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by

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The Number of Independent Sets in Unicyclic Graphs

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Subm. to Discrete Applied Mathematics

Abstract

In this paper, we determine upper and lower bounds for the number of independent sets in a unicyclic graph in terms of its order. This gives an upper bound for the number of independent sets in a connected graph which contains at least one cycle. We also determine the upper bound for the number of independent sets in a unicyclic graph in terms of order and girth. In each case we characterize the extremal graphs.

Keywords: Unicyclic graphs, independent sets, bounds, Fibonacci numbers.

MSC 05C69, 05C05

1 Notation

We denote by G a graph of order $n = |V(G)|$ and size $m = |E(G)|$. For a vertex x in $V(G)$ let $\deg_G(x)$ denote its degree. A leaf is a vertex of degree one and a stem is a vertex adjacent to at least one leaf. Let P_n denote the path on n vertices and let C_n denote the cycle on n vertices. A *corona graph* G is a graph in which each vertex is a leaf or a stem adjacent to exactly one leaf. If H is a graph, then $H \circ K_1$ denotes the corona graph constructed from H by attaching precisely one leaf at each vertex of H. Let $K_{1,n-1}$ denote the star consisting of one center vertex adjacent to $n-1$ leaves. A graph is called *unicyclic* if it is connected and contains exactly one cycle. A graph is unicyclic if and only if it is connected and has size equal to its order. We shall by $H_{n,k}$ denote the unicyclic graph constructed by attaching $n-k$ leaves to a cycle of length k. The *Fibonacci numbers*, 0, 1, 1, 2, 3, 5, 8, 13, 21, 34,... are defined recursively by $\mathrm{fib}(0) = 0, \mathrm{fib}(1) = 1$, and for $n \geq 2$, $\mathrm{fib}(n) = \mathrm{fib}(n-2) + \mathrm{fib}(n-1)$. The *Lucas numbers* are $L(n) = \mathrm{fib}(n-1) + \mathrm{fib}(n+1)$. Given a graph G, a subset $S \subseteq V(G)$ is

called independent if no two vertices of S are adjacent in G. The set of independent sets in G is denoted by $\mathrm{I}(G)$. The empty set is independent. The set of independent sets in G which contains the vertex x is denoted by $\mathrm{I}_x(G)$, while $\mathrm{I}_{-x}(G)$ denotes the set of independents sets which do not contain x. The number of independent sets in G is denoted by $i(G)$. In the chemical literature the graph parameter $i(G)$ is referred to as the *Merrifield-Simmons index* [5].

2 Introduction

The first papers about counting maximal independent sets in a graph are Miller and Muller [6] and Moon and Moser [7]. For a survey see [1, 2]. In the same spirit Prodinger and Tichy [8] initiated the study of the number $i(G)$ of independent sets in a graph. The problem of counting the number of independent sets in a graph is NP-complete (see for instance Roth [10]). However, for certain types of graphs the problem of determining their number of independent subsets is polynomial. For instance, Prodinger and Tichy [8] proved, by induction, that $i(P_n)$ and $i(C_n)$, respectively, is the sequence of Fibonacci and Lucas numbers.

Theorem 2.1 ([8])

$$\begin{array}{lrcl} \forall n \in \mathbb{N}: & i(P_n) & = & \mathrm{fib}(n+2). \\ \forall n \in \mathbb{N}_{\geq 3}: & i(C_n) & = & L(n) = \mathrm{fib}(n-1) + \mathrm{fib}(n+1). \end{array}$$

When dealing with a graph parameter for which the value is NP-complete to determine, it is often useful to find bounds for its value. Prodinger and Tichy [8] proved that every tree T on n vertices satisfies $\mathrm{fib}(n+2) \leq i(T) \leq 2^{n-1}+1$, while Lin and Lin [4] proved that $i(T) = \mathrm{fib}(n+2)$ iff $T \simeq P_n$ and $i(T) = 2^{n-1}+1$ iff $T \simeq K_{1,n-1}$.

