } n=3s+1;\\ \frac{2}{3}g(n), & \text{otherwise.} \end{cases} \tag{1.1}$$

Note that Hua and Hou [1] obtained that $i'(n)=\frac{97}{108}g(n)$ if $n=3s+1$ and $\frac{70}{81}g(n)$ otherwise, which is not correct by direct calculation. It is easy to see

$$i'(n)<i(n). \tag{1.2}$$

(♢) ([**Theorem 3.1**, 1]) *If G is a graph with $n \geqslant 3$ vertices and $G \ncong G(n)$, $H(n)$, then*

$$\mathrm{mi}(G) \leqslant \begin{cases} \frac{97}{108} g(n), & \text{if } n = 3s+1; \\ \frac{70}{81} g(n), & \text{otherwise.} \end{cases} \tag{1.3}$$

Furthermore, each of the equalities in (1.3) holds if and only if $G \cong I'(n)$.

Note that $I(n) \ncong G(n), H(n)$, hence in view of (1.2), Theorem 3.1 in [1] is not true. The following result characterizes the third largest number of maximal independent sets of n-vertex graphs ($n \geqslant 3$), the corresponding extremal graphs are identified.

Theorem 1.6. *Let G be an n-vertex graph with $n \geqslant 3$.*

(i) *If $G \ncong G(n), H(n)$ with $3 \leqslant n \leqslant 10$, then G is the graph with the third largest number of maximal independent set if and only if $G \in I''(n)$, where*

$$I''(n) = \begin{cases} 3K_1, & \text{if } n = 3; \\ 2K_1 \uplus K_2,\ K_1 \uplus P_3,\ K_{1,3}, \text{ or } C_4, & \text{if } n = 4; \\ K_1 \uplus 2K_2,\ K_1 \uplus K_4,\ K_2 \uplus P_3,\ P_5,\ K_4 * K_1,\ I_5^1 * K_1,\ I_5^2,\ I_5^3,\ I_5^4, \text{ or } I_5^5, & \text{if } n = 5; \\ K_4 * K_2,\ I_6^1,\ I_6^2,\ I_6^3, \text{ or } I_6^4, & \text{if } n = 6; \\ K_5 \uplus K_2,\ C_5 \uplus K_2,\ (K_3 * K_2) \uplus K_2,\ I_7^1 \uplus K_2,\ I_7^2,\ I_7^3,\ I_7^4, \text{ or } I_7^5, & \text{if } n = 7; \\ K_4 * K_4,\ (K_3 * K_2) \uplus K_3,\ K_5 \uplus K_3,\ C_5 \uplus K_3, \text{or } I_7^1 \uplus K_3, & \text{if } n = 8; \\ K_3 * (K_3 \uplus K_3), \text{or } (K_4 * K_3) \uplus K_2, & \text{if } n = 9; \\ K_4 \uplus (K_3 * K_3),\ K_4 \uplus 3K_2,\ 2K_4 \uplus K_2, (K_3 * K_3) \uplus 2K_2, \text{or } 5K_2, & \text{if } n = 10. \end{cases}$$

where I_5^2, I_5^3, I_5^4, I_5^5, I_6^1, I_6^2, I_6^3, I_6^4, I_7^2, I_7^3, I_7^4 and I_7^5 are depicted in Fig. 2.

(ii) *If $G \ncong G(n), H(n)$ with $n \geqslant 8$, then $\mathrm{mi}(G) \leqslant i(n)$ with equality if and only if $G \cong I(n)$.*

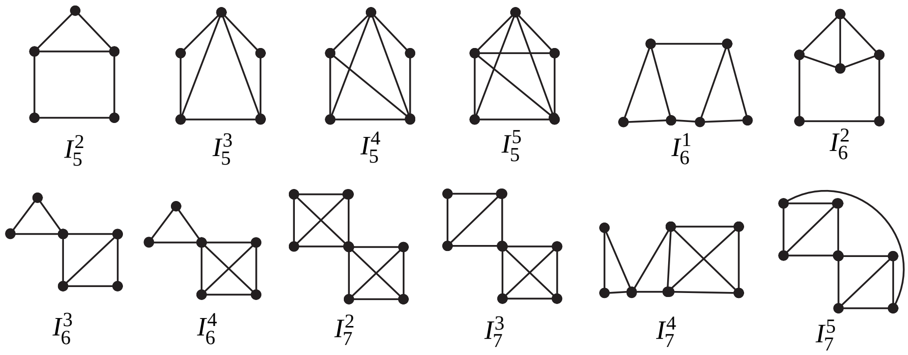

Figure 2: Graphs I_5^2, I_5^3, I_5^4, I_5^5, I_6^1, I_6^2, I_6^3, I_6^4, I_7^2, I_7^3, I_7^4 and I_7^5.

2. Proof of Theorem 1.6

We show Theorem 1.6 according to the following two possible cases.

Case 1. $3 \leqslant n \leqslant 10$.

It is straightforward to check that $I''(n) \ncong G(n),\ H(n)$ and $\mathrm{mi}(I''(n)) = h(n) - 1$ if $n = 3,4,5,6,7,8,10$ and $\mathrm{mi}(I''(9)) = h(9) - 2$. Suppose $G\ (\ncong G(n),\ H(n))$ is a graph of order n, $3 \leqslant n \leqslant 10$, such that $\mathrm{mi}(G)$ is as large as possible. By Theorem 1.5, we have that $h(n) - 1 = \mathrm{mi}(I''(n)) \leqslant \mathrm{mi}(G) \leqslant h(n) - 1$ for $n = 3,4,5,6,7,8,10$. Hence, $\mathrm{mi}(G) = h(n) - 1$. For $n = 9$, by Theorem 1.5, we have that $h(9) - 2 = \mathrm{mi}(I''(9)) \leqslant \mathrm{mi}(G) \leqslant h(9) - 1$, thus $\mathrm{mi}(G) = h(9) - 2$, or $h(9) - 1$. If $n = 3$, note that $g(3) = 3$, hence we get just one extremal graph $3K_1$. In the following, assume $n \geqslant 4$ and prove our results according to the following four subcases.

Subcase 1.1. $\delta(G)=0$.

In this subcase, we take a vertex $x\in V_G$ such that $d(x)=0$. Thus, we get $\mathrm{mi}(G)=\mathrm{mi}(G-x)$.

If $n=4$, note that $g(4)=4$, thus $\mathrm{mi}(G)=\mathrm{mi}(G-x)=2$ and $|V_{G-x}|=3$. Hence, we obtain that $G-x\cong P_3$ or $K_2\uplus K_1$, i.e., $G\cong P_3\uplus K_1$ or $K_2\uplus 2K_1$.

