Maximising the number of independent sets in connected graphs

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A Turán connected graph $\mathrm{TC}_{n,\alpha}$ is obtained from α cliques of size $\lfloor \frac{n}{\alpha} \rfloor$ or $\lceil \frac{n}{\alpha} \rceil$ by joining all cliques by an edge to one central vertex in one of the larger cliques. The graph $\mathrm{TC}_{n,\alpha}$ was shown recently by Bruyère and Mélot to maximise the number of independent sets among connected graphs of order n and independence number α. We prove a generalisation of this result by showing that $\mathrm{TC}_{n,\alpha}$ in fact maximises the number of independent sets of any fixed cardinality $\beta \leq \alpha$. Several results (both old and new) on the number of independent sets or maximum independent sets follow as corollaries.

1 Introduction

Turán's theorem [18], which characterises the K_r-free graphs with greatest number of edges, is probably the most classical result in extremal graph theory. It has been modified and extended in various ways: one such extension, due to Erdős [6, 7] (and rediscovered by Sauer [17] and Roman [15]), states that the complete $(r-1)$-partite graph whose partite sets are as equal in size as possible (this graph is often called a Turán graph, but we will rather use this name for its complement later) even has the greatest number of copies of K_k among all K_r-free graphs of given order for every $k \in \{1, 2, \ldots, r-1\}$ (and thus also the greatest total number of induced complete subgraphs); for $k > 1$, it is unique with this property. See also [1, Chapter VI, Corollary 1.10]. A similar result, due to Hedman [10], states that the same type of graph also has the greatest number of cliques (maximal complete subgraphs) among all graphs of order n with clique number ω if $\omega < \frac{n}{2}$.

We will be working with the dual setting, considering independent (stable) sets rather than complete subgraphs. The number of independent sets, known also as the *Fibonacci*

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number (in view of the fact that the number of independent sets of a path is a Fibonacci number, see [14] for the first reference) or *Merrifield-Simmons index* (a name that stems from the work of chemists Merrifield and Simmons [13]) of a graph, has received quite a lot of attention recently, with a specific focus on extremal problems, see the survey [19] for a collection of results. It is very natural to ask the following question: among all graphs of order n whose independence number is α, which graphs have the greatest number of independent sets? Of course, the answer to this question follows trivially from the aforementioned theorem of Erdős if no further assumptions are made, since independent sets of a graph correspond to complete subgraphs in the complement.

We note, however, that the complement of a complete multipartite graph is not connected; in a recent paper, Bruyère and Mélot [5] address the natural question how the situation changes if only connected graphs are considered. They prove that the answer in this case is given by what they call *Turán-connected graphs.* These graphs are obtained from a union of α cliques whose sizes are as equal as possible (the complement of the aforementioned complete multipartite graphs) by adding additional edges going out from a vertex in one of the "large" cliques to render the graph connected. For trees, Bruyère, Joret and Mélot considered the analogous minimisation problem (least number of independent sets) in [4] and obtained a partial characterisation of the extremal trees.

The main result of this paper is to show that a more general statement, paralleling the result of Erdős, holds: the Turán-connected graph has the greatest number of independent sets of *any cardinality* among connected graphs of given order and independence number. Apart from the theorem of Bruyère and Mélot, this has other implications as well: in particular, the Turán-connected graph maximises the number of maximum independent sets among connected graphs of given order and independence number. Comparing the number of maximum independent sets for different independence numbers, we find the greatest possible number of maximum independent sets a graph of order n can have, and characterise the corresponding extremal graphs. This result was originally obtained by Jou and Chang [11], based on work of Griggs, Grinstead and Guichard [9] and Füredi [8].

One also notes that the Turán-connected graph is a tree whenever $\alpha \geq \frac{n}{2}$ (there are no trees whose independence number is lower). Therefore, we obtain the solution to another problem, which was solved by Zito [20] (and generalised by Sagan and Vatter [16]), as a special case: which tree of order n has the greatest number of maximum independent sets?

This paper is organised as follows: we first review some important notation and preliminaries, then formally state and prove the main result in Section 3. Our approach mostly follows [5], adapted to the more general setting. Several corollaries conclude the paper.

2 Notions and preliminary results

As usual, let $\alpha(G)$ be the independence number of G, that is, $\alpha(G)$ is the greatest cardinality of an independent set in G. Denote by $i_\beta(G)$ the number of independent sets of size β in the graph G. Throughout this paper we say that a graph is extremal for β if it maximises i_β among all connected graphs with the same independence number.

Definition 2.1. Let $n, \alpha \in \mathbb{N}$. The *Turán graph* $\mathrm{T}_{n,\alpha}$ on n vertices is the disjoint union of α cliques of sizes $\lceil \frac{n}{\alpha} \rceil$ and $\lfloor \frac{n}{\alpha} \rfloor$. Note that this defines $\mathrm{T}_{n,\alpha}$ up to isomorphism because there is only one way to obtain n vertices.