In 1997 Jou and Chang [3] gave an upper bound on the number of maximal independent sets in graphs with at most one cycle. In this paper we consider the number of independent sets in unicyclic graphs. In particular, we prove that every unicyclic graph G on n vertices satisfies $L(n) \leq i(G) \leq 3 \cdot 2^{n-3} + 1$ and we characterize the extremal graphs for these inequalities.

3 The Number of Independent Sets in Unicyclic Graphs

We shall in the following give both lower and upper bounds for the number of independent sets in unicyclic graphs.

3.1 A Lower Bound for $i(G)$

Given integers n and k with $3 \leq k \leq n$, the *lollipop* $L_{n,k}$ is the unicyclic graph of order n obtained from the two vertex disjoint graphs C_k and P_{n-k} by adding an edge joining a vertex of C_k to an endvertex of P_{n-k}. The lollipops satisfy $i(L_{n,k}) = i(L_{n,n+3-k})$ and $i(L_{n,k})$ is minimized for $k = 3$ and $k = n$. The main result of this section shows that among all unicyclic graphs of order n, the two graphs $L_{n,3}$ and $L_{n,n} \simeq C_n$ have the smallest number of independent subsets.

Theorem 3.1
If G is a unicyclic graph of order n, then $i(G) \geq L(n)$ and equality occurs if and only if $G \simeq C_n$ or $G \simeq L_{n,3}$.

For the proof of Theorem 3.1 we shall use the following results.

Lemma 3.2
Given any integer $k \geq 1$, the corona tree $Q_k := P_k \circ K_1$ satisfies $i(Q_k) = g(k)$, where the function g is defined recursively by $g(0) = 1, g(1) = 3$ and $g(j) = 2\,(g(j-1) + g(j-2))$ for every integer $j \geq 2$. Moreover, $i(C_k \circ K_1) = 4g(k-3) + 2g(k-1)$ for every integer $k \geq 3$.

The proof of the above lemma is straightforward and is omitted.

Prodinger and Tichy [8] solved the recursion for $g(k)$ and found that

$$i(Q_k) = \frac{3+2\sqrt{3}}{6}(1+\sqrt{3})^k + \frac{3-2\sqrt{3}}{6}(1-\sqrt{3})^k.$$

Lemma 3.3
For any integer $k \geq 3$, $i(C_k \circ K_1) > i(C_{2k})$.

Proof. We prove by induction on k that $4g(k-3)+2g(k-1) > L(2k)$. The statement is easily verified for $k \in \{3,4\}$. Suppose that $k \geq 5$ and that $4g(j-3) + 2g(j-1) > L(2j)$ whenever $3 < j < k$. We then obtain

$$\begin{aligned}
&i(C_k \circ K_1) = \\
&4g(k-3) + 2g(k-1) = \; 4\,(2g((k-1)-3) + 2g((k-2)-3)) + \\
&\qquad\qquad\qquad\quad 2\,(2g((k-1)-1) + 2g((k-2)-1)) \\
&\qquad\qquad\qquad = \; 2\,(4g((k-1)-3) + 2g((k-1)-1)) + \\
&\qquad\qquad\qquad\quad 2\,(4g((k-2)-3) + 2g((k-2)-1)) \\
&\qquad\qquad\qquad > \; 2L(2(k-1)) + 2L(2(k-2)) \\
&\qquad\qquad\qquad = \; 2L(2k-2) + 2L(2k-4) > 2L(2k-2) + L(2k-3) \\
&\qquad\qquad\qquad = \; L(2k-2) + L(2k-1) = L(2k) = i(C_{2k}).
\end{aligned}$$

This completes the proof. ■

Furthermore, we shall use the inequality $2^s L(n-s) > L(n)$ for $s \geq 1$, which can be proved by induction.

Proof of Theorem 3.1. We apply induction on the order of the graph. The statement is easily verified for $n \in \{3, 4, 5\}$. Hence we may assume $n \geq 6$.

Among the unicyclic graphs of order n, let G denote one for which the number of independent vertex subsets is minimum.