If $n=5$, note that $g(5)=6$, thus $\mathrm{mi}(G)=\mathrm{mi}(G-x)=4$ and $|V_{G-x}|=4$. Hence, by Theorem 1.4, we have $G-x\cong K_4$ or $2K_2$, which is equivalent to $G\cong K_4\uplus K_1$ or $2K_2\uplus K_1$.

If $6\leqslant n\leqslant 7$, then, on the one hand, $\mathrm{mi}(G)=\mathrm{mi}(G-x)=h(n)-1$; on the other hand, by Theorem 1.4, we get $\mathrm{mi}(G-x)\leqslant g(n-1)$. Thus, we get $g(n)-2\leqslant g(n-1)$. But, in fact $6=g(5)<h(6)-1=7$ and $9=g(6)<h(7)-1=10$, a contradiction.

If $n=8$, then by Theorem 1.4, $\mathrm{mi}(G)=\mathrm{mi}(G-x)$ and $\mathrm{mi}(G-x)\leqslant g(7)=12$. Hence, $\mathrm{mi}(G)\leqslant 12<15=h(8)-1$, this is a contradiction. Similarly, we can also get a contradiction, respectively, for $n=9,10$, which is omitted here.

Subcase 1.2. $\delta(G)=1$.

In this subcase, we take a vertex $x\in V_G$ such that $d(x)=1$ and $xy\in E_G$. Let $G_1=G-x-y$. Note that $G-N[y]$ is a subgraph of G_1, then $1\leqslant \mathrm{mi}(G-N[y])\leqslant \mathrm{mi}(G_1)$.

First consider $G_1\cong G(n-2)$. If $n=3s\,(s=2,3)$, then we obtain that $G_1\cong K_4\uplus(s-2)K_3$ or $2K_2\uplus(s-2)K_3$. If $G-N[y]\cong K_4\uplus(s-2)K_3$ or $2K_2\uplus(s-2)K_3$, then $G\cong H(n)$, a contradiction. So $G-N[y]$ is a proper subgraph of $K_4\uplus(s-2)K_3$, i.e. $G-N[y]$ is a subgraph $(s-1)K_3$, $K_4\uplus K_2\uplus(s-3)K_3$, or $K_1\uplus K_2\uplus(s-2)K_3$. By a simple calculation, we have $\mathrm{mi}(G-N[y])\leqslant \max\{3^{s-1},\ 8\cdot 3^{s-3},\ 2\cdot 3^{s-3}\}=3^{s-1}$. By Lemma 1.1(ii), we have $\mathrm{mi}(G)=\mathrm{mi}(G_1)+\mathrm{mi}(G-N[y])\leqslant 4\cdot 3^{s-2}+3^{s-1}=7\cdot 3^{s-2}$, the equality holds if and only if $G-N[y]\cong(s-3)K_3$. Note that $\mathrm{mi}(G)=7$ for $n=6$ and $\mathrm{mi}(G)>21$ for $n=9$. In conclusion, $n=6,\ G\cong K_4*K_2$.

If $n=3s+1\,(s=1,2,3)$, then we obtain that $G_1\cong K_2\uplus(s-1)K_3$. If $G-N[y]\cong K_2\uplus(s-1)K_3$, then $G\cong G(n)$, a contradiction. So $G-N[y]$ is a proper subgraph of $K_2\uplus(s-1)K_3$, i.e. $G-N[y]$ is a subgraph $K_1\uplus(s-1)K_3$ or $2K_2\uplus(s-2)K_3$. By a simple calculation, we have $1\leqslant \mathrm{mi}(G-N[y])\leqslant \max\{3^{s-1},\ 4\cdot 3^{s-2}\}=4\cdot 3^{s-2}$. By Lemma 1.1(ii), we have

$$3\leqslant 2\cdot 3^{s-1}+1\leqslant \mathrm{mi}(G)=\mathrm{mi}(G_1)+\mathrm{mi}(G-N[y])\leqslant 2\cdot 3^{s-1}+4\cdot 3^{s-2}=10\cdot 3^{s-2},$$

the equality holds if and only if $G-N[y]\cong 2K_2\uplus(s-2)K_3$. Note that $\mathrm{mi}(G)=h(n)-1$ holds for $n=4,7,10$. In conclusion, $n=7$ and $G\cong(K_3*K_2)\uplus K_2$.

If $n=3s+2\,(s=1,2)$, then we obtain that $G_1\cong sK_3$. There are two such graphs $K_4*K_1,\ I_5^1*K_1$ for $n=5$. By a simple calculation, we get K_4*K_1 and $I_5^1*K_1$ are extremal graphs. In the following, we consider $n=8$. If $G-N[y]\cong sK_3$, then $G\cong G(n)$, a contradiction. Hence, $G-N[y]$ is a proper subgraph of sK_3 , i.e. $G-N[y]$ is a subgraph $K_1\uplus(s-1)K_3$ or $K_2\uplus(s-1)K_3$. By a simple calculation, we have $1\leqslant \mathrm{mi}(G-N[y])\leqslant \max\{3^{s-1},\ 2\cdot 3^{s-1}\}=2\cdot 3^{s-1}$. By Lemma 1.1(ii), we have $\mathrm{mi}(G)=\mathrm{mi}(G_1)+\mathrm{mi}(G-N[y])\leqslant 3^s+2\cdot 3^{s-1}=5\cdot 3^{s-1}$, the equality holds if and only if $G-N[y]\cong K_2\uplus(s-1)K_3$. Note that $\mathrm{mi}(G)=15$ for $n=8$. In conclusion, $n=8$ and $G\cong(K_3*K_2)\uplus K_3$.

Next consider $G_1\cong H(n-2)$. If $n=4$, it is easy to get that $G_1\cong 2K_1$. As $\delta(G)=1$, we obtain that $G\cong K_{1,3}$. For $n\geqslant 5$, note that $G-N[y]$ is a subgraph of G_1, we have $\mathrm{mi}(G-N[y])\leqslant \mathrm{mi}(G_1)=h(n-2)$. By Lemma 1.1(ii) and Theorem 1.5, we have $\mathrm{mi}(G)=\mathrm{mi}(G_1)+\mathrm{mi}(G-N[y])\leqslant 2h(n-2)$, the equality holds if and only if $G-N[y]\cong H(n-2)$. Note that $\mathrm{mi}(G)=2$ for $n=4$ and $h(4-2)=h(4-4)=1$, we get extremal graph $K_{1,3}$. Note that $\mathrm{mi}(G)=h(n)-1$ holds for $n=5,6,7,8,10$ and $\mathrm{mi}(G)\geqslant h(n)-2$ holds for $n=9$. In conclusion, we also get extremal graphs $K_2\uplus K_3,\ K_5\uplus K_2,\ C_5\uplus K_2,\ (K_3*K_2)\uplus K_2,\ I_7^1\uplus K_2,\ (K_4*K_3)\uplus K_2,\ K_4\uplus 3K_2,\ 2K_4\uplus K_2, (K_3*K_3)\uplus 2K_2,\ 5K_2$.