Definition 2.2. The *Turán connected graph* $\mathrm{TC}_{n,\alpha}$ on n vertices is obtained from $\mathrm{T}_{n,\alpha}$ by taking a vertex c in a clique of size $\lceil \frac{n}{\alpha} \rceil$ and connecting it via an edge to exactly one vertex in each of the other cliques. The vertex c is called the *central vertex* or *centre* of the Turán connected graph, the clique containing c is called the *central clique*.

The following recursion is standard, yet very useful:

Proposition 2.3. *For any vertex v of G, we have*

$$i_\beta(G) = i_{\beta-1}(G - N[v]) + i_\beta(G - v),$$

where $N[v]$ denotes the closed neighbourhood of v.

Proof. Every independent set of size β either contains v (and thus none of its neighbours) or it does not. □

Theorem 2.4 (see [15, Theorem 1])**.** *Let α, β, n be integers with $1 < \beta \leq \alpha \leq n$. For every graph G on n vertices with independence number α, the inequality*

$$i_\beta(G) \leq i_\beta(\mathrm{T}_{n,\alpha})$$

holds, with equality only if G is isomorphic to $\mathrm{T}_{n,\alpha}$.

Lemma 2.5. *If $\alpha, \beta \geq 1$ are fixed, then the value of $i_\beta(\mathrm{T}_{n,\alpha})$ is strictly increasing in n.*

Proof. Note that $\mathrm{T}_{n+1,\alpha}$ can be obtained from $\mathrm{T}_{n,\alpha}$ by adding a vertex v to one of the smaller cliques. In the larger graph we have all independent sets from the smaller graph and some independent sets obtained by swapping in the new vertex v for one of the vertices in the clique that v was added to, which proves that $i_\beta(\mathrm{T}_{n+1,\alpha}) > i_\beta(\mathrm{T}_{n,\alpha})$. □

Call an edge e of G *critical* for α if $\alpha(G - e) > \alpha(G)$. A graph is called critical if all of its edges are critical. It is known that a critical graph cannot have a cutset spanning a complete subgraph, thus in particular no cut vertex:

Lemma 2.6 (cf. [5, Lemma 1])**.** *If G is critical and connected, then G is 2-connected, i.e. $G - v$ is connected for every vertex v.*

For a proof, see [12, Problem 8.18].

If we remove edges from a graph, the number of independent sets (of any fixed cardinality β) cannot decrease. Starting from any extremal graph, we can thus remove edges until we reach an *edge minimal* graph, where removal of another edge either increases the independence number or renders the graph disconnected. It is clear that if an edge minimal extremal (in particular connected) graph is not critical, then every uncritical edge must be a bridge. Furthermore, the following lemma states that in this case we can find an uncritical bridge such that one component of $G - e$ is critical, and every edge contained in this component is also a critical edge of G (we call this a *critical decomposition*). It is essentially identical to [5, Lemma 11], but since our definition of extremality is different, we provide its proof for completeness.

Lemma 2.7 (cf. [5, Lemma 11])**.** *An edge minimal connected graph that is extremal for some β is either critical, or it has a critical decomposition.*

Proof. Let G be an edge minimal connected graph, and suppose that G is not critical. Any edge of G that is not critical has to be a bridge, for otherwise we could remove it to obtain a connected graph of the same order and independence number, contradicting edge minimality. Among all uncritical edges, pick an edge e for which the smaller of the two components of $G - e$, which we call G_1, has the smallest possible number of vertices. Note that G_1 cannot contain any uncritical bridge e' of G, since the smaller component of $G - e'$ would be strictly smaller than (and in fact contained in) G_1, contradicting the choice of e. Thus all edges of G_1 are critical edges of G.

We claim that G_1 itself is critical as well, which means that we have found the desired critical decomposition. If this is not the case, then G_1 has a noncritical edge f, i.e. $\alpha(G_1 - f) = \alpha(G_1)$. Now if G_2 is the other component of $G - e$, then we clearly have

$$\alpha(G - f) \leq \alpha(G - e - f) = \alpha(G_1 - f) + \alpha(G_2) = \alpha(G_1) + \alpha(G_2) = \alpha(G - e) = \alpha(G),$$

where the last identity is due to the fact that e is uncritical by assumption. This implies that f is uncritical for G as well, which is a contradiction, completing the proof. □

Remark 2.8. As can be seen from the proof, the result of Lemma 2.7 holds for all edge minimal graphs, it does not depend on extremality with respect to i_β.

3 Main result

Theorem 3.1. *Let α, β, n be integers with $1 \leq \beta \leq \alpha < n$. For every connected graph G on n vertices with independence number α, we have*

$$i_\beta(G) \leq i_\beta(\mathrm{TC}_{n,\alpha}).$$

For $\beta > 2$, the graph $\mathrm{TC}_{n,\alpha}$ is the only edge minimal extremal graph.