If G is a cycle, then, according to Theorem 2.1, $i(G) = L(n)$ and we are done. Suppose that G is not a cycle and let C_k denote the unique cycle of G. Let x denote a vertex of G having maximum distance to C_k.

(1) Suppose that $\mathrm{dist}(C_k, x) \geq 2$. The number of independent sets of G which contain x is equal to $i(G - N[x])$. The maximality of $\mathrm{dist}(C_k, x)$ and the assumption that $\mathrm{dist}(C_k, x) \geq 2$ imply that $G - N[x]$ consists of one component with precisely one cycle and possibly a number of isolated vertices, say $G - N[x] = H \cup \overline{K}_s$, where H is a unicyclic graph of order $n - 2 - s$. By induction on n, $i(G - N[x]) \geq 2^s L(n - 2 - s) \geq L(n - 2)$. In fact, we have $i(G - N[x]) > L(n - 2)$ if $s \geq 1$. The number of independent sets of G, which do not contain x, is equal to $i(G - x)$ and, by the induction on n, $i(G - x) \geq L(n - 1)$. Together these two inequalities imply $i(G) \geq L(n - 2) + L(n - 1) = L(n)$. If $i(G) = L(n)$, then we must have $s = 0$, $i(G - x) = L(n - 1)$ and $i(G - N[x]) = L(n - 2)$. Moreover, since $G - x$ is not a cycle, the induction on n implies that $G - x \simeq L_{n-1,3}$ and consequently $G \simeq L_{n,3}$.

(2) Assume $\mathrm{dist}(C_k, x) = 1$. We shall show that this assumption leads to a contradiction. Let the vertices of the cycle in G be consecutively labelled $v_1, v_2, \ldots, v_k$. It suffices to consider the following three cases.

(2.1) Suppose that some vertex v_j of G has more than one leaf attached, say v_1 has at least two leaves x and y. Define H by deleting the edges v_1v_2, v_1y and introducing two new edges xy and v_2y, that is, $H := (G - \{v_1y, v_1v_2\}) \cup \{xy, yv_2\}$. Now H is a unicyclic graph on n vertices. We intend to show $i(G) > i(H)$ and thus obtain a contradiction with the minimality of $i(G)$. We do this by constructing an injective, non-surjective mapping ϕ from $\mathrm{I}(H)$ to $\mathrm{I}(G)$. Let B denote an independent set in H and let $\phi(B)$ be defined by the table in Figure 1. The number beneath each vertex indicates whether or not the vertex is considered to be in the indendent set B. For instance, the third row reads 0010, which means that y is in B while neither v_1, v_2 nor x is in B.

The mapping ϕ is injective. Moreover, $\{x, y, v_k\} \in \mathrm{I}(G)$, but there exists no independent set $B \in \mathrm{I}(H)$ with $\phi(B) = \{x, y, v_k\}$. Hence ϕ is also non-surjective. It follows that $i(G) > i(H)$, which contradicts the minimality of $i(G)$. Hence, in the following we shall assume that every vertex v_i has at most one leaf attached.

v_1	x	y	v_2	$\phi(B)$
0	0	0	0	B
0	0	0	1	B
0	0	1	0	B
0	1	0	0	B
1	0	0	0	B
0	1	0	1	B
1	0	0	1	$(B - \{v_1\}) \cup \{x, y\}$
1	0	1	0	$(B - \{v_1\}) \cup \{x\}$

Figure 1: Definition of the mapping $\phi : \mathrm{I}(H) \to \mathrm{I}(G)$.

v_1	x	v_2	$\phi(B)$
0	0	0	B
0	0	1	B
0	1	0	B
1	0	0	B
1	0	1	$(B - \{v_2\}) \cup \{x\}$

Figure 2: Definition of the mapping $\phi : \mathrm{I}(H) \to \mathrm{I}(G)$.