Now consider $G_1\ncong G(n-2),\ H(n-2)$. By Theorem 1.5, we have $\mathrm{mi}(G_1)=1$ for $n=4$ and $\mathrm{mi}(G_1)\leqslant h(n-2)-1$ for $5\leqslant n\leqslant 10$. By Lemma 1.1(ii) and Theorem 1.5, we have $\mathrm{mi}(G)=\mathrm{mi}(G_1)+\mathrm{mi}(G-N[y])\leqslant 2h(n-2)-2<h(n)-1$ for $n=5,\ 6,\ 7,\ 8,\ 10$ and $\mathrm{mi}(G)=\mathrm{mi}(G_1)+\mathrm{mi}(G-N[y])\leqslant 2h(7)-2<h(9)-2$ for $n=9$. Thus there does not exist extremal graph in this subcase.

Subcase 1.3. $\delta(G)=2$ and $\Delta(G)=2$.

In this subcase, $G\cong C_n$. By direct calculation, $\mathrm{mi}(C_4)=2,\ \mathrm{mi}(C_5)=5>4,\ \mathrm{mi}(C_6)=5<7,\ \mathrm{mi}(C_7)=7<10$, $\mathrm{mi}(C_8)=10<15$, $\mathrm{mi}(C_9)=12<22$, $\mathrm{mi}(C_{10})=17<32$. Hence, we get the extremal graphs C_4 and $C_5\uplus K_3$.

Subcase 1.4. $\delta(G)\geqslant 2$ and $\Delta(G)\geqslant 3$.

In this subcase, we take a vertex $x\in V_G$ such that $d(x)=\Delta(G)\geqslant 3$. Let $G_2=G-N[x]$. If $n=4$, it is routine to check that $G\cong I_5^1$ since $G\ncong K_4$, i.e., $\mathrm{mi}(G)=3$, a contradiction. In the following, assume that $n\geqslant 5$.

First consider $\Delta(G)=3$ according to the following subcases.

• $n=5$. In this subcase we have $g(5)=6$ and $G_2=K_1$, hence $3 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1)=4$, i.e., $G-x \cong K_4,\ 2K_2,\ P_4,\ I_5^1,\ K_3 \uplus K_1$ or $K_3 * K_1$. Thus, we get $G \cong I_5^2$.

• $n=6$. In this subcase, we have $G_2 \cong 2K_1$ or K_2. If $G_2 \cong 2K_1$, then $6=7-1 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1)=6$, i.e., $\mathrm{mi}(G-x)=6$, i.e., $G-x \cong K_3 \uplus K_2$. But there is no such graph. If $G_2 \cong K_2$, then $5=7-2 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1)=6$, i.e., $\mathrm{mi}(G-x)=5$ or 6, which is equivalent to $G-x \cong K_3 \uplus K_2,\ C_5,\ K_5,\ K_3 * K_2,$ orI_7^1. Thus, we get $G \cong I_6^1$ or I_6^2.

• $n=7$. In this subcase, we have $G_2 \cong K_3,\ P_3,\ K_2 \uplus K_1$ or $3K_1$. If $G_2 \cong K_3$, note that $\mathrm{mi}(G)=10$ and $G \ncong G(n),\ H(n)$, hence there is no such graph. If $G_2 \cong P_3$ or $K_2 \uplus K_1$, then $\mathrm{mi}(G_2)=2$ and $8=10-2 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1)=9$, i.e., $\mathrm{mi}(G-x)=8$ or 9, which is equivalent to $G-x \cong 2K_3,\ K_3 * K_3,\ 3K_2$ or $K_4 \uplus K_2$. Thus, we get the only graph G, but $\mathrm{mi}(G)=9<10$, this is a contradiction. If $G_2 \cong 3K_1$, then $9=10-1 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1)=9$, i.e., $\mathrm{mi}(G-x)=9$, i.e., $G-x \cong 2K_3$. But such graph does not exist.

• $n=8$. Note that $G-x \ncong H(7)=K_4 * K_3$ since $\Delta(G)=3$. If $G-x \cong G(7)=K_4 \uplus K_3$, or $2K_2 \uplus K_3$, as $\Delta(G)=3$, we get $G \cong 2K_4=H(8)$, which is a contradiction. If $G-x \ncong G(7),\ H(7)$, by Theorem 1.5, we get $\mathrm{mi}(G-x) \leqslant h(7)-1=10$. Note that $|V_{G_2}|=8-4=4$, by Theorem 1.4, we have $\mathrm{mi}(G_2) \leqslant g(4)=4$. By Lemma 1.1(i), we obtain that $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-x)+\mathrm{mi}(G_2) \leqslant 10+4=14<15$, a contradiction.

• $n=9$. If $G-x \cong G(8)=K_2 \uplus 2K_3$, observe that $\Delta(G)=3$, then we get $G \cong (K_3 * K_3) \uplus K_3 = H(9)$, a contradiction. If $G-x \cong H(8)$, note that $\Delta(G)=3$, we get $G-x \cong (K_3 * K_3) \uplus K_2$, i.e., $G \cong W_0$; see Fig. 3. By direct calculation, $\mathrm{mi}(G)=21<22=h(9)-2$, a contradiction. If $G-x \ncong G(8),\ H(8)$, by Theorem 1.5, we get $\mathrm{mi}(G-x) \leqslant h(8)-1=15$. Note that $|V_{G_2}|=9-4=5$, by Theorem 1.4, we have $\mathrm{mi}(G_2) \leqslant g(5)=6$. By Lemma 1.1(i), we obtain that $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-x)+\mathrm{mi}(G_2) \leqslant 15+6=21<22=h(9)-2$, a contradiction.

