The minimum number of maximal independent sets in twin-free graphs

Stijn Cambie[a]   Stephan Wagner[b]

Abstract

The problem of determining the maximum number of maximal independent sets in certain graph classes dates back to a paper of Miller and Muller and a question of Erdős and Moser from the 1960s. The minimum was always considered to be less interesting due to simple examples such as stars. In this paper we show that the problem becomes interesting when restricted to twin-free graphs, where no two vertices have the same open neighbourhood. We consider the question for arbitrary graphs, bipartite graphs and trees. The minimum number of maximal independent sets turns out to be logarithmic in the number of vertices for arbitrary graphs, linear for bipartite graphs and exponential for trees. In the latter case, the minimum and the extremal graphs have been determined earlier by Taletskiĭ and Malyshev, but we present a shorter proof.

Mathematics Subject Classifications: 05C35, 05C69, 05C05

1   Introduction

1.1   History on the maximum number of maximal independent sets

Let $i_{\max}(G)$ denote the number of maximal independent sets of a graph G, i.e., the number of independent sets that are not contained in any larger independent set. Answering a question on the number of (maximal) cliques posed by Erdős and Moser, Moon and Moser [16], independently from Miller and Muller [15] (see also [21] for a short alternative proof) proved (by considering the complement) that for a graph G of order n, where $n \geqslant 2$,

$$
i_{\max}(G) \leqslant \begin{cases} 3^{\frac{n}{3}} & \text{if } n \equiv 0 \pmod{3}, \\ 4 \cdot 3^{\frac{n-4}{3}} & \text{if } n \equiv 1 \pmod{3}, \\ 2 \cdot 3^{\frac{n-2}{3}} & \text{if } n \equiv 2 \pmod{3}. \end{cases}
$$

[a]Department of Computer Science, KU Leuven Campus Kulak, Kortrijk, Belgium (`stijn.cambie@hotmail.com`).
[b]Institute of Discrete Mathematics, TU Graz, Graz, Austria (`stephan.wagner@tugraz.at`).
Department of Mathematics, Uppsala University, Uppsala, Sweden (`stephan.wagner@math.uu.se`).

The extremal graphs are disjoint unions of (at most two) K_2s and many K_3s. In the original setting (for the number of maximal cliques), the extremal graph is a balanced $\lceil \frac{n}{3} \rceil$−partite graph. Wilf [20] proved that among all trees of order n the spiders (presented in Figure 1) maximize the number of maximal independent sets. For a tree T with n vertices,

$$i_{\max}(T) \leqslant \begin{cases} 2^{\frac{n}{2}-1} + 1 & \text{if } n \equiv 0 \pmod{2}, \\ 2^{\frac{n-1}{2}} & \text{if } n \equiv 1 \pmod{2}. \end{cases}$$

(a) An odd spider   (b) An even spider

Figure 1: Two spiders.

By induction, one can verify with Wilf's idea that the extremal tree is unique when n is odd, but this is not the case when n is even. Sagan [18] provided an alternative proof for Wilf's result and also characterized the extremal trees of even order as batons of length 1 or 3. Here batons are subdivisions of trees of diameter at most 3 in which the pendent edges are subdivided once and the central edge (or one edge of a star) is not subdivided or subdivided twice. Examples of such batons are presented in Figure 2. From this one can also conclude that there are precisely $\frac{n}{2} - 1$ extremal trees if $n \geqslant 4$ is even.

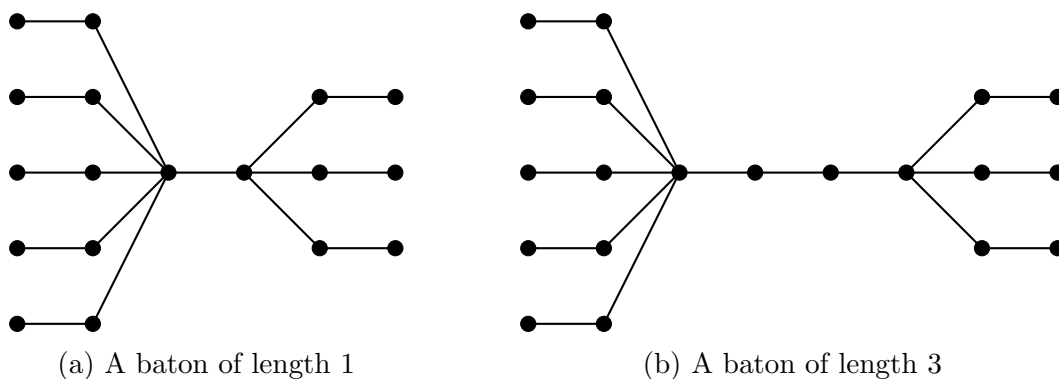(a) A baton of length 1   (b) A baton of length 3

Figure 2: Batons of length 1 and 3.

Wilf also asked about the maximum of $i_{\max}(G)$ when considering arbitrary connected graphs of given order. This question was answered independently by Füredi [6] (for

large n) and Griggs et al. [7]. They proved that for a connected graph G,

$$i_{\max}(G) \leqslant \begin{cases} 2 \cdot 3^{\frac{n}{3}-1} + 2^{\frac{n}{3}-1} & \text{if } n \equiv 0 \pmod 3, \\ 3^{\frac{n-1}{3}} + 2^{\frac{n-4}{3}} & \text{if } n \equiv 1 \pmod 3, \\ 4 \cdot 3^{\frac{n-5}{3}} + 3 \cdot 2^{\frac{n-8}{3}} & \text{if } n \equiv 2 \pmod 3. \end{cases}$$

For $n \geqslant 6$, the extremal graph is unique: if $n \equiv k \pmod 3$, where $k \in \{0, 1, 2\}$, the graph is obtained from a union of k complete graphs K_4 and $\frac{n-4k}{3} = \lfloor \frac{n}{3} \rfloor - k$ complete graphs K_3 by choosing one vertex from each of these complete graphs and connecting them to form a star of order $\lfloor \frac{n}{3} \rfloor$. The centre of this star has to belong to a K_4, if there is (at least) one. This is presented in Figure 3 in the case $n \equiv 2 \pmod 3$.
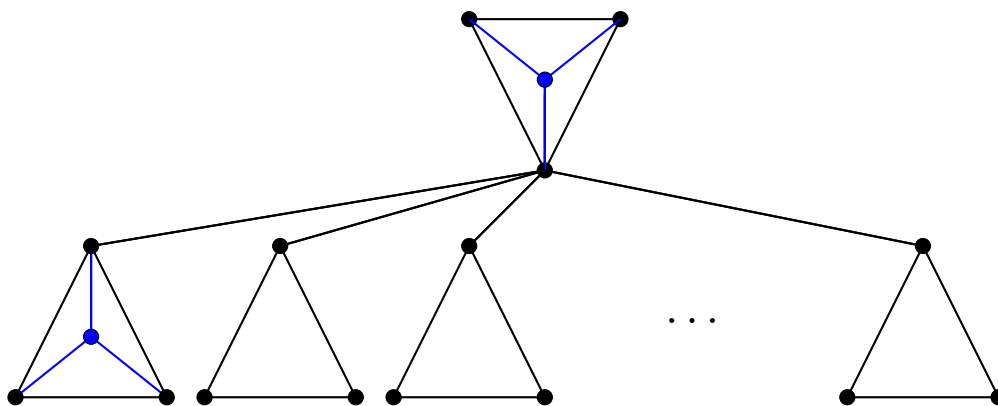

Figure 3: Connected graph with maximum value of $i_{\max}$.