(2.2) Suppose that no vertex v_i of G has more than one leaf attached and that G contains a vertex v_j which has no leaf attached. We may w.l.o.g. assume that the vertices of G have been numerated such that v_1 has no leaf attached while v_2 has exactly one leaf attached, say x. Define $H := (G - \{v_1v_2\}) \cup \{v_1x\}$. The graph H has order n and is unicyclic. Again, we obtain a contradiction be showing $i(G) > i(H)$. We construct an injective non-surjective mapping ϕ from $\mathrm{I}(H)$ to $\mathrm{I}(G)$. Let B denote an independent set in H and let $\phi(B)$ be defined by the table in Figure 2.

The mapping ϕ is injective. Recall that $n \geq 6$ and so, in this case, $k \geq 4$. This implies $\{x, v_1, v_3\} \in \mathrm{I}(G)$. However, there exists no independent set $B \in \mathrm{I}(H)$ with $\phi(B) = \{x, v_1, v_3\}$. Hence ϕ is also non-surjective and it follows that $i(G) > i(H)$. This contradiction implies that every vertex v_i of G must have exactly one leaf attached.

(2.3) Suppose that every vertex v_i has exactly one leaf attached. Then $G \simeq C_k \circ K_1$ where $k = n/2$ and it follows from Lemma 3.3 that $i(G) > i(C_n)$, a contradiction.

This completes the proof. ■

3.2 Two results used in proving an upper bound

Let $B_{n,d}$ denote the graph obtained from the path P_d with $n-d$ leaves attached to one of its ends. The following results were obtained in [9].

Theorem 3.4 ([9])
Let T denote a tree of order $n \geq 2$ and diameter d. Then

$$i(T) \leq \mathrm{fib}(d) + 2^{n-d}\mathrm{fib}(d+1) = i(B_{n,d}) \tag{1}$$

and equality occurs if and only $T \simeq B_{n,d}$.

Proposition 3.5 ([9])
For any $d \geq 3$ and $n \geq d+1$,

$$i(B_{n,d}) < i(B_{n,d-1})$$

These two results immediately give the following corollary.

Corollary 3.6
If T is a tree of order n and diameter at least k, then $i(T) \leq i(B_{n,k})$ and equality occurs if and only if $T \simeq B_{n,k}$.

3.3 An Upper bound for $i(G)$

Recall that $H_{n,k}$ is a k-cycle with $n-k$ leaves attached to one of its vertices.

Proposition 3.7
Given integers $k \geq 3$ and $n \geq k$. Then

$$i(H_{n,k}) = \mathrm{fib}(k-1) + 2^{n-k}\mathrm{fib}(k+1). \tag{2}$$

Proof. Let x denote the unique stem of $H_{n,k}$. The number of independent sets of $H_{n,k}$ containing x is equal to the number of independent sets in $G - N[x] \simeq P_{k-3}$, which, by Theorem 2.1, is $\mathrm{fib}(k-1)$. Similarly, the number of independent sets of $H_{n,k}$ not containing x is equal to the number of independent sets in $G - x \simeq P_{k-1} \cup \overline{K_{n-k}}$, which is $\mathrm{fib}(k+1)2^{n-k}$. This establishes (2). ■

Theorem 3.8
Let G denote a unicyclic graph with n vertices. Then $i(G) \leq 3 \cdot 2^{n-3} + 1$ and equality holds if and only if G is a 4-cycle or $G \simeq H_{n,3}$.

Proof. The statement is easily verified for $n \leq 5$, therefore let us assume $n \geq 6$.

Suppose that the cycle in G has length three. If G is obtained by attaching $n-3$ leaves at one vertex x of the 3-cycle, then, by (2), $i(G) = 3 \cdot 2^{n-3} + 1$ and we are done. Suppose that G cannot be constructed by attaching $n-3$ leaves to the 3-cycle of G. Now, either the 3-cycle of G contains at least two vertices of degree greater than two, or there is a vertex in G with distance at least two to the 3-cycle. In any event, G contains a spanning tree T of diameter at least four. According to Corollary 3.6 and Theorem 3.4,

$$i(G) < i(T) \leq i(B_{n,4}) = \text{fib}(4) + 2^{n-4}\text{fib}(5) = 3 + 5 \cdot 2^{n-4}. \qquad (3)$$

A simple calculation shows $i(B_{n,4}) < 3 \cdot 2^{n-3} + 1$ for all $n \geq 6$ and so the desired inequality follows.