Before we give the proof (in several steps), let us state and prove the following corollary:

Corollary 3.2. *For $2 < \beta \leq \min\{\alpha, n - \alpha\}$ the graph $\mathrm{TC}_{n,\alpha}$ is the only extremal graph.*

Proof. It suffices to prove that adding an edge to $\mathrm{TC}_{n,\alpha}$ strictly decreases the number of independent sets of size β. In other words, we must show that any two vertices that are not connected by an edge are contained in an independent set of size β.

Pick two arbitrary non-adjacent vertices u, v. Of the α cliques that form $\mathrm{TC}_{n,\alpha}$, there are at least $\min\{\alpha, n-\alpha\}$ whose size is at least 2. Since at most two of them can be fully contained in $N[u] \cup N[v]$, we can find $\beta - 2$ cliques which are not contained in this set. From each of these cliques select a vertex to obtain an independent set of size β containing both u and v. $\square$

Remark 3.3. For $\beta = 1$, evidently all graphs are extremal. The extremal graphs for $\beta = 2$ were characterised by Bougard and Joret in [2]: they are obtained from either a Turán graph or a graph whose components are odd cycles and/or single edges by adding the minimum number of edges (possibly zero) required to obtain a connected graph.

If $\alpha > \frac{n}{2}$ and $\beta > n - \alpha$, there are also other extremal graphs besides the Turán connected graph: they are obtained from $\mathrm{TC}_{n,\alpha}$ by adding additional edges incident with the central vertex.

The proof of Theorem 3.1 is inductive. It is easy to see that the theorem holds for $n \leq 3$. From now on we will assume that we have shown the theorem for all graphs on less than n vertices.

Lemma 3.4. *Complete graphs are extremal if and only if $\alpha = 1$.*

Proof. They are the only graphs with $\alpha = 1$. $\square$

Lemma 3.5. *Odd cycles are extremal if and only if $\alpha = \frac{n-1}{2}$ and $\beta = 2$.*

Proof. The independence number of an odd cycle is $\alpha = \frac{n-1}{2}$, hence we only consider graphs with this independence number.

Clearly being extremal for $\beta = 2$ is equivalent to having the smallest possible number of edges. The only connected graphs with fewer edges than cycles are trees. However, every tree with an odd number of vertices has an independent set of cardinality at least $\frac{n+1}{2}$ (the larger part of its bipartition). Thus a graph with independence number $\alpha = \frac{n-1}{2}$ cannot have more independent 2-sets than the cycle.

Conversely assume $\beta > 2$. In this case we will show that $\mathrm{TC}_{n,\frac{n-1}{2}}$ contains more independent sets of size β than C_n. Observe that the graph $\mathrm{TC}_{n,\frac{n-1}{2}}$ consists of a triangle with $\frac{n-3}{2}$ paths of length 2 attached to one of its vertices. Choosing v in Proposition 2.3 as one of the other two vertices of the triangle we obtain

$$i_\beta(\mathrm{TC}_{n,\frac{n-1}{2}}) = i_\beta(\mathrm{TC}_{n-1,\frac{n-1}{2}}) + i_{\beta-1}(\mathrm{T}_{n-3,\frac{n-3}{2}}).$$

On the other hand we have

$$i_\beta(C_n) = i_\beta(P_{n-1}) + i_{\beta-1}(P_{n-3}).$$

By our general induction hypothesis $i_\beta(P_{n-1}) \leq i_\beta(\mathrm{TC}_{n-1,\frac{n-1}{2}})$, and by Theorem 2.4 $i_{\beta-1}(P_{n-3}) < i_{\beta-1}(\mathrm{T}_{n-3,\frac{n-3}{2}})$. Hence C_n is not extremal. $\square$

Next we characterise all critical extremal graphs, paralleling part of the proof of Theorem 12 in [5]. This also fixes a small flaw of the proof in [5], where an upper bound for the number of independent sets of $\mathrm{TC}_{n,\alpha}$ is used in one case rather than a lower bound.

Lemma 3.6. *The only extremal critical graphs for $\beta \geq 2$ are complete graphs and odd cycles.*

Proof. Assume that we have a critical graph G which is neither complete nor an odd cycle. We will show that in this case G cannot be extremal.

