Filomat 28:3 (2014), 451–461
DOI 10.2298/FIL1403451H

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

Unicyclic Graphs with Given Number of Cut Vertices and the Maximal Merrifield - Simmons Index

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Abstract. The Merrifield-Simmons index of a graph G, denoted by $i(G)$, is defined to be the total number of independent sets in G, including the empty set. A connected graph is called a unicyclic graph, if it possesses equal number of vertices and edges. In this paper, we characterize the maximal unicyclic graph w.r.t. $i(G)$ within all unicyclic graphs with given order and number of cut vertices. As a consequence, we determine the connected graph with at least one cycle, given number of cut vertices and the maximal Merrifield-Simmons index.

1. Introduction

In this paper only simple graphs without loops and multiple edges are considered. For terminology and notation not defined here, the reader is referred to Bondy and Murty [2].

Given a graph G with vertex set $V(G)$ and edge set $E(G)$. If $S \subseteq V(G)$ and the subgraph induced by S has no edges, then S is said to be an *independent set* of G. Let $i(G)$ denote the total number of independent sets, including the empty set, in G.

Since, for the n-vertex path P_n, $i(P_n)$ is exactly equal to the Fibonacci number F_{n+1}, some researchers also call $i(G)$ the *Fibonacci number* of a graph G (see [1, 17]). Nowdays, $i(G)$ is commonly termed as 'Merrifield-Simmons index', which originated from [15]. This index is one of the most popular topological indices in chemistry, which has been extensively studied, as can be seen in the monograph [13]. During the past several decades, a number of research results on the Fibonacci number or Merrifield-Simmons index of graphs have been obtained, among which characterization of graphs with extremal $i(G)$ within a given class of graphs with special structure has been one of the most popular tendency. For instance, see [11] and [17] for trees, [16] for trees with given number of pendent vertices, [10] for trees with a given diameter, [7] for trees with bounded degree, [14] for unicyclic graphs, [9] for the unicyclic graphs with a given diameter, [12] for the cacti, [8] for the quasi-tree graphs, [4] for connected graphs with given number of cut edges, [5] for connected graphs with given number of cut vertices, [6] for 3-connected and 3-edge-connected graphs, [1] for maximal outerplanar graphs, and so on.

2010 *Mathematics Subject Classification*. Primary 05C35; Secondary 05C90
Keywords. independent set; Merrifield-Simmons index; unicyclic graph; cut vertices; upper bound; extremal graph
Received: 16 October 2012; Accepted: 13 September 2013
Communicated by Dragan Stevanović
Research supported in part by NSF of the Higher Education Institutions of Jiangsu Province (No. 12KJB110001), NNSF of China (No.s 11201227, 11171273), SRF of HIT (No. HGA1010) and Qing Lan Project of Jiangsu Province, PR China.
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In the current paper, we characterize the maximal unicyclic graph w.r.t. $i(G)$ within all unicyclic graphs with given order and number of cut vertices. As a consequence, we determine the connected graph with at least one cycle, given number of cut vertices and the maximal Merrifield-Simmons index.

Before proceeding, we introduce some notation and terminology. For a vertex $v \in V(G)$, we use $N_G(v)$ to denote the set of neighbors of v, and let $N_G[v] = N_G(v) \cup \{v\}$. For the sake of brevity, we write $[v]$ instead of $N_G[v]$. The degree of v in G, denoted by $d(v)$, is the number of its neighbors. A vertex v is said to be a *branched vertex*, if $d(v) \geq 3$. A vertex v is said to be a *pendent vertex*, if $d(v) = 1$. A *cut vertex* of a graph is any vertex that when removed increases the number of connected components of this graph. If S is a subset of $V(G)$, we use $G - S$ to denote the subgraph of G obtained by deleting the vertices in S and the edges incident with them. Suppose that $P = v_1v_2\cdots v_s$ $(s \geq 2)$ is a path lying within a graph G. If $d(v_1) \geq 3$, $d(v_s) = 1$ and $d(v_j) = 2(1 < j < s)$, then we call P a *pendant path* of G.

Denote, as usual, by S_n and C_n the star and cycle on n vertices, respectively. Let S_n^l denote the graph obtained from the cycle C_l by attaching $n - l$ pendent vertices to any one vertex of it. Let $P_{n,t}$ be the tree obtained by attaching $t - 2$ pendent edges to the second vertex (natural ordering) of the path P_{n-t+2}.