If the cycle in G is of length greater than three, then it is easy to see that G contains a spanning tree T of diameter at least four and so (3) implies $i(G) < 3 \cdot 2^{n-3} + 1$. This completes the proof. ■

Corollary 3.9
Let G denote a graph in which every component contains exactly one cycle. Then $i(G) \leq 3 \cdot 2^{n-3} + 1$ and equality holds if and only if G is a 4-cycle or $G \simeq H_{n,3}$.

Proof. Given any n, we consider the class $\mathcal{G}_n$ of graphs of order n with the property that every component has exactly one cycle. In this class of graphs, let G denote a graph for which the number of independent sets is maximum.

Suppose that G contains $k \geq 2$ components, say $G_1, \ldots, G_k$ and let n_j denote the order of G_j. Since each component contains exactly one cycle, we have $n_j \geq 3$ and, according to Theorem 3.8, $i(G_j) \leq 3 \cdot 2^{n_j-3} + 1$ for every $j \in \{1, \ldots, k\}$. Now it is easy to see that $2^p + 2^q + 6 < 2^{p+q}$ for every pair of integers $p, q \geq 3$. It follows that

$$\begin{aligned} i(G_1) \cdot i(G_2) &\leq 3 \cdot 2^{n_1-3} + 1 + 3 \cdot 2^{n_2-3} + 1 \\ &< \frac{3}{8}(2^{n_1} + 2^{n_2} + 6) \\ &< 3 \cdot 2^{n_1+n_2-3} < i(H_{n_1+n_2,3}). \end{aligned}$$

Hence the graph $G' := H_{n_1+n_2,3} \cup G_3 \cup \cdots \cup G_k$ has more independent sets than G and, since $G' \in \mathcal{G}_n$, we have a contradiction with the maximality of $i(G)$. It follows that G must be connected, and now the desired result follows directly from Theorem 3.8. ■

Theorem 3.10
Let G denote a connected graph. If G is not a tree, then $i(G) \leq 3 \cdot 2^{n-3} + 1$. Equality holds if and only if G is a 4-cycle or $G \simeq H_{n,3}$.

Proof. Let T denote a spanning tree of G and let e denote an edge in $E(G) - E(T)$. Now $G' := T + e$ is a unicyclic spanning subgraph of G and therefore, by Theorem 3.8, $i(G) \leq i(G') \leq 3 \cdot 2^{n-3} + 1$, where equality occurs if and only if $G \simeq H_{n,3}$. ■

3.4 An Upper Bound in terms of Order and Cycle Length

A *tree T rooted at v* is the pair (T, v) consisting of a tree T and a distinguished vertex $v \in V(T)$. By $G \simeq U((T_1, v_1), (T_2, v_2), \ldots, (T_k, v_k))$ we denote a unicyclic graph with cycle $C_k \simeq v_1 v_2 \ldots v_k$ and the connected component of $G - E(C_k)$ containing v_i is the tree T_i, $1 \leq i \leq k$. The tree T_i is said to be *pendent from v_i, attached to v_i or rooted at v_i*. Let $h_i = h(T_i) = h(T_i, v_i) = \max\{d(v_i, x) | x \in V(T_i)\}$ denote the *height* of T_i and let $h = \max\{h_i | 1 \leq i \leq k\}$. Analogously $L((T_1, v_1), \ldots, (T_k, v_k))$ denotes $U((T_1, v_1), (T_2, v_2), \ldots, (T_k, v_k)) - v_1 v_k$, i.e. a path $v_1 \ldots v_k$ with T_j rooted at v_j, $1 \leq j \leq k$. For short we may write $U(T_1, \ldots, T_k)$ and $L(T_1, \ldots, T_k)$.