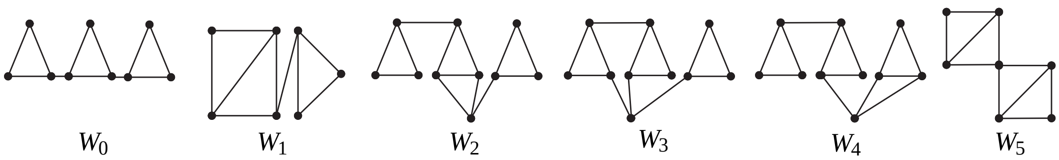

Figure 3: Graphs W_0, W_1, W_2, W_3, W_4 and W_5.

• $n=10$. If $G-x \cong G(9)=3K_3$, then it is routine to check that $G \cong K_1 * 3K_3$ or $W_1 \uplus K_3$ directly, where W_1 is depicted in Fig. 3. By elementary calculation, $\mathrm{mi}(G)=27<32$, a contradiction. If $G-x \cong H(9)$, observe that $\Delta(G)=3$, we get $G-x \cong (K_3 * K_3) \uplus K_3$ or $K_4 \uplus K_3 \uplus K_2$, which implies G must be isomorphic to W_2, W_3, W_4 (see Fig. 3) or $(K_3 * K_3) \uplus K_4$. By direct calculation, $\mathrm{mi}(W_2)=26<32,\ \mathrm{mi}(W_3)=\mathrm{mi}(W_4)=24<32,\ \mathrm{mi}((K_3 * K_3) \uplus K_4)=32$. Thus, we get the extremal graph $(K_3 * K_3) \uplus K_4$, as desired. If $G-x \ncong G(9),\ H(9)$, by Theorem 1.5, we get $\mathrm{mi}(G-x) \leqslant h(9)-1=23$. In this subcase, note that $|V_{G-N[x]}|=6$, hence if $G-N[x] \ncong G(6)$ for some vertex x with $d(x)=3$, then by Theorem 1.4, we have $\mathrm{mi}(G-N[x]) \leqslant g(6)-1=8$. Thus, by Lemma 1.1(i), we get $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-x)+\mathrm{mi}(G_2) \leqslant 23+8=31<32=h(10)-1$, a contradiction. If, for any vertex x of degree 3, satisfying $G-N[x] \cong G(6)$, then there is only one such graph $(K_1 * 2K_3) \uplus K_3$. By direct computing, $\mathrm{mi}((K_1 * 2K_3) \uplus K_3)=27<32$, a contradiction.

Next consider $\Delta(G)=4$.

If $n=5$, then we get G is a connected graph. By elementary calculation, we obtain extremal graphs $I_5^3,\ I_5^4,$ orI_5^5, as desired.

If $n=6$, then we have $G_2=K_1$ and $6=7-1 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1)=6$, i.e., $\mathrm{mi}(G-x)=6$, i.e., $G-x \cong K_3 \uplus K_2$. Thus, we get the extremal graph I_6^3.

If $n=7$, we have $G_2 \cong 2K_1$ or K_2. If $G_2 \cong 2K_1$, then $9=10-1 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1)=9$. Hence, $\mathrm{mi}(G-x)=9$, i.e., $G-x \cong 2K_3$. Thus, we get the only graph W_5 (see Fig. 3) with $\mathrm{mi}(W_5)=9<10$, a contradiction. If $G_2 \cong K_2$, then $8=10-2 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1)=9$, which implies $\mathrm{mi}(G-x)=8$ or 9, i.e., $G-x \cong 2K_3,\ K_3 * K_3,\ K_4 \uplus K_2$, or $3K_2$. Thus, we get the extremal graphs I_7^4 and I_7^5.

If $n=8$, note that $|V_{G_2}|=3$, by Theorem 1.4, we have $\mathrm{mi}(G_2) \leqslant g(3)=3$. If $G-x \cong G(7)=K_4 \uplus K_3$, or $2K_2 \uplus K_3$, then $\mathrm{mi}(G-x)=12$. Thus, by Lemma 1.1(i), $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-x)+\mathrm{mi}(G_2) \leqslant 12+3=15$, the equality holds if and only if $G_2 \cong K_3$, i.e., $G \cong K_4 * K_4,\ K_5 \uplus K_3$ or $I_7^1 \uplus K_3$. If $G-x \ncong G(7)$, then by Theorem 1.5, we have $\mathrm{mi}(G-x) \leqslant h(7)=11$. Thus, by Lemma 1.1(i), $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-x)+\mathrm{mi}(G_2) \leqslant 11+3=14<15$, a contradiction.

Similarly, we can show, when $\Delta(G)=4$, $G \cong K_3 * 2K_3$ if $n=9$; whereas G does not exist if $n=10$, which is omitted here.

Now consider $\Delta(G) \geqslant 5$. In this case, $n \geqslant 6$ and $|V_{G_2}| \leqslant n-6$. At first we consider $n = 6,\ 7$ with $\Delta(G) = 5$. If $n = 6$, we get $6 = 7-1 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1) = 6$, i.e., $\mathrm{mi}(G-x) = 6$, i.e., $G-x \cong K_3 \uplus K_2$, which implies $G \cong I_6^4$. If $n = 7$, we get $\mathrm{mi}(G_2) = 1$ and $9 = 10-1 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1) = 9$, i.e., $\mathrm{mi}(G-x) = 9$, i.e., $G-x \cong 2K_3$, which implies $G \cong I_7^3$.

If $\Delta(G) = 6$, then we have $n = 7$. By Theorem 1.4, $9 = 10-1 \leqslant \mathrm{mi}(G-x) \leqslant g(n-1) = 9$, hence $\mathrm{mi}(G-x) = 9$, which implies $G-x \cong 2K_3$. Thus, we get extremal graph I_7^2.

Now we consider $n = |V_G| = 8,\ 9,\ 10$ for $\Delta(G) \geq 5$.

If $n = 8$, then by Lemma 1.1(i) and Theorem 1.4, we have $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-x) + \mathrm{mi}(G_2) \leqslant g(7) + g(2) = 14 < 15 = h(8)-1$, a contradiction. Similarly, we can also get a contradiction, respectively, for $n = 9, 10$, which is omitted here.

This completes the proof of Theorem 1.6(i).

Case 2. $n \geqslant 8$.

In this case, it is easy to see that $I(n) \ncong G(n), H(n)$ and $\mathrm{mi}(I(n)) = i(n)$ for $n \geqslant 8$. We prove it by induction on n. For $n = 8, 9, 10$, in view of (i), our result holds. In what follows, we consider $n \geqslant 11$ and assume our result holds for $n-1$. We proceed to show our result holds for n. We first show the following two claims.