Let $\mathcal{U}_{n,k}$ denote the set of connected unicyclic graphs with n vertices and k cut vertices, and $\mathcal{U}_{n,k}^l$ denote a subset of $\mathcal{U}_{n,k}$, in which every graph has girth l. If $k = 0$, then $\mathcal{U}_{n,k}$ contains a single element C_n. So we will assume that $k \geq 1$. Obviously, we have $k \leq n - 3$, since $n \geq l + k \geq k + 3$.

For any graph G in $\mathcal{U}_{n,k}$, we let $P(G)$ be the set of pendent vertices in G and $C(G)$ be the set of cut vertices in G. For any graph G in $\mathcal{U}_{n,k}^l$, we let $OC(G)$ be the number of cut vertices in G lying outside of the unique cycle C_l.

2. Preliminary results

The following lemmas are needed in the proof of main results.

Lemma 2.1 ([3]). *Let G be a graph with m components $G_1, G_2, \ldots, G_m$. Then*

$$i(G) = \prod_{i=1}^{m} i(G_i).$$

Lemma 2.2 ([3]). *Let G be a graph, u be a vertex and vw be an edge of G. Then*
(i) $i(G) = i(G - u) + i(G - [u])$;
(ii) $i(G) = i(G - vw) - i(G - \{[v] \cup [w]\})$.

Lemma 2.2 (ii) implies the following lemma.

Lemma 2.3. *Let G_1 and G_2 be two graphs. If G_1 can be obtained from G_2 by deleting some edges, then $i(G_2) < i(G_1)$.*

Recall that $F_n = F_{n-1} + F_{n-2}$ with initial conditions $F_0 = F_1 = 1$. Thus,

$$i(P_n) = F_{n+1} = \frac{\sqrt{5}}{5}\left[\left(\frac{1+\sqrt{5}}{2}\right)^{n+2} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+2}\right].$$

Prodinger and Tichy [13] gave an upper bound for the $i(G)$ of trees, and later Lin and Lin [6] characterized the unique tree attaining this upper bound. Their results are summarized as follows:

Lemma 2.4. *Let T be a tree on n vertices. Then $i(T) \leq 2^{n-1} + 1$, with the equality if and only if $T \cong S_n$.*

Yu and Lv proved the following result concerning the $i(G)$ of trees with k pendent vertices.

Lemma 2.5 ([16]). *Let T be a tree with n vertices and k pendent vertices. Then*
(i) $i(T) \leq 2^{k-1}F_{n-k+1} + F_{n-k}$, with equality if and only if $T \cong P_{n,k}$;
(ii) $i(P_{n,k}) > i(P_{n,k-1})$.

By means of Lemma 2.5, we obtain the following result.

Lemma 2.6. *Let T be a tree, not isomorphic to S_n, with n vertices. Then $i(T) \leq 3 \cdot 2^{n-3} + 2$, with equality if and only if $T \cong P_{n,n-2}$.*

Proof. Let T be a tree, not isomorphic to S_n, with n vertices. Then T has $k' \leq n-2$ pendent vertices. By Lemma 2.5, we have

$$i(T) \leq i(P_{n,k'}) \leq i(P_{n,n-2}).$$

This completes the proof. □

Lemma 2.7 ([12]). *Let X, Y and Z be three pairwise disjoint connected graphs with $|X|, |Y|, |Z| \geq 2$. Suppose that u, v are two vertices of Z, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from X, Y and Z by identifying v with v' and u with u', respectively. Also, we let G_1 be the graph obtained from X, Y and Z by identifying vertices u, v', u' and G_2 be the graph obtained from X, Y and Z by identifying vertices v, v', u'; see Fig. 1 for instance. Then*

$$i(G_1) > i(G) \text{ or } i(G_2) > i(G).$$

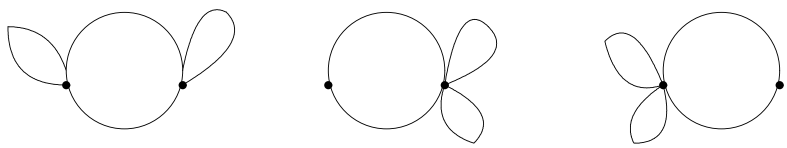


Fig. 1. The graphs G, G_1 and G_2.