Lemma 3.11
Let $G \simeq L(T_1, \ldots, T_k)$ be a tree of order n, where each T_j is a star $T_j \simeq K_{1,a_j}, a_j \geq 0$ rooted at its center v_j. Then $i(G) \leq 2^{n-k}\mathrm{fib}(k+2)$ and equality occurs if and only if $a_1 = \cdots = a_k = 0$.

Proof. We use induction on k. We see that the lemma holds for $k = 1, 2$. Suppose $k \geq 3$. Observe $\mathrm{I}(L(T_1, \ldots, T_k)) = \mathrm{I}_{v_k}(L(T_1, \ldots, T_k)) \cup \mathrm{I}_{-v_k}(L(T_1, \ldots, T_k))$. Therefore $i(L(T_1, \ldots, T_k)) = 2^{a_{k-1}} i(L(T_1, \ldots, T_{k-2})) + 2^{a_k} i(L(T_1, \ldots, T_{k-1}))$ and, by the induction hypothesis, we obtain

$$\begin{aligned} i(L(T_1, \ldots, T_k)) &\leq 2^{a_{k-1}} 2^{a_1 + a_2 + \ldots + a_{k-2}} \mathrm{fib}(k) + 2^{a_k} 2^{a_1 + \ldots + a_{k-1}} \mathrm{fib}(k+1) \\ &\leq 2^{n-k} \mathrm{fib}(k+2), \end{aligned}$$

where equality occurs if and only if $a_1 = \cdots = a_k = 0$. ■

Lemma 3.12
Let $G \simeq U(T_1, \ldots, T_k)$ be a unicyclic graph of order n, where each T_j is a star $T_j \simeq K_{1,a_j}, a_j \geq 0$ rooted at its center v_j. Then $i(G) \leq 2^{n-k}\mathrm{fib}(k+1) + \mathrm{fib}(k-1)$ and equality occurs if and only if $G \simeq H_{n,k}$.

Proof. We apply induction on $n - k$. If $n - k = 0$, then G is a cycle and the statement is true according to Theorem 2.1. Suppose $n - k \geq 1$. Let x denote a leaf of G and let v_1 denote the stem of x. Again, we use $\mathrm{I}(G) = \mathrm{I}_{-x}(G) \cup \mathrm{I}_x(G)$. By induction on $n - k$, we obtain

$$|\mathrm{I}_{-x}(G)| \leq 2^{n-1-k}\mathrm{fib}(k+1) + \mathrm{fib}(k-1). \tag{4}$$

Moreover, Lemma 3.11 implies

$$|\mathrm{I}_x(G)| = 2^{a_1 - 1} i(L(T_2, \ldots, T_k)) \leq 2^{a_1 - 1} 2^{a_2 + \cdots + a_k} \mathrm{fib}(k+1). \tag{5}$$

By summing up we obtain $i(G) \leq 2^{n-k}\text{fib}(k+1) + \text{fib}(k-1)$ as desired. If $i(G) = 2^{n-k}\text{fib}(k+1) + \text{fib}(k-1)$, then we must have equality in (4) and (5). Inequality (4) and the induction hypothesis implies $G - x \simeq H_{n-1,k}$. Finally, (5) implies $a_2 = \cdots = a_k = 0$ and therefore $G \simeq H_{n,k}$. ■

We can now prove that the expression in Proposition 3.7 is an upper bound for all unicyclic graphs.

Theorem 3.13
If G is a unicyclic graph of order n and cycle length k, then $i(G) \leq 2^{n-k}\text{fib}(k+1) + \text{fib}(k-1)$. Equality occurs if and only if $G \simeq H_{n,k}$.