1.2 The minimum number of maximal independent sets

Whenever a graph contains at least one edge, we must clearly have $i_{\max}(G) \geqslant 2$ (construct maximal independent sets greedily starting from each of the ends of one edge), and this bound is in fact attained by a star. As such, one can conclude that for trees or arbitrary connected graphs of order n, the best lower bound one can aim for is $i_{\max}(G) \geqslant 2$.

If two leaves v, v' of a tree have the same neighbour (we call such leaves *twins*), then v belongs to a maximal independent set if and only if v' does, so we can consider them as essentially being one vertex. Generally, if two vertices v and v' of a graph have the same open neighbourhood, i.e., $N(v) = N(v')$, then every maximal independent set either contains both or neither.

So by duplicating vertices (adding new vertices with the same open neighbourhood as existing vertices), we can construct infinitely many graphs with the same number of maximal independent sets. This is also the reason why the question for the minimum number of maximal independent sets appears to be less interesting than its counterpart for the maximum. As we will see, it becomes more interesting if we forbid duplicated vertices:

Definition 1. A graph is called *twin-free* if it has no two vertices with the same neighbours.

Twin-free graphs have been studied in the past, e.g. in [4] in connection with identifying codes. Note that every graph can be reduced to a twin-free graph (its "twin-free core") by removal of duplicates without affecting the number of maximal independent sets. We therefore study the problem of determining the minimum of $i_{\max}(G)$ for a twin-free graph G of given order n in different graph classes: specifically, arbitrary graphs, bipartite graphs, and trees.

We will see that for these three graph classes, the minimum of $i_{\max}(G)$ is logarithmic, linear and exponential in terms of the order n, respectively.

Our first main result determines the minimum of $i_{\max}(G)$ for arbitrary connected twin-free graphs of given order (in fact, it suffices to assume that there are no isolated vertices), and characterizes the extremal graph uniquely. We first prove that the extremal graph contains a clique of order $i_{\max}(G)$, and that the neighbourhoods satisfy certain conditions. Using a result from extremal set theory, we can then conclude with the following theorem. This is presented in Section 2.

Theorem 2. *Let $k \geqslant 2$ be an integer. If G is a twin-free graph of order n without isolated vertices and $i_{max}(G) = k$, then $n \leqslant 2^{k-1} + k - 2$. Furthermore, equality holds only if the graph G is formed by taking a clique K_{k-1} and adding, for every non-empty vertex subset S of this clique, a vertex whose neighbourhood is precisely S.*

The precise result for bipartite graphs is stated in the next theorem. In the proof in Section 3, we associate a unique maximal independent set to every vertex v in one partition class, which together with the other partition class gives the lower bound on the number of maximal independent sets.

Theorem 3. *Let G be a twin-free bipartite graph of order $n \geqslant 2$ without isolated vertices. Then $i_{max}(G) \geqslant \lceil \frac{n}{2} \rceil + 1$, and this inequality is sharp.*

The last result determines the minimum number of maximal independent sets in twin-free trees. This was previously proven by Taletskiĭ and Malyshev in [19]. We give a shorter proof in Section 4, which starts by deriving the bounds, in contrast to [19] where the extremal graphs are characterized first by excluding certain structures in the extremal graphs. We use an inductive approach, based on a lemma of Wilf [20].

Theorem 4. *Let $n \geqslant 4$ be an integer. Then for every twin-free tree T with n vertices, we have*

$$i_{max}(T) \geqslant \begin{cases} 4 \cdot 3^{\frac{n}{5}-1} & \text{if } n \equiv 0 \pmod 5, \\ 5 \cdot 3^{\frac{n-6}{5}} & \text{if } n \equiv 1 \pmod 5, \\ 2 \cdot 3^{\frac{n-2}{5}} & \text{if } n \equiv 2 \pmod 5, \\ 8 \cdot 3^{\frac{n-8}{5}} & \text{if } n \equiv 3 \pmod 5, \\ 3^{\frac{n+1}{5}} & \text{if } n \equiv 4 \pmod 5, \end{cases}$$

and this inequality is sharp.

For every n, Figure 4 depicts one example of a tree for which equality holds in Theorem 4. Here, the blue and red edges possibly have to be added depending on $n \pmod 5$. For large n, there are multiple extremal trees. In Subsection 4.1 we briefly make some comments on the characterization, which also already appears in [19].

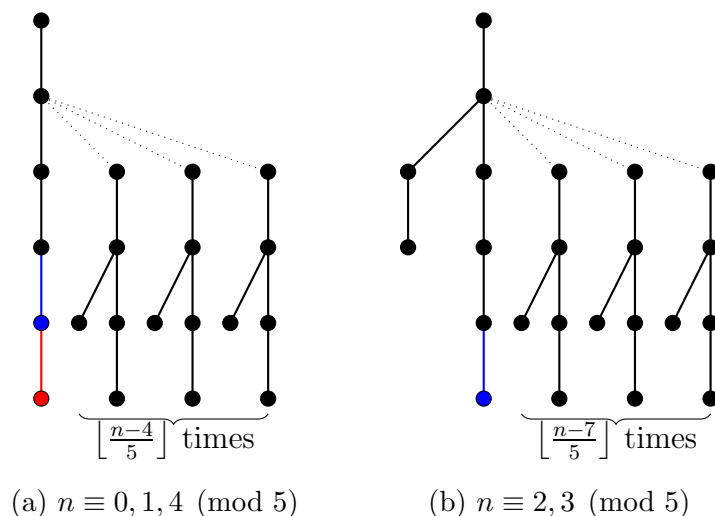(a) $n \equiv 0, 1, 4 \pmod 5$ (b) $n \equiv 2, 3 \pmod 5$

Figure 4: Constructions that attain equality in Theorem 4.

Finally, in Section 5, we conclude with some further directions related to the minimum of $i_{\max}(G)$ for twin-free graphs in other classes and some other related questions.

2 Twin-free graphs

We start with the proof that the minimum of the number of maximal independent sets in a connected twin-free graph is logarithmic in the order. We first provide the extremal construction and give a short argument for the lower bound $i_{\max}(G) > \log_2(n)$. The more precise Theorem 2 is proven afterwards in Subsection 2.1.