We call the graph transformation from G to G_1 (or G_2) **Operation I**. From Lemma 2.7, we know that Operation I increases the $i(G)$ of graphs under consideration.

3. Unicyclic graph with given number of cut vertices and the maximal Merrifield-Simmons index

Lemma 2.5 implies the following result.

Proposition 3.1. *Let T be a tree with n vertices and k cut vertices. Then $i(T) \leq 2^{n-k-1}F_{k+1} + F_k$, with equality if and only if $T \cong P_{n,n-k}$.*

Proposition 3.2. *Let T be a tree with n vertices and at least k cut vertices. Then $i(T) \leq 2^{n-k-1}F_{k+1} + F_k$, with equality if and only if $T \cong P_{n,n-k}$.*

Proof. For each $1 \leq k \leq n-3$,

$$\begin{aligned} i(P_{n,n-k}) - i(P_{n,n-k-1}) &= (2^{n-k-1}F_{k+1} + F_k) - (2^{n-k-2}F_{k+2} + F_{k+1}) \\ &= 2^{n-k-2}(2F_{k+1} - F_{k+2}) - (F_{k+1} - F_k) \\ &= 2^{n-k-2}F_{k-1} - F_{k-1} > 0. \end{aligned}$$

So, for any $1 \leq k < k' \leq n-2$,

$$i(P_{n,n-k}) > i(P_{n,n-k-1}) > \ldots > i(P_{n,n-k'}). \quad (1)$$

Suppose that T is a tree of n vertices and $k'(\geq k)$ cut vertices. Then by Proposition 3.1 and the above Ineq. (1), we have

$$i(P_{n,n-k}) \geq i(P_{n,n-k'}) \geq i(T),$$

with equality if and only if $k = k'$ and $T \cong P_{n,n-k'}$, i.e., $T \cong P_{n,n-k}$.

This completes the proof. □

Lemma 3.3. *For any* $3 \le l \le n-1$, $i(S_n^l) \le i(S_n^3)$, *with equality if and only if* $l = 3$.

Proof. Let u be a vertex of degree 2, adjacent to the vertex of degree $n-l+2$ in S_n^l. Write $S_n^l - u = T_{n-1}$. Then we have

$$i(S_n^l) = i(T_{n-1}) + i(P_{l-3} \cup (n-l)K_1)$$

and

$$i(S_n^3) = i(S_{n-1}) + i((n-3)K_1).$$

By Lemma 2.4, $i(T_{n-1}) \le i(S_{n-1})$ with equality if and only if $T_{n-1} \cong S_{n-1}$, i.e., $l = 3$. Note that $P_{l-3} \cup (n-l)K_1$ contains $(n-3)K_1$ as a proper spanning subgraph if $l \ge 4$. By Lemma 2.3, $i(P_{l-3} \cup (n-l)K_1) \le i((n-3)K_1)$ with equality if and only if $l = 3$. Consequently, $i(S_n^l) \le i(S_n^3)$, with equality if and only if $l = 3$. This completes the proof. □

Let $C_3(n, k)$ be a unicyclic graph constructed as follows.

- For $k = 1$, we let $Q_3(n, 1) = S_n^3$.
- For $k \ge 2$, we let $C_3(n, k)$ be the graph obtained by attaching a path of length $k-1$ to a vertex of degree 2 in $C_3(n-k+1, 1)$.

See Fig. 2 for instance.

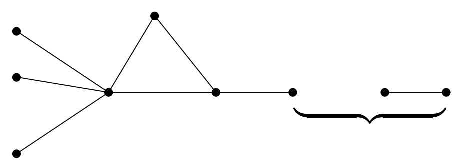


Fig. 2. The graph $C_3(n, k)$.

According to the above definition for $C_3(n, k)$, we have

$$i(C_3(n, k)) = \begin{cases} 3 \cdot 2^{n-3} + 1, & k = 1; \\ 2^{n-k-2}F_{k+2} + F_k, & k \ge 2. \end{cases}$$

Before proceeding, we prove the following two lemmas.

Lemma 3.4. *Let* G *be a unicyclic graph in* $\mathcal{U}_{n,k}^l$. *If* $|OC(G)| = 0$, *then* $i(G) \le i(C_3(n, k))$, *with equality if and only if* $G \cong C_3(n, k)$.