Proof. If all pendent trees have height 0 or 1, the theorem follows from Lemma 3.12. We may therefore assume that x is a leaf in G at distance ≥ 2 from the cycle. We have by induction assumption on n

$$|\mathrm{I}_{-x}(G)| \leq 2^{n-1-k}\text{fib}(k+1) + \text{fib}(k-1)$$

and assume the stem of x has t other leaves, $t \geq 0$. Then

$$|\mathrm{I}_x(G)| \leq 2^t \left(2^{n-k-t-2}\text{fib}(k+1) + \text{fib}(k-1)\right).$$

This gives $i(G) \leq 3 \cdot 2^{n-k-2}\text{fib}(k+1) + (2^t+1)\text{fib}(k-1)$ and, since $0 \leq t \leq n-k-2$, we obtain

$$\begin{aligned} i(G) &\leq 3 \cdot 2^{n-k-2}\text{fib}(k+1) + \text{fib}(k-1) + 2^{n-k-2}\text{fib}(k-1) \\ &\leq 2^{n-k}\text{fib}(k+1) + \text{fib}(k-1) + 2^{n-k-2}(\text{fib}(k-1) - \text{fib}(k+1)) \\ &< 2^{n-k}\text{fib}(k+1) + \text{fib}(k-1). \end{aligned}$$

This completes the proof. ■

3.5 Unicyclic Graphs with Long Cycles

It follows from the work of Lin and Lin [4] that if T is a tree on n vertices and T not isomorphic to the star $K_{1,n-1}$, then $i(T) \leq 3 \cdot 2^{n-3} + 2$. Moreover, $i(T) = 3 \cdot 2^{n-3} + 2$ if and only if T can be constructed from the star $K_{1,n-2}$ by subdividing a single edge. In this section we obtain a similar result for the unicyclic graphs which are not isomorphic to $H_{n,3}$.

Define $h : \mathbb{N}^2 \longrightarrow \mathbb{N}$ by $h(n,k) = \text{fib}(k-1) + 2^{n-k}\text{fib}(k+1)$. According to Theorem 3.13, every unicyclic graph G of order n and cycle length k satisfies $i(G) \leq h(n,k)$. The following lemma shows that for fixed n the function $h(n,k)$ is decreasing in k, so $k = 3$ gives its largest value and we have $i(G) \leq 2^{n-3}\text{fib}(4) + \text{fib}(2) = 3 \cdot 2^{n-3} + 1$, which is the inequality of Theorem 3.8.

Lemma 3.14
For any pair of integers n and k with $4 \leq k \leq n$ we have $h(n,k) \leq h(n,k-1)$. Equality occurs if and only if $n = k = 4$.

Proof. First, suppose $k \geq 5$. We shall prove that $h(n,k) < h(n,k-1)$ holds by means of the following inequalities.

$$\begin{aligned} h(n,k) &= \mathrm{fib}(k-1) + 2^{n-k}\mathrm{fib}(k+1) < \mathrm{fib}(k-2) + 2^{2-k+1}\mathrm{fib}(k) = h(n,k-1) \\ &\iff \mathrm{fib}(k-1) - \mathrm{fib}(k-2) < 2^{n-k+1}\mathrm{fib}(k) - 2^{n-k}\mathrm{fib}(k+1) \\ &\iff \mathrm{fib}(k-3) < 2^{n-k}(2\mathrm{fib}(k) - \mathrm{fib}(k+1)) \\ &\Longleftarrow \mathrm{fib}(k-3) < 2\mathrm{fib}(k) - \mathrm{fib}(k+1) = \mathrm{fib}(k-2). \end{aligned}$$

Secondly, if $k = 4$, then $\mathrm{fib}(k-3) = 1 < 2^{n-k}(2\mathrm{fib}(k) - \mathrm{fib}(k+1)) = 2^{n-4}$ if and only if $n \geq 5$. Hence $h(n,4) < h(n,3)$ whenever $n \geq 5$. Finally, for $k = 4$ and $n = 4$ we have $h(4,4) = 7 = h(4,3)$. ■

Theorem 3.15
Let $r \geq 3$ be an integer and G a unicyclic graph with n vertices and cycle length k. If $k \geq r$, then $i(G) \leq h(n,r) = \mathrm{fib}(r-1) + 2^{n-r}\mathrm{fib}(r+1)$. Equality occurs if and only if $G \simeq H_{n,r}$ $(k = r)$ or $G \simeq C_4$ $(k = 4 = r+1)$.