Claim 1. *If G is a connected graph with $\delta(G) = 1$, then $\mathrm{mi}(G) < i(n)$.*

Proof. Note that $\delta(G) = 1$, hence we take a leaf, say x, of G. Let $y \in N_G(x)$, then $d(y) \geqslant 2$. Thus, by Lemma 1.1(ii) and Theorem 1.4, we have $\mathrm{mi}(G) = \mathrm{mi}(G-N[x]) + \mathrm{mi}(G-N[y]) \leqslant g(n-2) + g(n-3)$.

• $n = 3s$. In this case, $g(n-2) = 4 \cdot 3^{s-2}$, $g(n-3) = 3^{s-1}$. Then we have $\mathrm{mi}(G) \leqslant g(n-2) + g(n-3) = 4 \cdot 3^{s-2} + 3^{s-1} = 7 \cdot 3^{s-2} = \frac{7}{9} g(n) < \frac{22}{27} g(n) = i(n)$.

• $n = 3s+1$. In this case, $g(n-2) = 2 \cdot 3^{s-1}$, $g(n-3) = 4 \cdot 3^{s-2}$. Then we have $\mathrm{mi}(G) \leqslant g(n-2) + g(n-3) = 2 \cdot 3^{s-1} + 4 \cdot 3^{s-2} = 10 \cdot 3^{s-2} = \frac{5}{6} g(n) < \frac{8}{9} g(n) = i(n)$.

• $n = 3s+2$. In this case, $g(n-2) = 3^s$, $g(n-3) = 2 \cdot 3^{s-1}$. Then we have $\mathrm{mi}(G) = \mathrm{mi}(G-N[x]) + \mathrm{mi}(G-N[y]) \leqslant g(n-2) + g(n-3) = 3^s + 2 \cdot 3^{s-1} = 5 \cdot 3^{s-1} = \frac{5}{6} g(n) = i(n)$. Thus $\mathrm{mi}(G) = \frac{5}{6} g(n)$ if and only if $G - N[x] \cong G(n-2)$ and $G - N[y] \cong G(n-3)$, which implies $G \cong K_3 * K_2$ and $n = 5$. Obviously, this is a contradiction for $n \geqslant 11$. Therefore, $\mathrm{mi}(G) < \frac{5}{6} g(n)$ if $n \geqslant 11$.

This completes the proof of Claim 1. □

Claim 2. *If $G \cong C_n$ with $n \geqslant 8$, then $\mathrm{mi}(G) < i(n)$.*

Proof. For $n \geqslant 8$, we have

$$\mathrm{mi}(C_n) = \mathrm{mi}(C_{n-2}) + \mathrm{mi}(C_{n-3}) \leqslant \begin{cases} \frac{19}{27} g(n), & \text{if } n = 3s; \\ \frac{3}{4} g(n), & \text{if } n = 3s+1; \\ \frac{20}{27} g(n), & \text{if } n = 3s+2. \end{cases}$$

The last inequality follows from [4]. Hence, in view of the expression of $i(n)$ in (1.1) we have $\mathrm{mi}(C_n) < i(n)$. This completes the proof of Claim 2. □

Now we come back to the proof of Theorem 1.6(ii). It suffices to show the following three subcases.

Subcase 2.1. $n = 3s$.

Firstly, we consider that G is disconnected. Obviously, we can always find two vertex-disjoint graphs G_1 and G_2 such that $G = G_1 \uplus G_2$, where $|V_{G_1}| = n_1,\ |V_{G_2}| = n_2$. Without loss of generality, assume that $n_1 = 3s_1$ and $n_2 = 3s_2$, or $n_1 = 3s_1 + 1$ and $n_2 = 3s_2 + 2$.

For the subcase $n_1 = 3s_1$ and $n_2 = 3s_2$. If $G_1 \cong G(n_1)$, then $G_2 \ncong G(n_2),\ H(n_2)$ since $G \ncong G(n),\ H(n)$. Thus, we obtain

$$\begin{aligned} \mathrm{mi}(G) &= \mathrm{mi}(G_1) \cdot \mathrm{mi}(G_2) \qquad \text{(by Lemma 1.3)} \\ &\leqslant g(n_1) i(n_2) \qquad \text{(by Theorem 1.4 and induction hypothesis)} \qquad (2.1) \\ &= \frac{22}{27} \cdot 3^{s_1} \cdot 3^{s_2} \\ &= \frac{22}{27} g(n) = i(n). \end{aligned}$$

The equality in (2.1) holds if and only if $G_1 \cong G(n_1) = s_1K_3$ and $G_2 \cong I(n_2)$, which implies $G \cong I(n)$, as desired.

Similarly, if $G_2 \cong G(n_2)$, we can also get $G \cong I(n)$, as desired. So, we may assume that $G_1 \ncong G(n_1)$ and $G_2 \ncong G(n_2)$. Then, by Lemma 1.3 and Theorem 1.5, we have

$$\mathrm{mi}(G) = \mathrm{mi}(G_1)\cdot \mathrm{mi}(G_2) \leqslant h(n_1)h(n_2) = \frac{64}{81}\cdot 3^{s_1}\cdot 3^{s_2} = \frac{64}{81}g(n) < \frac{22}{27}g(n) = i(n).$$

Now we consider for case $n_1 = 3s_1+1$ and $n_2 = 3s_2+2$. If $s_1 = 0$, then $\mathrm{mi}(G) = \mathrm{mi}(G_2) \leqslant g(n_2) = \frac{2}{3}g(n) < \frac{22}{27}g(n) = i(n)$. So, we assume that $s_1 \geqslant 1$ in the following.

If $G_1 \cong G(n_1)$, then $G_2 \ncong G(n_2)$ since $G \ncong H(n)$. Thus, we obtain that

$$\mathrm{mi}(G) = \mathrm{mi}(G_1)\cdot \mathrm{mi}(G_2) \leqslant g(n_1)h(n_2) = \frac{8}{9}\cdot 4\cdot 3^{s_1-1}\cdot 2\cdot 3^{s_2} = \frac{64}{81}g(n) < \frac{22}{27}g(n) = i(n).$$

If $G_2 \cong G(n_2)$, then $G_1 \ncong G(n_1)$ since $G \ncong H(n)$. Thus, we have

$$\begin{aligned} \mathrm{mi}(G) &= \mathrm{mi}(G_1)\cdot \mathrm{mi}(G_2) && \text{(by Lemma 1.3)} \\ &\leqslant h(n_1)g(n_2) && \text{(by Theorems 1.4 and 1.5)} \\ &= \frac{11}{12}4\cdot 3^{s_1-1}\cdot 2\cdot 3^{s_2} \\ &= \frac{22}{27}g(n) = i(n). \end{aligned} \tag{2.2}$$

The equality in (2.2) holds if and only if $G_1 \cong H(n_1) = (K_3 * K_4) \uplus (s_1-1)K_3$ and $G_2 \cong G(n_2) = K_2 \uplus s_2K_3$, which implies that $G \cong (K_3*K_4)\uplus K_2 \uplus (s-3)K_3$, as desired.