Proof. If $k = 1$, then $G \cong S_n^l$. Thus, by Lemma 3.3, we have

$$i(G) \le i(S_n^3) = i(C_3(n, 1))$$

with equality if and only if $l = 3$, that is, $G \cong C_3(n, 1)$.

So, we may assume that $k \ge 2$. If $k = 2$, then G is the graph $G_{s,t}(l)$, obtained by attaching s and t pendent edges to any two vertices of the cycle C_l, where $s + t + l = n$. If $\min\{s, t\} \ge 2$, then by Lemma 2.6, we have $i(G) = i(G_{s,t}(l)) < i(G_{1,s+t-1}(l))$. Thus, $i(G) = i(G_{s,t}(l)) \le i(G_{1,s+t-1}(l))$.

In view of Lemmas 2.1 and 2.2(i),

$$i(C_3(n, 2)) = i(S_{n-1}^3) + i(S_{n-2})$$

and

$$i(G_{1,s+t-1}(l)) = i(S^l_{n-1}) + i(T_{n-2}),$$

where T_{n-2} is a tree of order $n-2$.

Evidently, $i(T_{n-2}) \le i(S_{n-2})$, with equality if and only if $T_{n-2} \cong S_{n-2}$, and $i(S^l_{n-1}) \le i(S^3_{n-1})$, with equality if and only if $l = 3$. So

$$i(G) \le i(G_{1,s+t-1}(l)) \le i(C_3(n, 2))$$

with equality if and only if $T_{n-2} \cong S_{n-2}$, $l = 3$ and $G \cong G_{1,s+t-1}(l)$, that is, $G \cong C_3(n, 2)$, as claimed.

So, we may assume that $k \ge 3$.

Since $|OC(G)| = 0$, for $k \ge 3$, we must have $G \not\cong C_3(n, k)$. By Lemmas 2.1 and 2.2(i),

$$i(C_3(n, k)) = i(P_{n-1,n-k-1}) + 2^{n-k-2} i(P_{k-1})$$

and

$$i(G) = i(G - v_0) + i(G - [v_0]).$$

Notice that $G - v_0$ is a tree of order $n-1$ and at least k cut vertices; then, by Proposition 3.2, we have

$$i(G - v_0) \le i(P_{n-1,n-k-1}),$$

with equality if and only if $G - v_0 \cong P_{n-1,n-k-1}$.

By our assumption that $|OC(G)| = 0$, we know that all k cut vertices of G lie on C_l. If $k = 2$, then $G - [v_0]$ is an empty graph of $n-3$ isolated vertices. If $k \ge 3$, $G - [v_0]$ is a forest composed of x $(0 \le x \le n-k-3)$ isolated vertices and a nontrivial component of $n-x-3$ vertices and at least $k-2$ cut vertices. Also, the largest component of $G - [v_0]$ contains the path P_k as a subgraph. Thus, $G - [v_0]$ contains $(n-k-2)K_1 \cup P_{k-1}$ as a spanning subgraph. Then by Lemma 2.3,

$$\begin{aligned} i(G - [v_0]) &\le i((n-k-2)K_1 \cup P_{k-1}) \\ &= 2^{n-k-2} i(P_{k-1}), \end{aligned}$$

with equality if and only if $k = 2$.

So, $i(G) \le i(C_3(n, k))$, with equality if and only if $G \cong C_3(n, k)$ $(k = 2)$. □

Lemma 3.5. *Let G be a graph in $\mathcal{U}^l_{n,k}$. If $|OC(G)| \ge 1$ and there exists a pendent path of length ≥ 2 in G, then $i(G) \le i(C_3(n, k))$, with the equality if and only if $G \cong C_3(n, k)$.*

Proof. Obviously, $V(G) \setminus V(C_l) \ne \emptyset$. For any given vertex $x \in V(G) \setminus V(C_l)$, we let $d_G(x, C_l) = \min\{d_G(x, y) | y \in V(C_l)\}$. By the assumption that $|OC(G)| \ge 1$, we have $k \ge 2$.

We shall complete the proof by induction on $|OC(G)|$.

We first check the validity of the lemma for $|OC(G)| = 1$. Let v be the unique cut vertex, not belonging to C_l, in G. Since $|OC(G)| = 1$, we have $d_G(v, C_l) = 1$. Also, $d(v) = 2$, for otherwise, G has no pendent path of length ≥ 2, a contradiction. Let u be the pendent vertex adjacent to v. Clearly, $|OC(G-u)| = |OC(G-[u])| = 0$, $|C(G-u)| = k-1$ and $|C(G-[u])| = k-2$ or $k-1$.