Brooks' theorem [3] tells us that the chromatic number χ of G is less or equal to the maximum degree Δ. Using the trivial lower bound $\frac{n}{\alpha}$ for the chromatic number we obtain

$$\Delta \geq \chi \geq \frac{n}{\alpha},$$

which immediately implies that

$$n - \Delta - 1 \leq n - \left\lceil \frac{n}{\alpha} \right\rceil - 1.$$

Let v be a vertex of G with maximum degree. Since G is critical, $G - v$ must be connected by Lemma 2.6. Hence we have

$$\begin{aligned} i_\beta(G) &= i_\beta(G - v) + i_{\beta-1}(G - N[v]) \\ &\leq i_\beta(\mathrm{TC}_{n-1,\alpha}) + i_{\beta-1}\left(\mathrm{T}_{n-\Delta-1,\alpha-1}\right) \\ &\leq i_\beta(\mathrm{TC}_{n-1,\alpha}) + i_{\beta-1}\left(\mathrm{T}_{n-\lceil \frac{n}{\alpha} \rceil -1,\alpha-1}\right). \end{aligned}$$

If $n \equiv 1 \bmod \alpha$, there is exactly one clique of size $\lceil \frac{n}{\alpha} \rceil$ in $\mathrm{TC}_{n,\alpha}$. In this case, applying Proposition 2.3 to a vertex in this clique other than the central vertex gives us

$$\begin{aligned} i_\beta(\mathrm{TC}_{n,\alpha}) &= i_\beta(\mathrm{TC}_{n-1,\alpha}) + i_{\beta-1}\left(\mathrm{T}_{n-\lceil \frac{n}{\alpha} \rceil,\alpha-1}\right) \\ &> i_\beta(\mathrm{TC}_{n-1,\alpha}) + i_{\beta-1}\left(\mathrm{T}_{n-\lceil \frac{n}{\alpha} \rceil -1,\alpha-1}\right), \end{aligned}$$

the inequality being a consequence of Lemma 2.5. Otherwise, we choose a clique of size $\lceil \frac{n}{\alpha} \rceil$ that does not contain the central vertex and apply Proposition 2.3 to a vertex in this clique that is not adjacent to the central vertex. This gives us

$$\begin{aligned} i_\beta(\mathrm{TC}_{n,\alpha}) &= i_\beta(\mathrm{TC}_{n-1,\alpha}) + i_{\beta-1}\left(\mathrm{TC}_{n-\lceil \frac{n}{\alpha} \rceil,\alpha-1}\right) \\ &\geq i_\beta(\mathrm{TC}_{n-1,\alpha}) + i_{\beta-1}\left(\mathrm{T}_{n-\lceil \frac{n}{\alpha} \rceil -1,\alpha-1}\right), \end{aligned}$$

where the inequality is due to fact that $\mathrm{T}_{n-\lceil \frac{n}{\alpha} \rceil -1,\alpha-1}$ is a proper subgraph of $\mathrm{TC}_{n-\lceil \frac{n}{\alpha} \rceil,\alpha-1}$ (it is obtained by removing the central vertex). In either case, we end up with

$$i_\beta(G) \leq i_\beta(\mathrm{TC}_{n,\alpha}).$$

Hence for G being extremal it is necessary that all the inequalities hold with equality. In the first case ($n \equiv 1 \bmod \alpha$), we have already seen that this is impossible. In the second case, we must have

$$i_{\beta-1}\left(\mathrm{T}_{n-\lceil \frac{n}{\alpha} \rceil -1,\alpha-1}\right) = i_{\beta-1}\left(\mathrm{TC}_{n-\lceil \frac{n}{\alpha} \rceil,\alpha-1}\right),$$

which can only happen if there is no independent set of cardinality $\beta-1$ in $\mathrm{TC}_{n-\lceil \frac{n}{\alpha} \rceil, \alpha-1}$ that contains the central vertex, or equivalently no independent set of cardinality β in $\mathrm{TC}_{n,\alpha}$ that contains the central vertex. This happens if and only if $\alpha \geq n-\beta+1$ (cf. the proof of Corollary 3.2). But then $2\alpha \geq \alpha+\beta \geq n+1$, so $\lceil \frac{n}{\alpha} \rceil = 2$. Now Lemma 2.5 tells us that the inequality

$$i_{\beta-1}\left(\mathrm{T}_{n-\Delta-1,\alpha-1}\right) \leq i_{\beta-1}\left(\mathrm{T}_{n-\lceil \frac{n}{\alpha} \rceil-1,\alpha-1}\right)$$

can only be sharp if $\Delta = \lceil \frac{n}{\alpha} \rceil = 2$. Since G is connected, this means that G is either a path or a cycle. Even cycles are not critical, and neither are paths with more than two vertices, so this completes the proof. □

Before we start the proof of our main theorem, we need one last definition:

Definition 3.7. Call a graph *almost Turán connected* if there is a vertex v (the central vertex) such that $G-v$ is the disjoint union of cliques, there is a clique (the central clique, possibly empty) such that v is adjacent to each of its vertices, and for every other clique there is exactly one edge connecting it to v. In other words, it has the same structure as a Turán connected graph, but the sizes of the cliques are not necessarily balanced.

Proof of Theorem 3.1. For $\beta = 1$, every graph is extremal, and the case $\beta = 2$ is settled by [2, Proposition 5] (cf. Remark 3.3). For the rest of this proof assume that $\beta \geq 3$ and that G is an edge-minimal extremal graph for β.