If $G_1 \ncong G(n_1)$ and $G_2 \ncong G(n_2)$, then by Lemma 1.3 and Theorem 1.4, we get

$$\mathrm{mi}(G) = \mathrm{mi}(G_1)\cdot \mathrm{mi}(G_2) \leqslant h(n_1)h(n_2) = \frac{11}{12}g(n_1)\cdot\frac{8}{9}g(n_2) = \frac{22}{27}\cdot\frac{8}{9}g(n) < \frac{22}{27}g(n) = i(n).$$

Secondly, we consider that G is connected. From Claims 1 and 2, it suffices to consider the case that $\delta(G) \geqslant 2$ and $\Delta(G) \geqslant 3$. Choose a vertex $x \in V_G$ such that $d(x) = \Delta(G)$.

If $d(x) \geqslant 4$, then we get

$$\begin{aligned} \mathrm{mi}(G) &\leqslant \mathrm{mi}(G-x) + \mathrm{mi}(G-N[x]) && \text{(by Lemma 1.1(i))} \\ &\leqslant g(n-1)+g(n-5) && \text{(by Theorem 1.4)} \\ &= 2\cdot 3^{s-1} + 4\cdot 3^{s-3} \\ &= \frac{22}{27}g(n) = i(n). \end{aligned} \tag{2.3}$$

The equality in (2.3) holds if and only if $G-x \cong G(n-1) = K_2 \uplus (s-1)K_3$ and $G-N[x] \cong G(n-5) = K_4 \uplus (s-3)K_3$. But there is no such graph since $G-N[x]$ is a subgraph of $G-x$, hence $\mathrm{mi}(G) < i(n)$.

Now assume that $d(x) = 3$. If $G-x \cong G(n-1)$, then we have $G \cong (K_3*K_3)\uplus(s-2)K_3$, i.e., $G \cong H(n)$, a contradiction.

If $G-x \ncong G(n-1)$, then by Lemma 1.1 and Theorems 1.4 and 1.5, we get

$$\begin{aligned} \mathrm{mi}(G) &\leqslant \mathrm{mi}(G-x) + \mathrm{mi}(G-N[x]) && \text{(by Lemma 1.1(i))} \\ &\leqslant h(n-1)+g(n-4) && \text{(by Theorems 1.4 and 1.5)} \\ &= 16\cdot 3^{s-3} + 2\cdot 3^{s-2} \\ &= \frac{22}{27}g(n) = i(n). \end{aligned} \tag{2.4}$$

The equality in (2.4) holds if and only if $G-x \cong H(n-1) = (K_3*K_3)\uplus K_2 \uplus (s-3)K_3$, $4K_2 \uplus (s-3)K_3$, $K_4 \uplus 2K_2 \uplus (s-3)K_3$, or $2K_4 \uplus (s-3)K_3$ and $G-N[x] \cong G(n-4) = K_2 \uplus (s-2)K_3$. But there is no such graph since $\delta(G) \geqslant 2$ and $d(x) = 3$, hence $\mathrm{mi}(G) < i(n)$.

Subcase 2.2. $n = 3s+1$.

Firstly, we consider that G is disconnected. Obviously, we can always find two vertex-disjoint graphs G_1 and G_2 such that $G = G_1 \uplus G_2$, where $|V_{G_1}| = n_1,\ |V_{G_2}| = n_2$. Without loss of generality, assume that $n_1 = 3s_1$ and $n_2 = 3s_2 + 1$, or $n_1 = 3s_1 + 2$ and $n_2 = 3s_2 + 2$.

For the subcase $n_1 = 3s_1$ and $n_2 = 3s_2 + 1$. If $s_2 = 0$, then $\mathrm{mi}(G) = \mathrm{mi}(G_1) \leqslant g(n_1) = \frac{3}{4}g(n) < \frac{8}{9}g(n) = i(n)$. So, we assume that $s_2 \geqslant 1$ in the following.

If $G_1 \cong G(n_1)$, then $G_2 \ncong G(n_2),\ H(n_2)$ since $G \ncong G(n),\ H(n)$. Thus, we obtain that

$$\begin{aligned}
\mathrm{mi}(G) &= \mathrm{mi}(G_1)\cdot\mathrm{mi}(G_2) \qquad \text{(by Lemma 1.3)}\\
&\leqslant g(n_1)i(n_2) \qquad \text{(by Theorem 1.4 and induction hypothesis)}\\
&= \frac{8}{9}\cdot 3^{s_1}\cdot 4\cdot 3^{s_2-1}\\
&= \frac{8}{9}g(n) = i(n).
\end{aligned} \tag{2.5}$$

The equality in (2.5) holds if and only if $G_1 \cong G(n_1) = s_1K_3$ and $G_2 \cong I(n_2)$, this means $G \cong I(n)$.

If $G_2 \cong G(n_2)$, then $G_1 \ncong G(n_1)$ since $G \ncong H(n)$. Thus, we have

$$\begin{aligned}
\mathrm{mi}(G) &= \mathrm{mi}(G_1)\cdot\mathrm{mi}(G_2) \qquad \text{(by Lemma 1.3)}\\
&\leqslant h(n_1)g(n_2) \qquad \text{(by Theorems 2.1 and 2.2)}\\
&= \frac{8}{9}\cdot 3^{s_1}\cdot 4\cdot 3^{s_2-1}\\
&= \frac{8}{9}g(n) = i(n).
\end{aligned} \tag{2.6}$$

The equality in (2.7) holds if and only if $G_1 \cong H(n_1)$ and $G_2 \cong G(n_2)$, this means $G \cong I(n)$.

If $G_1 \ncong G(n_1)$ and $G_2 \ncong G(n_2)$, then by Lemma 1.3 and Theorem 1.4, we get

$$\mathrm{mi}(G) = \mathrm{mi}(G_1)\cdot\mathrm{mi}(G_2) \leqslant h(n_1)h(n_2) = \frac{8}{9}\cdot 3^{s_1}\cdot\frac{11}{12}\cdot 4\cdot 3^{s_2-1} = \frac{8}{9}\cdot\frac{11}{12}g(n) < \frac{8}{9}g(n) = i(n).$$

Now, we consider the subcase $n_1 = 3s_1 + 2$ and $n_2 = 3s_2 + 2$.