Proposition 5. *There exists a connected twin-free graph with $n = 2^{k-1} + k - 2$ vertices for which $i_{max}(G) = k$.*

Proof. Let K_{k-1} be a clique on $k - 1$ vertices. For every non-empty vertex subset S of this clique, we add a new vertex whose neighbours are exactly the vertices in S. Then the graph G obtained by this process has $k - 1 + (2^{k-1} - 1)$ vertices, and all neighbourhoods are different, i.e., G is twin-free. Every independent set contains at most one vertex of the clique K_{k-1}. We note that a maximal independent set I is uniquely determined by $I \cap V(K_{k-1})$, since $V(G) \setminus V(K_{k-1})$ is an independent set. If $I \cap V(K_{k-1}) = \emptyset$, then $V(G) \setminus V(K_{k-1})$ becomes a maximal independent set on its own. If $I \cap V(K_{k-1}) = \{v\}$, then $I = V(G) \setminus N(v)$. As such, we conclude that $i_{\max}(G) = k$. $\square$

On the other hand, we can prove a lower bound that is based on the following observation.
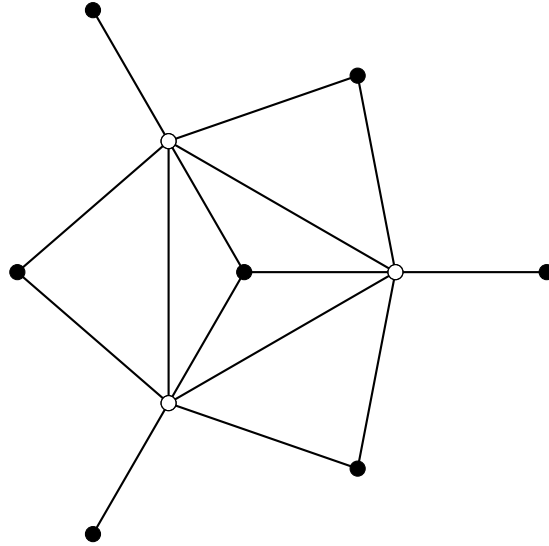
Figure 5: The construction in Proposition 5 for $k = 4$. The clique K_3 is indicated in white.

Lemma 6. *Two vertices u and v belong to the same maximal independent sets of a graph G if and only if they are twins.*

Proof. If u and v belong to the same maximal independent sets, then they cannot be neighbours, and they must have exactly the same neighbours: if for instance there is a vertex w adjacent to u, but not to v, then there must be a maximal independent set containing $\{v, w\}$, but not u. Hence u and v have to be twins. The converse is immediate. $\square$

The following proposition already shows that the minimum of $i_{\max}$ is of logarithmic order.

Proposition 7. *For every connected twin-free graph G with n vertices, $i_{max}(G) > \log_2(n)$.*

Proof. Let $k = i_{\max}(G)$, and let the maximal independent sets of G be $I_1, \ldots, I_k$. For every vertex v, consider the associated vector $\vec{v} = (1_{v \in I_1}, 1_{v \in I_2}, \ldots, 1_{v \in I_k})$. Since every vertex belongs to at least one maximal independent set, no vertex gets assigned the zero vector. Moreover, Lemma 6 shows that no two vertices have the same associated vector, as G is assumed to be twin-free. Since there are only $2^k - 1$ distinct non-zero vectors, we conclude that $n \leqslant 2^k - 1$, i.e., $k > \log_2(n)$. $\square$

This argument is further refined in the following subsection.

2.1 Proof of Theorem 2

Let us now prove Theorem 2, whose statement we first recall.

Theorem 2. *Let $k \geqslant 2$ be an integer. If G is a twin-free graph of order n without isolated vertices and $i_{max}(G) = k$, then $n \leqslant 2^{k-1} + k - 2$. Furthermore, equality holds only if the graph G is formed by taking a clique K_{k-1} and adding, for every non-empty vertex subset S of this clique, a vertex whose neighbourhood is precisely S.*

For $k = 2$, the statement holds by Proposition 7 and the fact that $i_{max}(K_3) = 3 > 2$. Suppose for contradiction that Theorem 2 does not hold, and let $k \geqslant 3$ be the minimum value for which this is the case. Let G be a graph of maximum order for which $i_{max}(G) = k$, and let $I_1, \ldots, I_k$ be its maximal independent sets. As in the proof of Proposition 7, we can conclude that every vertex of G belongs to at least one of these sets.

Lemma 8. *Every maximal independent set I_i has a vertex u_i that belongs to no maximal independent set I_j with $j \neq i$.*

Proof. If this is not the case, add a vertex u_i to the graph that is adjacent to all vertices except those in I_i. Then I_i is extended by this new vertex, but all other maximal independent sets remain the same. Note that the new vertex does not belong to any maximal independent sets other than the extension of I_i. By Lemma 6, the new graph G' is still twin-free, and $i_{max}(G') = i_{max}(G)$, contradicting the choice of G. □

Lemma 9. *In every graph H, we have $i_{max}(H) \geqslant \chi(H) \geqslant \omega(H)$.*

Proof. It is sufficient to observe that every colour class of an optimal proper colouring is an independent set, but the union of two colour classes is not. Since every independent set can be (e.g. greedily) extended to at least one maximal independent set, $i_{max}(H) \geqslant \chi(H)$ is immediate. The inequality $\chi(H) \geqslant \omega(H)$ is well known. □

In the graph G that we took as counterexample to Theorem 2, any two vertices u_i and u_j as defined in Lemma 8 with $i \neq j$ have to be adjacent. Otherwise, $\{u_i, u_j\}$ could be extended to a maximal independent set, contradicting the choice of u_i and u_j. So $U = \{u_1, \ldots, u_k\}$ spans a complete graph, implying that $\omega(G) \geqslant k = i_{max}(G)$, which means that we have equality in Lemma 9 when applied to G.

Lemma 10. *A vertex v belongs to I_j if and only if it is not adjacent to u_j.*

Proof. If v belongs to I_j, then it can clearly not be adjacent to u_j (which also belongs to I_j). Conversely, if v, u_j are not adjacent, then $\{v, u_j\}$ can be extended to a maximal independent set, which must necessarily be I_j (by Lemma 8). □

Remembering that the vectors $\vec{v}$ as defined in the proof of Proposition 7 are all distinct and neither equal to the all-0 vector (as every vertex belongs to a maximal independent set) nor the all-1 vector (the corresponding vertex would be isolated), we know that every vertex has at least one neighbour in the clique induced by U, and no two vertices $v, v' \notin U$ satisfy $N(v) \cap U = N(v') \cap U$.