If $k = 2$, then $|C(G-u)| = 1$ and $|C(G-[u])| = 0$ or 1. Thus, $G - u \cong S^l_{n-1}$ and $G - [u] \cong C_{n-2}$ or S^l_{n-2}. By Lemma 2.7, $i(S^l_{n-1}) \le i(S^3_{n-1})$. Also, $i(C_{n-2}) < i(P_{n-2}) < i(S_{n-2})$ and $i(S^l_{n-2}) \le i(S^3_{n-2}) < i(S_{n-2})$ by Lemmas 2.3, 2.4 and 2.7. Thus,

$$\begin{aligned} i(G) &= i(G-u) + i(G-[u]) \\ &< i(S^3_{n-1}) + i(S_{n-2}) \\ &= i(C_3(n, 2)), \end{aligned}$$

as claimed.

Assume now that $k \ge 3$. , Since $d_G(u, C_l) = 2$, $|C(G-u)| = k-1$ and $|C(G-[u])| = k-2$ or $k-1$, we have $G - u \in \mathcal{U}^l_{n-1,k-1}$ and $G - [u] \in \mathcal{U}^l_{n-2,k-2}$ or $\mathcal{U}^l_{n-2,k-1}$.

Note that $|OC(G-u)| = |OC(G-[u])| = 0$; then by Lemma 3.4,

$$i(G-u) \le i(C_3(n-1, k-1)), \tag{2}$$

with the equality if and only if $G-u \cong C_3(n-1, k-1)$.

Also, by Lemma 3.4,

$$i(G-[u]) \le i(C_3(n-2, k-2)), \tag{3}$$

with the equality if and only if $G-[u] \cong C_3(n-2, k-2)$, or

$$i(G-[u]) \le i(C_3(n-2, k-1)), \tag{4}$$

with the equality if and only if $G-[u] \cong C_3(n-2, k-1)$.

We shall prove that for $k \ge 3$,

$$i(C_3(n-2, k-1)) < i(C_3(n-2, k-2)). \tag{5}$$

The above Ineq. (5) is equivalent to

$$2^{n-k-3}F_{k+1} + 2F_{k-2} < 2^{n-k-2}F_k + 2F_{k-3}.$$
$$\Leftrightarrow 2^{n-k-3}F_{k+1} - 2^{n-k-2}F_k < 2F_{k-3} - 2F_{k-2}.$$
$$\Leftrightarrow 2^{n-k-3}F_{k-2} > 2F_{k-4}.$$

The last inequality holds due to the fact that $n-k-3 \ge 0$.

By Ineqs. (2)-(5), for $k \ge 4$, we obtain

$$i(G) \le i(C_3(n-1, k-1)) + i(C_3(n-2, k-2)) = i(C_3(n, k))$$

with the equality if and only if $G-u \cong C_3(n-1, k-1)$ and $G-[u] \cong C_3(n-2, k-2)$, i.e., $G \cong C_3(n, k)$.

If $k = 3$, then $G \ncong C_3(n, 3)$, as $|OC(G)| = s \ge 1$. Since $C_3(n-2, 1) = S^3_{n-2}$ contains $P_{n-2,n-4}$ as a proper spanning subgraph, $i(C_3(n-2, 1)) < i(P_{n-2,n-4})$ by Lemma 2.3. By Ineqs. (2)-(5), for $k = 3$, we have

$$\begin{aligned} i(G) &\le i(C_3(n-1, 2)) + i(C_3(n-2, 1)) \\ &< i(C_3(n-1, 2)) + i(P_{n-2,n-4}) \\ &= i(C_3(n, 3)), \end{aligned}$$

as claimed.

Suppose now that $|OC(G)| = s \ge 2$ and the statement of lemma is true for smaller values of $|OC(G)|$. Then $k \ge s+1 \ge 3$.

Let P be a pendent path of length ≥ 2 in G with pendent vertex u and $N(u) = v$. By the definition of pendent path, we have $d(v) = 2$. Then we have $|OC(G-u)| = s-1$ and $|OC(G-[u])| = |OC(G-u-v)| = s-2$ or $s-1$, $|C(G-u)| = k-1$ and $|C(G-[u])| = k-2$ or $k-1$.