If $G_1 \cong G(n_1)$, then $G_2 \ncong G(n_2)$ since $G \ncong G(n)$. Thus, we have

$$\begin{aligned}
\mathrm{mi}(G) &= \mathrm{mi}(G_1)\cdot\mathrm{mi}(G_2) \qquad \text{(by Lemma 1.3)}\\
&\leqslant g(n_1)h(n_2) \qquad \text{(by Theorems 2.1 and 2.2)}\\
&= \frac{8}{9}\cdot 2\cdot 3^{s_1}\cdot 2\cdot 3^{s_2}\\
&= \frac{8}{9}g(n) = i(n).
\end{aligned} \tag{2.7}$$

The equality in (2.7) holds if and only if $G_1 \cong G(n_1) = K_2 \uplus s_1K_3$ and $G_2 \cong H(n_2)$, this means $G \cong K_4 \uplus 3K_2 \uplus (s-3)K_3$, $2K_4 \uplus K_2 \uplus (s-3)K_3$, $(K_3 * K_3) \uplus 2K_2 \uplus (s-3)K_3$, or $5K_2 \uplus (s-3)K_3$.

Similarly, if $G_2 \cong G(n_2)$, we can also get $G \cong K_4 \uplus 3K_2 \uplus (s-3)K_3$, $2K_4 \uplus K_2 \uplus (s-3)K_3$, $(K_3 * K_3) \uplus 2K_2 \uplus (s-3)K_3$, or $5K_2 \uplus (s-3)K_3$.

If $G_1 \ncong G(n_1)$ and $G_2 \ncong G(n_2)$. Then by Lemma 1.3 and Theorem 1.5, we get

$$\mathrm{mi}(G) = \mathrm{mi}(G_1)\cdot\mathrm{mi}(G_2) \leqslant h(n_1)h(n_2) = \frac{8}{9}\cdot 2\cdot 3^{s_1}\cdot\frac{8}{9}\cdot 2\cdot 3^{s_2} = \frac{64}{81}g(n) < \frac{8}{9}g(n) = i(n).$$

Next, we consider that G is connected. From Claims 1 and 2, we just need to consider the case that $\delta(G) \geqslant 2$ and $\Delta(G) \geqslant 3$. Choose a vertex $x \in V_G$ such that $d(x) = \Delta(G)$.

Suppose that $d(x) \geqslant 4$. For the case $G - x \cong G(n-1) = sK_3$, we get $G - N[x] \ncong G(n-5)$ since $G \ncong H(n)$. If $G - N[x] \cong H(n-5)$, we get $G - N[x] \cong 4K_2 \uplus (s-4)K_3$ since $G - N[x]$ is a subgraph of $G - x$. So, we can obtain that $n = 13,\ G \cong K_1 * 4K_3$. By direct computing, we have $\mathrm{mi}(G) = 81 < i(13) = 96$. Hence, assume that $G - N[x] \ncong H(n-5)$. By induction hypothesis, we get $\text{mi}(G-N[x]) \leqslant \max\{g(n-6),\ i(n-5)\} = \max\{4\cdot 3^{s-3},\ 5\cdot 3^{s-3}\} = 5\cdot 3^{s-3}$. Thus, we obtain

$$\begin{aligned}\text{mi}(G) &\leqslant \text{mi}(G-x)+\text{mi}(G-N[x]) && \text{(by Lemma 1.1(i))}\\ &\leqslant g(n-1)+5\cdot 3^{s-3} && \text{(by Theorem 1.4)}\\ &= 32\cdot 3^{s-3}\\ &= \frac{8}{9}g(n)=i(n).\end{aligned} \tag{2.8}$$

The equality in (2.8) holds if and only if $G-x \cong G(n-1) = sK_3$ and $G-N[x] \cong I(n-5)$. But there is no such graph since $G-N[x]$ is a subgraph of $G-x$. Hence $\text{mi}(G) < i(n)$.

For the case $G-x \ncong G(n-1)$, by Lemma 1.1(i) and Theorems 1.4 and 1.5, we get $\text{mi}(G) \leqslant \text{mi}(G-x)+\text{mi}(G-N[x]) \leqslant h(n-1)+g(n-5) = 8\cdot 3^{s-2}+2\cdot 3^{s-2} = \frac{5}{6}g(n) < \frac{8}{9}g(n) = i(n)$, which is impossible.

Now assume that $d(x) = 3$. If $G-x \cong G(n-1)$, since G is connected, G is of order at most 10, this is a contradiction. If $G-x \ncong G(n-1)$ and $G-N[x] \ncong G(n-4)$. Thus, we get

$$\begin{aligned}\text{mi}(G) &\leqslant \text{mi}(G-x)+\text{mi}(G-N[x]) && \text{(by Lemma 1.1(i))}\\ &\leqslant h(n-1)+h(n-4) && \text{(by Theorem 1.5)}\\ &= \frac{8}{9}\cdot 3^{s}+\frac{8}{9}3^{s-1}\\ &= \frac{8}{9}g(n)=i(n).\end{aligned} \tag{2.9}$$

The equality in (2.9) holds if and only if $G-x \cong H(n-1) = sK_3$ and $G-N[x] \cong H(n-4) = (s-1)K_3$, this means $G \cong K_4$, this is a contradiction. Hence $\text{mi}(G) < i(n)$.

Now, we just need to consider that for any vertex $v \in V_G$ such that $d(v) = 3$, we can assume that $G-v \ncong G(n-1)$ and $G-N[v] \cong G(n-4)$. Since G is connected, G is of order at most 7, this is a contradiction.

Subcase 2.3. $n = 3s+2$.

Firstly we consider that G is disconnected. Obviously, we can always find two vertex-disjoint graphs G_1 and G_2 such that $G = G_1 \uplus G_2$, where $|V_{G_1}| = n_1,\ |V_{G_2}| = n_2$. Without loss of generality, assume that $n_1 = 3s_1+1$ and $n_2 = 3s_2+1$, or $n_1 = 3s_1$ and $n_2 = 3s_2+2$.