By Lemma 2.7 we know that either G is critical, or there is a critical decomposition of G. In the first case Lemma 3.6 provides a full answer: G is complete, since it cannot be an odd cycle for $\beta \geq 3$ in view of Lemma 3.5.

Hence consider the case where there is a critical decomposition of G. The induction step in this case consists of four parts:

(i) show that the critical component of a critical decomposition must be extremal as well,

(ii) show that there is a critical decomposition where the critical component is complete,

(iii) show that G is almost Turán connected, and

(iv) show that it is best possible to have balanced clique sizes.

For the first step, assume that we have a critical decomposition of G into parts G_1 and G_2; we will denote their orders by n_1 and n_2 and their independence numbers by α_1 and α_2 respectively. Without loss of generality assume that G_1 is the critical component. Let $e = uv$ be the bridge connecting G_1 and G_2, with $u \in G_1$ and $v \in G_2$. Since e is an uncritical bridge, the independence number of G is $\alpha = \alpha_1 + \alpha_2$. Proposition 2.3 gives

$$i_\beta(G) = \sum_{\gamma \geq 0} \left(i_\gamma(G_1) i_{\beta-\gamma}(G_2 - v) + i_\gamma(G_1 - u) i_{\beta-\gamma-1}(G_2 - N[v])\right). \tag{1}$$

Note that this sum contains only finitely many non-zero summands and that at least one of the summands must be non-zero unless $\beta > \alpha$. By the induction hypothesis,

$$i_\gamma(G_1) \le i_\gamma(\mathrm{TC}_{n_1,\alpha_1}). \tag{2}$$

Furthermore we have $\alpha(G_1 - u) \le \alpha_1$ and hence

$$i_\gamma(G_1 - u) \le i_\gamma(\mathrm{T}_{n_1-1,\alpha_1}). \tag{3}$$

Note here that $G_1 - u$ need not be connected. Summing up yields

$$i_\beta(G) \le \sum_{\gamma=0}^{\beta} \big(i_\gamma(\mathrm{TC}_{n_1,\alpha_1}) i_{\beta-\gamma}(G_2 - v) + i_\gamma(\mathrm{T}_{n_1-1,\alpha_1}) i_{\beta-\gamma-1}(G_2 - N[v])\big).$$

Equality holds for every γ if G_1 is the Turán connected graph $\mathrm{TC}_{n_1,\alpha_1}$, u being the central vertex. Thus equality in (2) must hold for every $\gamma \le \alpha_1$ where $i_{\beta-\gamma}(G_2 - v) \ne 0$ as we assumed G to be extremal. If $\beta \le \alpha_1$, we can take $\gamma = \beta$, for which we trivially have $i_0(G_2 - v) = 1 \ne 0$. Thus G_1 is extremal for β in this case. Otherwise, we take $\gamma = \alpha_1$. Since the independence number of $G_2 - v$ is at least $\alpha_2 - 1 = \alpha - \alpha_1 - 1$, we have $i_{\beta-\gamma}(G_2 - v) \ne 0$ unless $\beta - \gamma \ge \alpha_2$, which is only possible if $\beta = \alpha$. So G_1 is extremal for α_1, except perhaps for the case that $\beta = \alpha$ and $i_{\alpha_2}(G_2 - v) = 0$. In that case, every maximum independent set of G_2 (and thus also every maximum independent set of G) contains v.

In conclusion, either G_1 is extremal for $\min\{\beta, \alpha_1\}$, or every maximum independent set of G contains v (and hence does not contain u). In the latter case, any edge incident to u in G_1 is uncritical for G and hence G_1 is either a singleton (which already proves (i) and (ii)) or it contains an uncritical edge, which is a contradiction. Thus the proof of (i) is complete.

Note that we only used the criticality of G_1 at the end. So by the same arguments as above we can show that G_2 either is extremal for $\min\{\beta, \alpha_2\}$, or every maximum independent set of G contains u and does not contain v. We will use this fact later.

For step (ii) assume that neither G_1 nor G_2 is complete, otherwise there is nothing to show. In particular, $\alpha_1 \ge 2$ and $\alpha_2 \ge 2$. We already know that G_1 is extremal for $\gamma = \min\{\alpha_1, \beta\}$ and thus it must be an odd cycle.

There is a maximum independent set in G_1 that does not contain the vertex u, so G_2 is extremal for $\min\{\beta, \alpha_2\}$ by the remark at the end of step (i). Since $\beta \ge 3$ we can use the induction hypothesis to show that either G_2 is a Turán connected graph or $\alpha_2 = 2$. If G_2 is a Turán connected graph, then it contains an uncritical bridge that we can remove to obtain a critical decomposition with a complete critical component.

If G_2 is not a Turán connected graph then $\alpha_2 = 2$, and since G_2 is extremal for α_2 as well, G_2 is a C_5.