Lemma 11. *Two vertices v, v' are adjacent if and only if $U \subseteq N(v) \cup N(v')$.*

Proof. If v, v' are adjacent and $u \in U$ does not belong to $N(v) \cup N(v')$, then $\{u, v\}$ and $\{u, v'\}$ can be extended to distinct maximal independent sets containing u. This contradicts the construction of U (Lemma 8), so $U \subseteq N(v) \cup N(v')$ in this case. Conversely, if v, v' are not adjacent, then the set $\{v, v'\}$ can be extended to a maximal independent set, which must contain a vertex of U by construction. As this vertex is not in $N(v) \cup N(v')$, U is not fully contained in $N(v) \cup N(v')$ in this case. $\square$

If the union of the neighbourhoods of the vertices in an independent set in $V(G) \setminus U$ contains all of U, it can be extended to a maximal independent set without any vertices in U, leading to a contradiction again. Equivalently, if the union of the neighbourhoods of some vertices in $V(G) \setminus U$ contains all of U, then it cannot be an independent set, so it must contain two adjacent vertices whose neighbourhoods cover U by Lemma 11. This observation naturally leads us to the following concept.

Definition 12. We say that a family $\mathcal{F} \subseteq 2^{[n]}$ is *union-efficient* if for every subfamily $\{A_1, \ldots, A_m\}$ of $\mathcal{F}$ for which $\cup_{i \in [m]} A_i = [n]$, there are two indices $i, j \in [m]$ for which $A_i \cup A_j = [n]$.

For every vertex $v_i \in V(G) \setminus U$, we consider the index set $A_i = \{j \mid u_j \in N(v_i), 1 \leqslant j \leqslant k\}$. As explained before, the family $\mathcal{F} \subseteq 2^{[k]}$ consisting of all these A_i is union-efficient.
Note that $\mathcal{F}$ does not include $\emptyset, [k]$ (as observed before), nor $[k] \setminus j$ for any $j \in [k]$. The latter holds because $A_i = [k] \setminus j$ would mean that v_i is adjacent to (a) all vertices in U except u_j, and (b) precisely those vertices in $V(G) \setminus U$ that are adjacent to u_j (by Lemma 11). But then v_i and u_j would be twins, a contradiction. It is easy to see that $\mathcal{F}$ stays union-efficient if we add these $k + 2$ sets to $\mathcal{F}$.
Formulated in the terminology of union-efficient families (the equivalence is explained in [2]), the following theorem is a result by Milner (see [5]), with the uniqueness result proven by Bollobás and Duchet [1], and by Mulder [17].

Theorem 13. *Let* $n \geqslant 3$, *and let* $\mathcal{E} \subseteq 2^{[n]}$ *be a union-efficient family. Then* $|\mathcal{E}| \leqslant 2^{n-1} + n$. *Equality is attained if and only if (up to isomorphism)* $\mathcal{E} = 2^{[n-1]} \cup \binom{[n]}{\geqslant n-1}$ *(i.e., $\mathcal{E}$ contains all subsets of $[n-1]$ and all subsets of $[n]$ with at least $n-1$ elements).*

Theorem 13 implies that $|\mathcal{F}| \leqslant 2^{k-1} - 2$, thus

$$|V(G)| = |U| + |V(G) \setminus U| \leqslant k + 2^{k-1} - 2,$$

and equality holds if and only if (up to renaming) $\mathcal{F} = 2^{[k-1]} \setminus \{[k-1], \emptyset\}$. In this case, G consists of the clique induced by $u_1, \ldots, u_{k-1}$ and the $2^{k-1} - 1$ vertices in $V(G) \setminus \{u_1, \ldots, u_{k-1}\}$ whose neighbourhoods are precisely all the different nonempty subsets of $\{u_1, \ldots, u_{k-1}\}$ (u_k is the unique vertex adjacent to all of them). This is precisely the characterization of the extremal graph described in Theorem 2, completing our proof. $\square$

Note that a twin-free graph has at most one isolated vertex, and that adding an isolated vertex does not change the number of maximal independent sets. Thus, if we drop the condition that there are no isolated vertices, we obtain the following version of Theorem 2.

Corollary 14. *Let $k \geqslant 2$ be an integer. If G is a twin-free graph of order n and $i_{max}(G) = k$, then $n \leqslant 2^{k-1} + k - 1$. Furthermore, equality holds only if the graph G is formed by taking a clique K_{k-1} and adding, for every vertex subset S of this clique, a vertex whose neighbourhood is precisely S.*

3 Twin-free bipartite graphs

In this section, we show that the minimum value of $i_{\max}(G)$ for twin-free bipartite graphs is linear in the order. We start by proving Theorem 3, which we recall for convenience.

Theorem 3. *Let G be a twin-free bipartite graph of order $n \geqslant 2$ without isolated vertices. Then $i_{max}(G) \geqslant \left\lceil \frac{n}{2} \right\rceil + 1$, and this inequality is sharp.*

Proof. For the lower bound, we prove a stronger statement: if G is a twin-free bipartite graph without isolated vertices whose bipartition classes A, B have sizes $a \leqslant b$ ($b \leqslant 2^a - 1$ is necessary for existence), then $i_{\max}(G) \geqslant b + 1$.

For every vertex $v \in B$, consider the set $I_v = (A \setminus N(v)) \cup \{u \in B \mid N(u) \subseteq N(v)\}$. This is a maximal independent set by construction. Since for every two vertices $u, v \in B$ their neighbourhoods $N(u)$ and $N(v)$ are different, we have $I_u \neq I_v$ if $u \neq v$. Finally, A is also a maximal independent set (since G has no isolated vertices) that does not coincide with any of the I_v. Thus G has at least $b + 1$ maximal independent sets. Since $b \geqslant \left\lceil \frac{n}{2} \right\rceil$, the lower bound is clear.

Equality is attained by K_2 and for example by taking a balanced complete bipartite graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ and removing a matching M of size $\left\lceil \frac{n}{2} \right\rceil - 1$ when $n \geqslant 4$ (note that no bipartite twin-free connected graph of order 3 exists). The graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil} \setminus M$ is clearly bipartite, connected and twin-free (note that a bipartite graph is twin-free if and only if its bipartite complement is, provided that neither of the two has two isolated vertices). It has two types of maximal independent sets: each of the bipartition classes is a maximal independent set, and for each of the $\left\lceil \frac{n}{2} \right\rceil - 1$ edges in M, the ends form a maximal independent set of cardinality 2. There are no others: once two vertices from the same bipartition class are contained in an independent set I, no vertices from the other class can be included. By maximality, I must be one of the bipartition classes in this case. If an independent set I contains vertices from both classes, then they have to be the ends of an edge in M, as they would otherwise be adjacent. Hence $i_{\max}\left(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil} \setminus M\right) = \left\lceil \frac{n}{2} \right\rceil + 1$. $\qquad\square$

The same bound seems to hold more generally for triangle-free graphs, but we do not have a proof at this point.