Note that $G-u \in \mathcal{U}^l_{n-1,k-1}$ and $G-[u] \in \mathcal{U}^l_{n-2,k-1}$ or $\mathcal{U}^l_{n-2,k-2}$; thus by the induction hypothesis, we have

$$i(G-u) \le i(C_3(n-1, k-1))$$

with the equality if and only if $G-u \cong C_3(n-1, k-1)$.

Also, by Lemma 3.4 (when $|OC(G-[u])| = s-2 = 0$) or by the induction assumption (when $|OC(G-[u])| = s-2 \ge 1$), we have: if $C(G-[u]) = k-2$, then

$$i(G-[u]) \le i(C_3(n-2, k-2))$$

with the equality if and only if $G-[u] \cong C_3(n-2, k-2)$, and if $C(G-[u]) = k-1$, then

$$i(G-[u]) \le i(C_3(n-2, k-1))$$

with the equality if and only if $G-[u] \cong C_3(n-2, k-1)$.

Now, by the same way as used in the case of $|OC(G)| = 1$, we can obtain the desired result.

This completes the proof. □

A graph is called a *sun graph* if it can be obtained by attaching a pendent edge to each vertex of a cycle. A *damaged sun graph* is a graph obtained from sun graph by deleting part of its pendent edges. Denoted by $\mathcal{DSG}(N, l)$ the set of damaged sun graphs having N vertices and a cycle of length l. Obviously, we have $l + 1 \leq N \leq 2l - 1$.

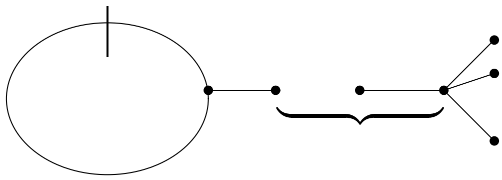
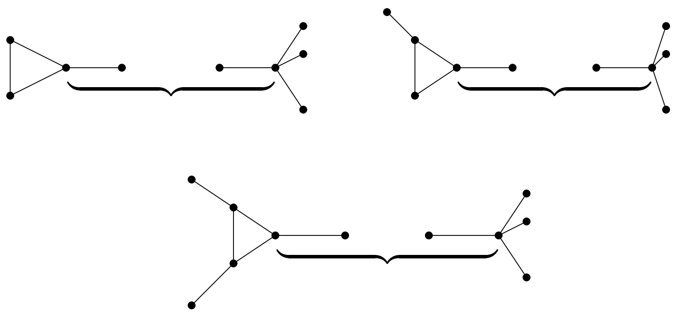


Fig. 3. The graph occurred in the proof of Theorem 1.



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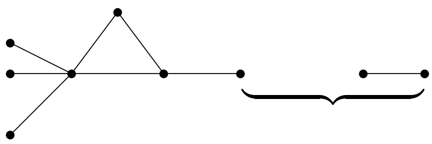

Fig. 5. The graph $H_3(n, k)$ occurred in the proof of Theorem 1.

Now, we are in a position to state and prove our maim theorem.

Theorem 3.6. *Let G be a graph in $\mathcal{U}_{n,k}$. Then $i(G) \leq i(C_3(n, k))$, with the equality if and only if $G \cong C_3(n, k)$.*

Proof. Let G_{max} be a graph chosen from $\mathcal{U}^l_{n,k}$ for some $l\,(3 \leq l \leq n - k)$ such that $i(G_{max}) \geq i(G)$ for any $G \in \mathcal{U}_{n,k} \setminus \{G_{max}\}$. Next, we shall prove that $G_{max} \cong C_3(n, k)$.

By contradiction. Suppose that $G_{max} \ncong C_3(n, k)$.

If $|OC(G_{max})| = 0$, then $i(G_{max}) < i(C_3(n, k))$ by Lemma 3.4, a contradiction to our choice of G_{max}. So we may suppose that $|OC(G_{max})| \geq 1$.

We first prove the following two claims.

Claim 3.1. *G_{max} has exactly one branched vertex lying outside C_l. Also, all neighbors but one of this branched vertex are pendent vertices.*

Proof. If G_{max} has no branched vertices lying outside C_l, then G_{max} must contain a pendent path of length ≥ 2, as $|OC(G_{max})| \geq 1$. Then by Lemma 3.5, $i(G_{max}) < i(C_3(n, k))$, a contradiction to our choice of G_{max}. So G_{max} has at least one branched vertex lying outside C_l.