So the only remaining problematic case is when G consists of a 5-cycle and another odd cycle connected by a single edge. In this scenario, we have $\alpha = \frac{n}{2} - 1$ (recall that n is the number of vertices), so the corresponding Turán connected graph $\mathrm{TC}_{n,\alpha} = \mathrm{TC}_{n,\frac{n}{2}-1}$ has two cliques of three vertices, all other cliques are of size 2. Apply Proposition 2.3 to an arbitrary vertex x of G that is not adjacent to either endpoint of the bridge, and to a vertex of the 3-vertex clique in $\mathrm{TC}_{n-1,\frac{n}{2}-1}$ that does not contain the central vertex, to obtain the following inequality:

$$\begin{aligned} i_\beta(G) &= i_\beta(G-x) + i_{\beta-1}(G-N[x]) \\ &< i_\beta(\mathrm{TC}_{n-1,\frac{n}{2}-1}) + i_{\beta-1}(\mathrm{TC}_{n-3,\frac{n}{2}-2}) \\ &= i_\beta(\mathrm{TC}_{n,\frac{n}{2}-1}) \end{aligned}$$

This shows that G is not extremal, completing the proof of (ii). In the following, we can assume that G_1 is complete.

For the proof of (iii) once again recall that G_2 must be extremal for $\gamma = \min\{\beta, \alpha_2\}$ unless every independent set of size β in G uses the vertex u.

Since G_1 is complete it is easy to see that in the latter case G_1 can only be a singleton, so that (1) reduces to

$$i_\beta(G) = i_\beta(G_2) + i_{\beta-1}(G_2 - v) \leq i_\beta(\mathrm{TC}_{n-1,\alpha_2}) + i_{\beta-1}(\mathrm{T}_{n-2,\alpha_2}).$$

The only way that equality can hold here if G_2 is not isomorphic to TC_{n-2,a_2} is that $\beta > \alpha_2$, so $\alpha_2 = \beta - 1$. However, $G_2 - v$ must still be isomorphic to $\mathrm{T}_{n-1,\alpha_2}$. Every component of $G - v$ must be connected to v by at least one edge in G. Since G is edge minimal, we conclude that there is exactly one edge from each component to v and hence G is almost Turán connected in this case.

Hence we may assume that G_2 is extremal for $\min\{\beta, \alpha_2\}$. If this minimum is 1 then $\alpha_2 = 1$ and G_2 is a clique. If the minimum is 2 then $\alpha_2 = 2$ and we can argue as before: either G_2 is a C_5, or it is Turán connected. The former possibility can be ruled out directly again: in this case, $\alpha = \beta = 3$, $i_3(G) = 5n - 27$ (recall that G_1 is complete), and

$$i_3(\mathrm{TC}_{n,3}) = \begin{cases} \frac{n^3-18n+27}{27} & n \equiv 0 \bmod 3, \\ \frac{n^3-21n+47}{27} & n \equiv 1 \bmod 3, \\ \frac{n^3-21n+34}{27} & n \equiv 2 \bmod 3, \end{cases}$$

so it is easily verified that $i_3(G) < i_3(\mathrm{TC}_{n,3})$.

Thus G_2 is Turán connected if $\min\{\beta, \alpha_2\} = 2$, and if $\min\{\beta, \alpha_2\} \geq 3$ this is also the case by the induction hypothesis. For the proof of (iii) it only remains to show that it is best possible to have v at the centre c of the Turán connected graph. Assume that $v \neq c$ and let G' be the graph obtained from G by replacing $e = uv$ by $e' = uc$. Every independent set of G which does not contain u is also an independent set of G' and vice versa. Similarly the independent sets which do contain u but neither v nor c are the same for G and G'. Hence we only have to compare the number of independent sets of G containing u and c to the number of independent sets in G' containing u and v.

To investigate those numbers, observe that $G - (N[u] \cup N[c])$ and $G' - (N[u] \cup N[v])$ are both disjoint unions of cliques, and that the cliques of $G' - (N[u] \cup N[v])$ are even balanced, i.e., it is a Turán graph. Thus

$$i_{\beta-2}(G - (N[u] \cup N[c])) \leq i_{\beta-2}\left(\mathrm{T}_{n_2 - \lceil \frac{n_2}{\alpha_2} \rceil - \alpha_2 + 1, \alpha_2 - 1}\right)$$

with equality if and only if v is a neighbour of c, and

$$i_{\beta-2}(G' - (N[u] \cup N[v])) \geq i_{\beta-2}\left(\mathrm{T}_{n_2-\left\lceil\frac{n_2}{\alpha_2}\right\rceil-1,\alpha_2-1}\right)$$

with equality if and only if v is contained in a non-central clique of size $\left\lceil\frac{n_2}{\alpha_2}\right\rceil$. Since $\beta \geq 3$ and $\alpha_2 \geq 3$, Lemma 2.5 tells us that

$$i_{\beta-2}(G - (N[u] \cup N[c])) < i_{\beta-2}(G' - (N[u] \cup N[v])),$$

and hence G cannot be extremal. This contradiction completes the proof of (iii).