Conjecture 15. Let G be a twin-free and triangle-free graph of order n without isolated vertices. Then $i_{\max}(G) \geqslant \left\lceil \frac{n}{2} \right\rceil + 1$. Furthermore, if n is even, graphs that attain equality are bipartite.

If we drop the condition that there are no isolated vertices, the minimum only changes by at most 1 by the same reasoning that gave us Corollary 14: a twin-free graph has at

most one isolated vertex, and adding an isolated vertex does not change the number of maximal independent sets. The same is true for triangle-free graphs under Conjecture 15.

Corollary 16. *For every twin-free bipartite graph G of order n, we have $i_{max}(G) \geqslant \left\lceil \frac{n-1}{2} \right\rceil + 1 = \left\lfloor \frac{n}{2} \right\rfloor + 1$, and this inequality is sharp.*

The graphs in the proof that were constructed to show that the inequality is sharp are not unique—there are many more extremal graphs, see Table 1.

n	$\min i_{\max}(G)$	# extremal bip. graphs	# extremal K_3-free graphs
4	3	1	1
5	4	1	1
6	4	2	2
7	5	4	5
8	5	4	4
9	6	16	18
10	6	11	11
11	7	73	79
12	7	33	33

Table 1: The number of connected twin-free bipartite/triangle-free graphs for which the minimum in Theorem 3 is attained.

Let us also present a bijection with certain binary matrices.

Proposition 17. *The connected twin-free bipartite graphs of order $2k$ for which $i_{max}(G) = k+1$ are in one-to-one correspondence with $k \times k$-binary matrices satisfying the following conditions:*

- *there is an all-1 row and an all-1 column,*

- *all columns are distinct, and all rows are distinct,*

- *the union (bitwise maximum) of any two rows is a row of the matrix itself.*

Proof. In the proof of Theorem 3, it was shown that $i_{\max}(G) \geqslant \max\{|A|, |B|\} + 1$, where $V(G) = A \cup B$ is the bipartition of G. Hence the equality $i_{\max}(G) = k+1$ can only occur among balanced bipartite graphs, i.e., when $|A| = |B|$. The bipartite graph can now be presented by its reduced adjacency matrix $\mathcal{M}$, which is a $k \times k$-matrix. From the proof, we also conclude that there is a vertex $v \in B$ for which $I_v = B$ and thus $N(v) = A$. Similarly, there is a vertex $w \in A$ with $N(w) = B$. Thus $\mathcal{M}$ has a row and a column containing only 1s. The graph G being twin-free is equivalent to $\mathcal{M}$ having distinct rows and distinct columns.

If there is a bipartition class, say B, of G for which the union of the neighbourhoods of some of its vertices, $B_1 \subseteq B$ ($B_1 \neq \emptyset$), is not equal to the neighbourhood of a vertex in B, then $A \setminus N(B_1) \cup \{u \in B \mid N(u) \subseteq N(B_1)\}$ would be another maximal independent

set not counted in the proof of Theorem 3. So for every $B_1 \subseteq B$, there is a $b \in B$ with $N(B_1) = N(b)$. The latter is the case if and only if this is true for every subset B_1 of size 2, which is equivalent with the union of any 2 rows being a row itself.

In the reverse direction, assuming $\mathcal{M}$ does satisfy the conditions, we know that it is the adjacency matrix of a connected twin-free bipartite graph G. Assume a maximal independent set of G different from A consists of precisely the vertices in $A_1 \subseteq A$ and $B_1 \subseteq B$. Due to the third condition, there is a vertex b for which $N(B_1) = N(b)$. Then B_1 has to be precisely equal to $\{u \in B \mid N(u) \subseteq N(b)\}$, and $A_1 = A \backslash N(b)$ since $A_1 \cup B_1$ is a maximal independent set. Therefore the maximal independent sets are exactly those of the form $\{I_b \mid b \in B\} \cup \{A\}$, and we have $i_{\max}(G) = k + 1$. We conclude that we really have a bijection. $\square$

Remark 18. This also gives a combinatorial proof that among square binary matrices $\mathcal{M}$ with all columns resp. rows distinct and containing an all-1 row and an all-1 column, the condition that the union of any set of columns of $\mathcal{M}$ is a column of $\mathcal{M}$ is equivalent with the condition that the union of any set of rows of $\mathcal{M}$ is a row of $\mathcal{M}$.

From this characterization, it can be derived that there are at least exponentially many bipartite graphs G of order $2k$ for which $i_{\max}(G) = k + 1$. For example, $2^{\lfloor \frac{k}{3} \rfloor}$ different matrices satisfying the constraints in Proposition 17 can be obtained by taking a $k \times k$ binary lower-triangular matrix $\mathcal{M}$ all of whose lower-triangular elements are 1 and then additionally setting some entries $\mathcal{M}_{3i+1,3i+3}$ equal to 1 for some $0 \leqslant i < \lfloor \frac{k}{3} \rfloor$. For $k = 6$, this gives four possibile matrices of this form (a red entry can be either 0 or 1)

$$
\mathcal{M} = \begin{pmatrix}
1 & 0 & 0/1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 0 & 0/1 \\
1 & 1 & 1 & 1 & 1 & 0 \\
1 & 1 & 1 & 1 & 1 & 1
\end{pmatrix}.
$$

4 Twin-free trees

In this section, we consider the problem for trees. Let us start again by recalling the theorem we want to prove. We first define a function f by $f(1) = 1, f(2) = f(3) = 2$, and for $n \geqslant 4$

$$
f(n) = \begin{cases}
4 \cdot 3^{\frac{n}{5} - 1} & \text{if } n \equiv 0 \pmod 5, \\
5 \cdot 3^{\frac{n-6}{5}} & \text{if } n \equiv 1 \pmod 5, \\
2 \cdot 3^{\frac{n-2}{5}} & \text{if } n \equiv 2 \pmod 5, \\
8 \cdot 3^{\frac{n-8}{5}} & \text{if } n \equiv 3 \pmod 5, \\
3^{\frac{n+1}{5}} & \text{if } n \equiv 4 \pmod 5.
\end{cases}
$$

The main theorem of this section can thus be stated as follows.

Theorem 4. *Let $n \geqslant 4$ be an integer. Then for every twin-free tree T with n vertices, we have $i_{max}(T) \geqslant f(n)$, and this inequality is sharp.*

Note that the inequality $i_{\max}(T) \geqslant f(n)$ is also true for $n \in \{1, 2, 3\}$, although the statement is void for $n = 3$ as there are no twin-free trees with 3 vertices (however, $i_{\max}(P_3) = 2$).

For $n \leqslant 8$, the values can be verified by determining $i_{\max}(T)$ for all trees of order n (these are the base cases of our induction proof). So from now on, we consider $n \geqslant 9$ and assume that the statement has been proven for every smaller order.