For the subcase $n_1 = 3s_1+1$ and $n_2 = 3s_2+1$. If $s_1 = 0$, then by Lemma 1.3 and Theorem 1.4, we have $\text{mi}(G) = \text{mi}(G_2) \leqslant g(n_2) = g(n-1) = \frac{2}{3}g(n) < \frac{5}{6}g(n) = i(n)$. Hence, assume $s_1 \geqslant 1$ in what follows. Similarly, we assume that $s_2 \geqslant 1$.

If $G_1 \cong G(n_1)$, then we get $G_2 \ncong G(n_2)$ since $G \ncong H(n)$. By Lemma 1.3 and Theorems 1.4 and 1.5, we get $\text{mi}(G) = \text{mi}(G_1)\cdot\text{mi}(G_2) \leqslant g(n_1)h(n_2) = \frac{11}{12}\cdot 4\cdot 3^{s_1-1}\cdot 4\cdot 3^{s_2-1} = \frac{22}{27}g(n) < \frac{5}{6}g(n) = i(n)$.

If $G_1 \ncong G(n_1)$, then by Lemma 1.3 and Theorems 1.4 and 1.5, we get $\text{mi}(G) = \text{mi}(G_1)\cdot\text{mi}(G_2) \leqslant h(n_1)g(n_2) = \frac{11}{12}\cdot 4\cdot 3^{s_1-1}\cdot 4\cdot 3^{s_2-1} = \frac{22}{27}g(n) < \frac{5}{6}g(n) = i(n)$.

Now, consider the subcase $n_1 = 3s_1$ and $n_2 = 3s_2+2$. If $G_1 \cong G(n_1)$, then we get $G_2 \ncong G(n_2),\ H(n_2)$ since $G \ncong G(n),\ H(n)$. Thus, we obtain that

$$\begin{aligned}\text{mi}(G) &= \text{mi}(G_1)\cdot\text{mi}(G_2) && \text{(by Lemma 1.3)}\\ &\leqslant g(n_1)i(n_2) && \text{(by Theorems 1.4 and 1.5)}\\ &= \frac{5}{6}\cdot 3^{s_1}\cdot 2\cdot 3^{s_2}\\ &= \frac{5}{6}g(n)=i(n).\end{aligned} \tag{2.10}$$

The equality in (2.10) holds if and only if $G_1 \cong G(n_1) = s_1K_3$ and $G_2 \cong I(n_2)$, this means $G \cong I(n)$.

If $G_2 \cong G(n_2)$, then we get $G_1 \ncong G(n_1),\ H(n_1)$ since $G \ncong G(n),\ H(n)$. By Lemma 1.3, Theorem 1.4 and induction hypothesis, we get $\text{mi}(G) = \text{mi}(G_1)\cdot\text{mi}(G_2) \leqslant i(n_1)g(n_2) = \frac{22}{27}\cdot 3^{s_1}\cdot 2\cdot 3^{s_2} = \frac{22}{27}g(n) < \frac{5}{6}g(n) = i(n)$.

If $G_1 \ncong G(n_1)$ and $G_2 \ncong G(n_2)$, then by Lemma 1.3 and Theorem 1.5, we get $\text{mi}(G) = \text{mi}(G_1)\cdot\text{mi}(G_2) \leqslant h(n_1)h(n_2) = \frac{64}{81}\cdot 3^{s_1}\cdot 2\cdot 3^{s_2} = \frac{64}{81}g(n) < \frac{5}{6}g(n) = i(n)$.

Next, we consider that G is connected. From Claims 1 and 2, we just need to consider the case that $\delta(G) \geqslant 2$ and $\Delta(G) \geqslant 3$. Choose a vertex $x \in V_G$ such that $d(x) = \Delta(G)$.

If $d(x) \geqslant 4$, then we get

$$\begin{aligned} \mathrm{mi}(G) &\leqslant \mathrm{mi}(G-x)+\mathrm{mi}(G-N[x]) && \text{(by Lemma 1.1(i))} \\ &\leqslant g(n-1)+g(n-5) && \text{(by Theorem 1.4)} \\ &= 4\cdot 3^{s-1}+3^{s-1} \\ &= \frac{5}{6}g(n)=i(n). \end{aligned} \tag{2.11}$$

The equality in (2.11) holds if and only if $G-x \cong G(n-1) = K_4 \uplus (s-1)K_3$ and $G-N[x] \cong G(n-5) = (s-1)K_3$, which implies $G \cong K_5 \uplus (s-1)K_3$ or $(K_4 * K_4) \uplus (s-2)K_3$.

Now assume that $d(x) = 3$. If $G-x \cong G(n-1)$, then it is easy to see either $G-x \cong 2K_2 \uplus (s-1)K_3$ or $K_4 \uplus (s-1)K_3$. Since $\delta(G) \geqslant 2$ and $\Delta(G) = 3$, it follows that $G-x \ncong 2K_2 \uplus (s-1)K_3$. Since $\Delta(G) = 3$ and G is connected, it follows that $G-x \ncong K_4 \uplus (s-1)K_3$.

If $G-x \ncong G(n-1)$, since $\Delta(H(n-1)) = 4$, we get $G-x \ncong H(n-1)$. By induction hypothesis, we get $\mathrm{mi}(G-x) \leqslant i(n-1)$. Thus by Lemma 1.1(i) and Theorem 1.4, we get $\mathrm{mi}(G) \leqslant \mathrm{mi}(G-x)+\mathrm{mi}(G-N[x]) \leqslant i(n-1)+g(n-4) = \frac{8}{9}\cdot 4\cdot 3^{s-1}+4\cdot 3^{s-2} = \frac{22}{27}g(n) < \frac{5}{6}g(n) = i(n)$.

By Subcases 2.1-2.3, Theorem 1.6 (ii) holds. This completes the proof.

References

[1] H.B. Hua, Y.P. Hou, On graphs with the third largest number of maximal independent sets, Inform. Process. Lett. 109 (4) (2009) 248-253.

[2] H.B. Hua, Private communications.

[3] Z. Füredi, The number of maximal independent sets in connected graphs, J. Graph Theory, 11 (1987) 463-470.

[4] Z. Jin, X. Li, Graphs with the second largest number of maximal independent sets, Discrete Math. 308 (2008) 5864-5870.

[5] M.J. Jou, G. J. Chang, Maximal independent sets in graphs with at most one cycle, Discrete Appl. Math. 79 (1997) 67-73 .

[6] J.W. Moon, L. Moser, On Cliques in graphs, Israel J. Math. 3 (1965) 23-28.

[7] M.J. Jou, J. J. Lin, Trees with the second largest number of maximal independent sets, Discrete Math. 309 (2009) 4469-4474.