So we know that G is almost Turán connected. It only remains to show that balanced clique sizes are best possible and that the central clique must be one of the larger cliques. For this purpose let k be the size of some clique C and let l be the size of the central clique C_0. If $k = l$ or $k = l - 1$ there is nothing to show. We now consider the cases $k > l$ and $k < l - 1$ and show that in both cases G is not extremal.

This will be done by moving a vertex from a larger clique to a smaller clique, i.e., disconnecting this vertex from all of its neighbours and connecting it to every vertex of the smaller clique. It is readily verified that the number of independent sets of size β containing a vertex in at most one of the two involved cliques is invariant under this transformation. For convenience, we simply denote this number by A_β. We will show that the number of independent sets of size β containing vertices in both cliques increases, so that we obtain a graph with the same independence number and more independent sets of size β.

In the case where $k > l$ we move a vertex from C to C_0 to obtain a new graph G'. Before moving the vertex we have

$$i_\beta(G) = (k-1)I^-_{\beta-2} + k(l-1)I_{\beta-2} + A_\beta,$$

where $I_{\beta-2}$ denotes the number of independent sets of size $\beta - 2$ in the remaining cliques and $I^-_{\beta-2}$ denotes the number of such cliques which do not contain vertices adjacent to the centre.

After moving the vertex we have

$$i_\beta(G') = (k-2)I^-_{\beta-2} + (k-1)lI_{\beta-2} + A_\beta.$$

The difference of the two values is now easily seen to be positive:

$$\begin{aligned} i_\beta(G') - i_\beta(G) &= -I^-_{\beta-2} + kI_{\beta-2} - lI_{\beta-2} \\ &> -I_{\beta-2} + kI_{\beta-2} - lI_{\beta-2} \\ &= (k-l-1)I_{\beta-2} \\ &\geq 0 \end{aligned}$$

because $k > l$ and both k and l are integers. Hence $i_\beta(G') > i_\beta(G)$. Since the independence numbers of G and G' coincide this contradicts G being extremal.

Now assume that $k < l-1$. In this case we move a vertex from C_0 to C to obtain a new graph G''. We have

$$i_\beta(G'') = kI^-_{\beta-2} + (k+1)(l-2)I_{\beta-2} + A_\beta.$$

Taking differences gives

$$i_\beta(G'') - i_\beta(G) = I^-_{\beta-2} + (l-k-2)I_{\beta-2} > 0$$

by similar arguments as above. But this again contradicts G being extremal.

Hence we have shown that if G is edge minimal but not critical, then it must be a Turán connected graph. Together with Lemma 3.6 this completes the proof of the theorem. □

4 Consequences

As it has already been mentioned in the introduction, our main result has a number of implications. First and foremost, it obviously implies the result of Bruyère and Mélot that was the original motivation for this paper:

Corollary 4.1 (cf. [5, Theorem 12]). *The Turán-connected graph* $\mathrm{TC}_{n,\alpha}$ *has the greatest number of independent sets among all connected graphs of order* n *whose independence number is* α.

Since Theorem 3.1 holds in particular for $\beta = \alpha$ (i.e., the number of independent sets whose cardinality is equal to the independence number), we also have the following corollary:

Corollary 4.2. *The Turán-connected graph* $\mathrm{TC}_{n,\alpha}$ *has the greatest number of maximum independent sets among all connected graphs of order* n *whose independence number is* α.

Any tree of order n has independence number at least $\frac{n}{2}$. We notice that for any $\alpha \geq \frac{n}{2}$, the Turán-connected graph $\mathrm{TC}_{n,\alpha}$ is indeed a tree. Therefore, we also immediately obtain the following results:

Corollary 4.3 (cf. [5, Corollary 13]). *For any* $\alpha \geq \frac{n}{2}$, *the Turán-connected graph* $\mathrm{TC}_{n,\alpha}$ *has the greatest number of independent sets among all trees of order* n *whose independence number is* α.

Corollary 4.4. *For any* $\alpha \geq \frac{n}{2}$, *the Turán-connected graph* $\mathrm{TC}_{n,\alpha}$ *has the greatest number of maximum independent sets among all trees of order* n *whose independence number is* α.