In the proof of Theorem 4, we will use the following estimates.

Lemma 19. *The following statements hold:*

(a) *except for the pair $(n, m) = (3, 3)$, we have $f(n) \cdot f(m) \geqslant f(n+m)$ for all $n, m \geqslant 2$, and*

(b) *$f(n - 1) \cdot f(m - 1) \geqslant f(n + m - 1)$ for all $n, m \geqslant 5$.*

Proof. Note that for $n \geqslant 5$, the function $g(n) = f(n-1)3^{-\frac{n}{5}} \geqslant 1$ only depends on the residue class modulo 5, namely

$$g(n) = \begin{cases} 1 & \text{if } n \equiv 0 \pmod 5, \\ 4 \cdot 3^{-\frac{6}{5}} & \text{if } n \equiv 1 \pmod 5, \\ 5 \cdot 3^{-\frac{7}{5}} & \text{if } n \equiv 2 \pmod 5, \\ 2 \cdot 3^{-\frac{3}{5}} & \text{if } n \equiv 3 \pmod 5, \\ 8 \cdot 3^{-\frac{9}{5}} & \text{if } n \equiv 4 \pmod 5. \end{cases}$$

A direct verification shows that

$$\frac{g(i)g(j)}{g(i+j)} \in \left\{ 1, \frac{25}{24}, \frac{16}{15}, \frac{10}{9}, \frac{32}{27} \right\},$$

thus in particular $g(i)g(j) \geqslant g(i + j)$ in all cases. So it follows that

$$f(n - 1)f(m - 1) = 3^{(n+m)/5}g(n)g(m) \geqslant 3^{(n+m)/5}g(n + m) = f(n + m - 1)$$

for all $n, m \geqslant 5$. Thus statement (b) holds. Since $f(n)$ is increasing for $n \geqslant 4$, we have

$$f(n)f(m) \geqslant f(n + m + 1) > f(n + m)$$

for all $n, m \geqslant 4$. Thus we only need to verify (a) in those cases where either n or m (without loss of generality n) is equal to 2 or 3. If both n and m are equal to 2 or 3, then the inequality holds unless $n = m = 3$, as $f(6) = 5 > f(2)^2 = f(2)f(3) = f(3)^2 = 4 = f(5) > f(4) = 3$.

Moreover, since $f(2) = f(3) = 2$, it actually suffices to consider $n = 3$ (again because f is an increasing function: $f(3)f(m) \geqslant f(m+3)$ implies $f(2)f(m) = f(3)f(m) \geqslant f(m+2)$).

The inequality $f(3)f(m) = 2f(m) \geqslant f(m+3)$ is easily verified for $m \geqslant 4$ by checking all five possible cases modulo 5 and finding that

$$\frac{f(3)f(m)}{f(3+m)} \in \left\{1, \frac{16}{15}, \frac{10}{9}\right\}.$$

$\square$

Next, we explain the inductive idea used by Wilf [20]. Let x be a leaf of T and y its neighbour. Let $u_1, u_2, \ldots, u_r$ be the neighbours of y different from x. Let U_i be the component (subtree) of $T \setminus \{x, y\}$ that contains u_i, and let $W_{i,j}$, $1 \leqslant j \leqslant s_i$, be the components of $U_i \setminus u_i$. Finally, let $w_{i,j}$ be the neighbour of u_i belonging to $W_{i,j}$. This is illustrated in Figure 6.
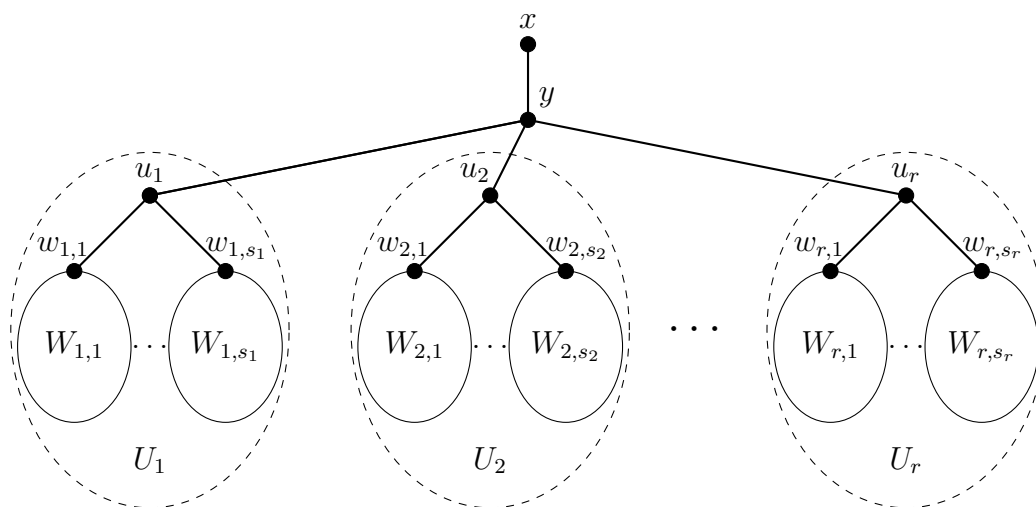

Figure 6: Tree with subtrees.

Then the following formula holds, see [20, Lemma 1].

Lemma 20 ([20]). *If T is a tree decomposed as in Figure 6, then*

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

With this formula, it is immediate to prove that the five constructions in Figure 4 give equality in Theorem 4.

Let us now continue with our induction proof. Assume that T is a twin-free tree of order $n \geqslant 9$. In the decomposition of Figure 6, assume without loss of generality that x is a leaf that is an end of a diametral path. This implies that all but one of y's neighbours are leaves, and since we are only considering twin-free trees, it actually implies that y has

degree 2, i.e., $r = 1$. Writing $s = s_1$, $U = U_1$, $W_j = W_{1,j}$, $u = u_1$ and $w_j = w_{1,j}$ for simplicity, the formula in Lemma 20 is reduced to

$$i_{\max}(T) = i_{\max}(U) + \prod_{j=1}^{s} i_{\max}(W_j). \tag{1}$$

Note that $|U| = n - 2$. The core of our induction lies in the following lemma.

Lemma 21. *At least one of the following holds:*

1. $i_{max}(U) \geqslant f(n-3)$ *and* $\displaystyle\prod_{j=1}^{s} i_{max}(W_j) \geqslant f(n-3)$, *or*

2. $i_{max}(U) \geqslant f(n-2)$ *and* $\displaystyle\prod_{j=1}^{s} i_{max}(W_j) \geqslant f(n-4)$, *or*

3. $i_{max}(U) \geqslant 2f(n-5)$ *and* $\displaystyle\prod_{j=1}^{s} i_{max}(W_j) \geqslant f(n-5)$.