Suppose that G_{max} has two branched vertices lying outside C_l. Then we can employ Operation I on G_{max} and obtain a new graph G' such that $G' \in \mathcal{U}^l_{n,k}$. But, $i(G_{max}) < i(G')$ by Lemma 2.6, a contradiction to the maximality of G_{max}. Consequently, G_{max} has exactly one branched vertex lying outside C_l.

Suppose that the unique branched vertex, lying outside C_l, has two neighbors of degree ≥ 2. Then G_{max} must contain a pendent path of length ≥ 2, as G_{max} has exactly one branched vertex lying outside C_l. As above, we can obtain a contradiction. This proves the claim. □

Claim 3.2. *Each vertex on the cycle C_l of G_{max} is either of degree 2 or of degree 3. Also, all vertices but one, of degree 3, on the cycle C_l are adjacent to a pendent vertex.*

Proof. Suppose to the contrary that G_{max} has a branched vertex, of degree ≥ 4, lying along C_l. By Claim 3.1, G_{max} has a branched vertex lying outside C_l. Then we can employ Operation I on G_{max} and obtain a new graph G'' such that $G'' \in \mathcal{U}^l_{n,k}$. But then, $i(G_{max}) < i(G'')$ by Lemma 2.6, a contradiction to the maximality of G_{max}. Thus, each vertex on the cycle C_l of G_{max} is either of degree 2 or of degree 3.

Assume that there are two branched vertices on the cycle C_l whose all neighbors are not pendent vertices. By Claim 3.1, G_{max} has exactly one branched vertex lying outside C_l. Thus, G_{max} must contain a pendent path of length ≥ 2. Then by Lemma 3.5, $i(G_{max}) < i(C_3(n, k))$, a contradiction to the maximality of G_{max}. This proves the claim. □

By Claims 3.1 and 3.2, G_{max} must be isomorphic to the graph as shown in Fig. 3.

If $l = 3$, then G_{max} must be isomorphic to one of the graphs (a), (b) and (c), as shown in Fig. 4.

• G_{max} is the graph (a). By our assumption that $|OC(G_{max})| \geq 1$, we have $k \geq 2$. Also, we have $n - k \geq 3$, since $n \geq l + k$. Thus,

$$\begin{aligned} i(G_{max}) &= i(P_{n-1,n-k-1}) + i(P_{n-3,n-k-1}) \\ &= 2^{n-k-2}F_{k+1} + F_k + 2^{n-k-2}F_{k-1} + F_{k-2} \\ &< 2^{n-k-2}F_{k+2} + 2F_{k-1} \\ &= i(C_3(n, k)), \end{aligned}$$

a contradiction to the maximality of G_{max}.

• G_{max} is the graph (b). Since $|OC(G_{max})| \geq 1$, we have $k \geq 3$. Also, we have $n - k \geq 3$.
Thus,

$$\begin{aligned} i(G_{max}) &= i(P_{n-1,n-k-1}) + 2i(P_{n-4,n-k-1}) \\ &= 2^{n-k-2}F_{k+1} + F_k + 2(2^{n-k-2}F_{k-2} + F_{k-3}) \\ &< 2^{n-k-2}F_{k+2} + 2F_{k-1} \\ &= i(C_3(n, k)), \end{aligned}$$

a contradiction to the maximality of G_{max}.

• G_{max} is the graph (c). Since $|OC(G_{max})| \geq 1$, we have $k \geq 4$. Also, we have $n - k \geq 4$ (see Fig. 4).
Thus,

$$\begin{aligned} i(G_{max}) &= 2i(P_{n-2,n-k-1}) + 2i(P_{n-5,n-k-1}) \\ &= 2(2^{n-k-2}F_k + F_{k-1}) + 2(2^{n-k-2}F_{k-3} + F_{k-4}) \\ &< 2^{n-k-2}F_{k+2} + 2F_{k-1} \\ &= i(C_3(n, k)), \end{aligned}$$

a contradiction to the maximality of G_{max}.

Now, we assume that $l \geq 4$.

Let w be the branched vertex of G_{max} such that w lies along C_l and the unique neighbor, not belonging to C_l, of w is of degree ≥ 2.