Comparing the numbers for different values of α, we also find the extremal connected graphs or trees without restrictions on the independence number. Let us first consider arbitrary connected graphs. Griggs, Grinstead and Guichard [9] and independently by Füredi [8] for sufficiently large n determined the connected graphs of order n with the greatest number of maximal independent sets (maximal with respect to set inclusion rather than cardinality), but since every maximum independent set is necessarily maximal independent as well, and conversely all maximal independent sets in the extremal graphs are in fact also maximum independent sets, the result remains true for maximum independent sets, as pointed out by Jou and Chang in [11]:

Corollary 4.5 (cf. [11, Theorem 17])**.** *A connected graph of order $n \leq 5$ has at most n maximum independent sets, with equality for the complete graph or (if $n = 5$) the Turán connected graph $\mathrm{TC}_{5,2}$. For $n \geq 6$, the unique connected graph of order n with the greatest number of maximum independent sets is the Turán connected graph $\mathrm{TC}_{n,\lfloor \frac{n}{3} \rfloor}$.*

Proof. For $n \leq 5$, the statement can be verified directly, so assume that $n \geq 6$. In view of Corollary 4.4, the maximum must be attained by a Turán connected graph $\mathrm{TC}_{n,\alpha}$ for some α. Consider such a Turán connected graph, assume that it has the greatest number of maximum independent sets, and let l be the number of vertices in the central clique. There are $r = \alpha l - n$ small cliques of size $l-1$ and $\alpha - r - 1$ large non-central cliques of size l, so we obtain the following formula for the number $i_\alpha(\mathrm{TC}_{n,\alpha})$ of maximum independent sets of $\mathrm{TC}_{n,\alpha}$:

$$i_\alpha(\mathrm{TC}_{n,\alpha}) = l^{\alpha-r-1}(l-1)^{r+1} + (l-1)^{\alpha-r-1}(l-2)^r.$$

If $l \geq 5$, we replace the central clique by a clique of $l - 2$ vertices and add another clique of size 2 that is joined to the central vertex by an edge. Then the number of maximum independent vertices changes to

$$2(l-3) \cdot l^{\alpha-r-1}(l-1)^r + (l-1)^{\alpha-r-1}(l-2)^r \geq i_\alpha(\mathrm{TC}_{n,\alpha}),$$

with equality only if $l = 5$. In the latter case, however, the resulting graph is not Turán connected (since $n \geq 6$). Thus we can rule out the possibility that $l \geq 5$. On the other hand, if $l = 2$, then we replace two non-central cliques by a single one (two 2-cliques become one 4-clique, a 2-clique and a singleton become a 3-clique, or two singletons become a 2-clique). Again, the number of maximum independent sets does not decrease, and the resulting graph is not Turán connected, so we reach a contradiction. Thus $l = 3$ or $l = 4$. Now we note that for $l = 3$, the function

$$3^{\alpha-r-1}2^{r+1} + 2^{\alpha-r-1} = 3^{n-2\alpha-1}2^{3\alpha-n+1} + 2^{n-2\alpha-1}$$

is decreasing in α, while for $l = 4$, the function

$$4^{\alpha-r-1}3^{r+1} + 3^{\alpha-r-1}2^r = 4^{n-3\alpha-1}3^{4\alpha-n+1} + 3^{n-3\alpha-1}2^{4\alpha-n}$$

is increasing in α. This leaves us with the following options:

- if $n = 3s$, $i_s(\mathrm{TC}_{3s,s}) = 2 \cdot 3^{s-1} + 2^{s-1}$ or $i_{s-1}(\mathrm{TC}_{3s,s-1}) = 16 \cdot 3^{s-3} + 9 \cdot 2^{s-4}$,
- if $n = 3s+1$, $i_{s+1}(\mathrm{TC}_{3s+1,s+1}) = 8 \cdot 3^{s-2} + 2^{s-2}$ or $i_s(\mathrm{TC}_{3s+1,s}) = 3^s + 2^{s-1}$,
- if $n = 3s+2$, $i_{s+1}(\mathrm{TC}_{3s+2,s+1}) = 4 \cdot 3^{s-1} + 2^{s-1}$ or $i_s(\mathrm{TC}_{3s+2,s}) = 4 \cdot 3^{s-1} + 3 \cdot 2^{s-2}$.

Direct comparison shows that $\mathrm{TC}_{n,\lfloor \frac{n}{3} \rfloor}$ is extremal in all cases. $\square$

In the same way, we also obtain the following corollary:

Corollary 4.6 (cf. [14, Theorem 2.1] and [20, Theorems 3 and 4])**.** *The unique tree (connected graph) of order n with the greatest number of independent sets is the star, and the unique tree of order n with the greatest number of maximum independent sets is the extended star $\mathrm{TC}_{n,\lceil \frac{n}{2} \rceil}$, obtained by subdividing all but two edges of a star of order $\frac{n+3}{2}$ (if n is odd) or all but one edge of a star of order $\frac{n+2}{2}$ (if n is even).*

Proof. Simply note that for $\alpha \geq \frac{n}{2}$,

$$i(\mathrm{TC}_{n,\alpha}) = 3^{n-\alpha-1}2^{2\alpha-n+1} + 2^{n-\alpha-1},$$

which is increasing in α, while

$$i_\alpha(\mathrm{TC}_{n,\alpha}) = 2^{n-\alpha-1} + \begin{cases} 1 & \alpha = \frac{n}{2}, \\ 0 & \text{otherwise}, \end{cases}$$

which is decreasing in α. $\square$

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