Proof. We divide the proof into two cases, depending on the root degree of U.
Case 1: $s = 1$.
Observe that if U is not twin-free (in which case u and a leaf of U are at distance 2 from each other), then W_1 is twin-free and by the induction hypothesis $i_{\max}(U) = i_{\max}(W_1) \geqslant f(n-3)$, so the first of the three statements holds. If U is twin-free, W_1 might not be, but can in this case be made twin-free by removing a vertex without affecting $i_{\max}$. Hence we have $i_{\max}(U) \geqslant f(n-2)$ and $i_{\max}(W_1) \geqslant f(n-4)$, so the second statement holds.
Case 2: $s \geqslant 2$.
First we observe that U is now always a twin-free tree and thus $i_{\max}(U) \geqslant f(n-2)$ by the induction hypothesis. We also observe that $i_{\max}(W_j) \geqslant f(|W_j|)$ if W_j is twin-free and otherwise $i_{\max}(W_j) \geqslant f(|W_j|-1)$ by the same argument as in Case 1; only the vertex w_j can become a twin of another vertex, and in that case $W \setminus w_j$ is twin-free.
If $|W_j| \leqslant 4$, then we have $i_{\max}(W_j) = f(|W_j|)$: in each case, there is only one possible tree up to isomorphism (W_j cannot be a star of order 4, since T would then not be twin-free). Hence $i_{\max}(W_j) < f(|W_j|)$ can only happen if $|W_j| \geqslant 5$.
We consider two subcases now: assume first that $|W_j| > 1$ for all j. We have $i_{\max}(W_j) \geqslant f(|W_j|-1)$ whenever $|W_j| \geqslant 5$, and iterating part (b) of Lemma 19 gives us

$$\prod_{j:|W_j|\geqslant 5} i_{\max}(W_j) \geqslant f\left(\left(\sum_{j:|W_j|\geqslant 5} |W_j|\right) - 1\right),$$

provided there are W_j of order 5 or greater. For all j with $W_j < 5$, we can use the fact that $i_{\max}(W_j) = f(|W_j|)$. Applying part (a) of the same lemma repeatedly now, we end up with

$$\prod_{j=1}^{s} i_{\max}(W_j) \geqslant f\left(\left(\sum_{j=1}^{s}|W_j|\right) - 1\right) = f(n-4), \tag{2}$$

so statement 2 holds in this case. If there are no W_j of order 5 or greater, we can skip the first step and only apply part (a) of Lemma 19. The exceptional case $(3,3)$ only occurs at most once in the process, and we have $f(3)^2 = 4 = f(5)$, thus (2) still applies. In either case, we are done.

Let us finally consider the case that there is a j (without loss of generality $j = 1$) such that $|W_j| = 1$. There can only be one, as T is assumed to be twin-free. The same argument as in the other subcase now yields

$$\prod_{j=1}^{s} i_{\max}(W_j) = \prod_{j=2}^{s} i_{\max}(W_j) \geqslant f\left(\sum_{j=2}^{s} |W_j| - 1\right) = f(n-5).$$

Moreover, this bound can be improved if there is a twin-free W_j of order at least 4: in this case, we have $i_{\max}(W_j) \geqslant f(|W_j|)$. Iterating part (b) of Lemma 19 then yields

$$\prod_{j:|W_j|\geqslant 4} i_{\max}(W_j) \geqslant f\left(\sum_{j:|W_j|\geqslant 4} |W_j|\right)$$

and thus (2) again, in which case we are done. Likewise, since $f(2) = f(3) = 2$, we can improve the bound to $f(n-4)$ if there is a W_j of order 2.

So if (2) does not hold, then W_j cannot be twin-free for any $j \geqslant 2$ (there are no twin-free trees of order 3, and all other orders have been ruled out). This is only possible if the degree of w_j is 2. Moreover, $i_{\max}(W_j \setminus w_j) = i_{\max}(W_j)$ in this case. Taking w_1 (which by our assumption is a leaf) as the new root, we can apply Lemma 20 to U and deduce that

$$i_{\max}(U) = \prod_{j=2}^{s} i_{\max}(W_j) + \prod_{j=2}^{s} i_{\max}(W_j \setminus w_j) = 2\prod_{j=2}^{s} i_{\max}(W_j) \geqslant 2f(n-5).$$

Thus statement 3 applies in this case, which completes the proof. □

Applying the inequalities in Lemma 21 to the formula in (1), we obtain

$$i_{\max}(T) \geqslant \min\left(2f(n-3), f(n-2) + f(n-4), 3f(n-5)\right).$$

It is however straightforward to verify from the definition of $f(n)$ that $f(n) \leqslant 2f(n-3)$ (with equality if and only if $n \equiv 0, 2, 3 \pmod{5}$), $f(n) \leqslant f(n-2) + f(n-4)$ (with equality if and only if $n \equiv 1, 3 \pmod{5}$) and $f(n) = 3f(n-5)$ for all $n \geqslant 9$, so the inequality $i_{\max}(T) \geqslant f(n)$ follows immediately as a consequence, which finally completes the proof of Theorem 4. □

Theorem 4 also easily extends to forests, as the following corollary shows.

Corollary 22. *For every twin-free forest F of order $n \geqslant 2$, we have $i_{max}(F) \geqslant f(n-1)$.*

Proof. We use induction on n. For $n \leqslant 4$, the inequality is easy to check, so let us consider $n \geqslant 5$. Suppose that F is disconnected and has a connected component T of order m with $n - 1 > m \geqslant 2$. Taking the smallest such component, we can assume that $m \leqslant \frac{n}{2}$ and thus $n - m \geqslant \lceil \frac{n}{2} \rceil \geqslant 3$. By Theorem 4 and the induction hypothesis, we have

$$i_{\max}(F) = i_{\max}(T) \cdot i_{\max}(F - T) \geqslant f(m) \cdot f(n - m - 1) \geqslant f(n - 1),$$

where the final inequality follows from part (a) of Lemma 19. Note here that $m \neq 3$, since there are no twin-free trees of order 3. The only remaining possibilities are that F is connected (i.e., a tree), or that F consists of a tree and one isolated vertex. In either case, the conclusion follows from Theorem 4. □

4.1 The extremal trees

The extremal trees can be constructed iteratively by tracking the cases of equality in the proof. A complete characterization is provided in [19]. Here we add a small correction for $n = 8$: there are three extremal trees (rather than two as claimed in [19]), see Figure 7. Due to the different constructions, it is not too surprising that the number of extremal trees is not monotone as a function of n. The number of extremal trees for $4 \leqslant n \leqslant 19$ is summarized in Table 2.

n	# Extremal trees
$\{4, 5, 7, 9\}$	1
$\{6, 14\}$	2
$\{8, 10, 11, 12\}$	3
13	11
$\{15, 16\}$	12
17	10
18	60
19	5

Table 2: Number of extremal trees (i.e., trees satisfying $i_{\max}(T) = f(n)$) of order n.