Proof. By Theorem 3.13, $i(G) \leq h(n,k)$ and, by Lemma 3.14, $h(n,k) \leq h(n,r)$. Hence $i(G) \leq h(n,r)$. If $i(G) = h(n,r)$, then $h(n,k) = h(n,r)$. This occurs if and only if $k = r$ or $n = k = r+1 = 4$. If $k = r$, then Theorem 3.13 implies $G \simeq H_{n,k}$. If $n = k = r+1 = 4$, then $G \simeq C_4$. ■

Observe that if $e = uv$ is an edge of a graph G then

$$\mathrm{I}(G) = \mathrm{I}(G-e) - \big\{\{v_1, v_2\} \cup S | S \in \mathrm{I}(G - N[v_1, v_2])\big\},$$

and so $i(G) = i(G-e) - i(G - N[v_1, v_2])$.

Theorem 3.16
Let G denote a unicyclic graph with n vertices. If $G \not\simeq H_{n,3}$, then $i(G) \leq h(n,4) = 5 \cdot 2^{n-4} + 2$. Equality occurs if and only if (i) $G \simeq H_{n,4}$ or (ii) G is obtained from a C_3 by attaching one leaf to one of its vertices and $n-4$ leaves to another of its vertices.

Proof. Let T denote a spanning tree of G such that $\mathrm{diam}(T)$ is maximum. Then T is obtained by removing some edge, say v_1v_2, on the cycle $C_k : v_1v_2 \ldots v_k$ in G. If $\mathrm{diam}(T) \geq 5$, then it follows easily from Corollary 3.6 that $i(G) \leq i(T) < h(n,4)$. Hence we may assume that $\mathrm{diam}(T) \leq 4$.

If $k \geq 5$, then it follows from Theorem 3.15 that $i(G) < h(n,4)$. Hence we may suppose $k \geq 4$.

If $k = 4$, then, by Theorem 3.15, $i(G) \leq i(H_{n,4})$ and equality occurs if and only if $G \simeq H_{n,4}$.

Suppose $k = 3$. The assumption $G \not\simeq H_{n,3}$ implies $\mathrm{diam}(T) \geq 4$ and so, by Corollary 3.6, $i(T) \leq 3 + 5 \cdot 2^{n-4}$. Now it suffices to consider the following three cases.

(i) $\deg(v_1) \geq 3$ and $\deg(v_2) = \deg(v_3) = 2$. In this case $\mathrm{diam}(T) \geq 4$ implies $i(T - N[v_1, v_2]) \geq 2$ and therefore $i(G) = i(T) - i(T - N[v_1, v_2]) \leq 3 + 5 \cdot 2^{n-4} - 2 < i(H_{n,4})$.

(ii) $\deg(v_1), \deg(v_2) \geq 3$ and $\deg(v_3) = 2$. Since $\mathrm{diam}(T) \leq 4$, we find that G is the graph obtained from C_3 by attaching s_1 leaves at v_1 and s_2 leaves at v_2 such that $n = s_1 + s_2 + 3$. Now it is easy to see that $i(G) = 2^{s_1+s_2+1} + 2^{s_1} + 2^{s_2}$. Assume $s_1 \leq s_2$. For $s_1 = 1$ we obtain $s_2 = n - 4$ and the equality $i(G) = 2^{s_1+s_2} + 2 + 2^{s_2} = 5 \cdot 2^{n-4} + 2$. For $2 \leq s_1 \leq s_2$ we get $i(G) = 2^{s_1+s_2-1}(5 + 2^{1-s_2} + 2^{1-s_1} - 1) \leq 2^{n-4} \cdot 5 < 5 \cdot 2^{n-4} + 2 = h(n, 4)$.

(iii) $\deg(v_1), \deg(v_2), \deg(v_3) \geq 3$. This case is similar to case (ii).

■

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