5 Further thoughts

Füredi [6, Conjecture 4.3] asked about the maximum of $i_{\max}$ for other graph classes. This was done e.g. for triangle-free graphs in [3, 9], connected unicyclic graphs [13] and graphs with bounded degrees [14]. Let $\max i_{\max}(\mathcal{G})$ denote the maximum number of maximal independent sets in a graph class $\mathcal{G}$. This maximum grows exponentially in all cases mentioned, and $\lim_{n \to \infty} (\max i_{\max}(\mathcal{G}))^{1/n}$ equals $\sqrt{2}$ and $\sqrt[3]{3}$ for trees and graphs respectively.

In this paper, we proved that the minimum number of i_{max} for twin-free graphs, bipartite graphs and trees is logarithmic, linear and exponential, respectively. Due to this big
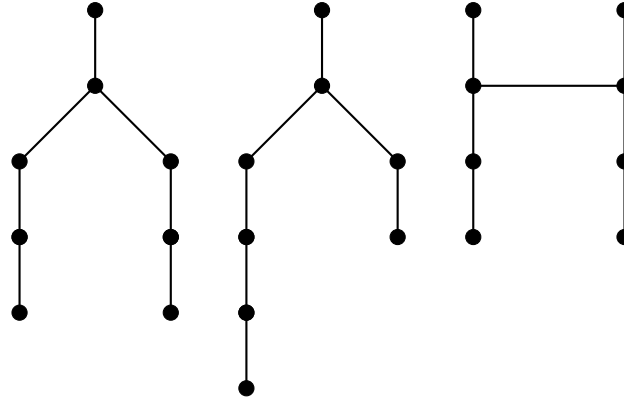
Figure 7: The three twin-free trees for $n = 8$ satisfying $i_{\max}(T) = 8$.

difference in behaviour of the minimum of $i_{\max}$, it may even be considered more interesting to study $\min i_{\max}(\mathcal{G})$ for some other graph classes $\mathcal{G}$ (restricted to twin-free graphs), since even the behaviour in terms of the order may be unclear.

Question 23. What is the behaviour of $\min i_{\max}(\mathcal{G})$ for twin-free graphs in a graph class $\mathcal{G}$?

One plausible interesting direction can be to wonder what happens for k-partite graphs as $n \to \infty$. For bipartite graphs, the bound was linear, while the extremal construction in Theorem 2 satisfies $\chi(G) \sim \log_2(n)$. Similarly, one can wonder about graphs with bounded clique number, with Conjecture 15 as a particular case.

Let $\nu(G)$ be the size of a maximum induced matching in G. Since every independent set can be extended to a maximal independent set and a set containing one end of each edge in an induced matching is an independent set, we conclude that $i_{\max}(G) \geqslant 2^{\nu(G)}$. Note that $\nu(G) \geqslant \frac{Cn}{\Delta^2}$ (see [10]) grows linearly in n for graphs with fixed maximum degree independent of n. For such sparse graph classes (bounded maximum degree independent of n), $\min i_{\max}(G)$ is exponential in terms of n. Kahn and Park [11] proved that for hypercubes Q_n of order $N = 2^n$, we have $\lim_{n\to\infty} i_{\max}(Q_n)^{1/N} = 2^{1/4}$, while also $\nu(Q_n) = \frac{N}{4}$ for every $n \geqslant 2$: in other words, $i_{\max}(Q_n)$ is of the form $2^{(1+o(1))\nu(G)}$. Note here that the hypercube Q_n is a twin-free graph if $n \geqslant 3$. For the twin-free trees in Figure 4, we note that $\lim_{n\to\infty} i_{\max}(T)^{1/n} = 3^{1/5}$ while $\nu(G) = \frac{n}{5} + 1$ (when $5 \mid n$), so here $2^{\nu(G)/n}$ is a lower bound for the limit that is not sharp. Studying $\lim_{n\to\infty}(\min i_{\max}(\mathcal{G}))^{1/n}$ for twin-free graphs in a graph class $\mathcal{G}$ might be interesting, especially if there is a natural graph class for which the constant is larger than $3^{1/5}$. One natural graph class to consider are r-regular graphs for fixed r. It is known that $i_{\max}(C_n) = P(n)$, where $P(n)$ denotes the nth Perrin number, which is defined by $P(0) = 3, P(1) = 0, P(2) = 2$ and the relation $P(n) = P(n-2) + P(n-3)$ for $n \geqslant 3$. For $n \geqslant 3$, the quantity $P(n)^{1/n}$ is minimized by $n = 4$, and the second smallest value is attained for $n = 6$. Since C_4 is not twin-free, for the class $\mathcal{G}$ of twin-free 2-regular graphs, $\lim_{n\to\infty}(\min i_{\max}(\mathcal{G}))^{1/n} = i_{\max}(C_6)^{1/6} = 5^{1/6}$. On the other side of the spectrum, when G is r-regular with $r = n-1-t$, i.e. $\overline{G}$ has small

degree, the question may be interesting as well. Such graphs satisfy $\frac{n}{t+1} \leqslant i_{\max} \leqslant 2^t n$. For $t = n^{1/s}$ and $\overline{G}$ being the Cartesian product of s K_ts, we have for example that $i_{\max}(G) \sim sn^{1-1/s}$.

There may well be quite a number of other problems where a parameter A can be unbounded in terms of another parameter B if A can increase when adding twins while B does not. This was for example also the obstruction in the related problem for $\nu(G)$, see [12].

One further direction is the relation between the vertex covering number $\tau(G)$ and $i_{\max}(G)$. Hoang and Trung [8] proved that $i_{\max}(G) \leqslant 2^{\tau(G)}$ for every graph G. In the other direction there is no such bound, since the complete bipartite graph $K_{n,n}$ satisfies $i_{\max}(G) = 2$ and $\tau(G) = n$. When restricting to twin-free graphs, we know that $\tau(G) \leqslant n - 1 < 2^{i_{\max}(G)}$ by Proposition 7 and thus $\tau(G)$ is bounded by a function of $i_{\max}(G)$. So the following question would tell us about the essential relationship between the two parameters.

Question 24. What is the maximum possible vertex covering number τ of a twin-free graph with $i_{\max}(G) = k$?

Plausible candidates are $\tau(G) = O(i_{\max}(G)^2)$, and for given order n, $\tau(G) - i_{\max}(G) \leqslant \left\lfloor \frac{n}{2} \right\rfloor - 3$. The first bound is attained by the complement of the Cartesian product $K_r \square K_r$ (one can connect every K_r with an additional vertex), and the second one by the complement of a cycle of K_3s (i.e., a cycle C_r for which every edge is connected to a new vertex).

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