Since $l \geq 4$, there is always a vertex $v \in V(C_l)$ such that $d_{G_{max}}(v, w) \geq 2$. Let $A = \{v \in V(C_l) | d_{G_{max}}(v, w) \geq 2\}$. Consider the following two cases.

Case 3.1. *There exists a vertex v in A such that $d(v) = 3$.*

By Claim 3.2, v has a pendent vertex as one of its neighbors in G_{max}. Let $u'v'$ be a pendent edge in $C_3(n, k)$ such that $d(u') = 1$ and $d(v') = 3$ (note that when $n = k + 3$ or $k = 3$, the way of choosing vertices v' and u' in $C_3(n, k)$ is not unique). By Lemmas 2.1 and 2.2(i), we obtain

$$\begin{aligned} i(C_3(n, k)) &= i(C_3(n, k) - v') + i(C_3(n, k) - [v']) \\ &= 2i(P_{n-2, n-k-1}) + 2^{n-k-2} i(P_{k-2}) \end{aligned}$$

and

$$\begin{aligned} i(G_{max}) &= i(G_{max} - v) + i(G_{max} - [v]) \\ &= 2i(T_1) + i(G_{max} - [v]), \end{aligned}$$

where T_1 is a subtree of $G_{max} - v$ with $n - 2$ vertices.

Obviously, T_1 has at least $k - 1$ cut vertices. Let $G_{max} - [v] = xK_1 \cup T_2$ $(0 \leq x \leq 2, x + n' = n - 4)$, where T_2 is the largest component of $G_{max} - [v]$ with n' vertices. Then T_2 has at least $k - 3$ cut vertices.

By Proposition 3.2, we obtain

$$i(T_1) \leq i(P_{n-2, (n-2)-(k-1)})$$

and

$$i(T_2) \leq i(P_{n', n'-(k-3)}).$$

Thus,

$$\begin{aligned} i(G_{max} - [v]) &= i(xK_1 \cup T_2) \\ &= 2^x i(T_2) \\ &\leq 2^x i(P_{n', n'-(k-3)}) \\ &= i(xK_1 \cup P_{n', n'-(k-3)}). \end{aligned}$$

Note that $P_{n', n'-(k-3)}$ contains $(n' - k + 1)K_1 \cup P_{k-1}$ as a proper spanning subgraph. Thus, $xK_1 \cup P_{n', n'-(k-3)}$ contains $(n - k - 2)K_1 \cup P_{k-2}$ as a proper spanning subgraph. By Lemma 2.3, we have

$$\begin{aligned} i(G_{max} - [v]) &\leq i(xK_1 \cup P_{n', n'-(k-3)}) \\ &< i((n - k - 2)K_1 \cup P_{k-2}) \\ &= 2^{n-k-2} i(P_{k-2}). \end{aligned}$$

So, $i(G_{max}) < i(C_3(n, k))$, a contradiction to our choice of G_{max}.

Case 3.2. *For each vertex v in A, we have $d(v) = 2$.*

Let v be a vertex in A. Then $G_{max} - v$ is a tree having $n - 1$ vertices and at least k cut vertices. Let $G_{max} - [v] = xK_1 \cup T_0$ $(0 \leq x \leq 2, x + n' = n - 3)$, where T_0 is the largest component of $G_{max} - [v]$ with n' vertices. Evidently, T_0 has at least $k - 2$ cut vertices.

We shall prove that $i(G_{max}) < i(H_3(n, k))$ in the following, see Fig. 5 for $H_3(n, k)$.

By Lemmas 2.1 and 2.2(i), we obtain

$$i(H_3(n, k)) = i(P_{n-1, n-k-1}) + 2^{n-k-2} i(P_{k-1})$$

and

$$\begin{aligned} i(G_{max}) &= i(G_{max} - v) + i(G_{max} - [v]) \\ &= i(G_{max} - v) + i(xK_1 \cup T_0). \end{aligned}$$

By Proposition 3.2, we obtain

$$i(G_{max} - v) \leq i(P_{n-1,(n-1)-k})$$

and

$$i(T_0) \leq i(P_{n',n'-(k-2)}).$$

Thus,

$$\begin{aligned} i(G_{max} - [v]) &= i(xK_1 \cup T_0) \\ &= 2^x i(T_0) \\ &\leq 2^x i(P_{n',n'-(k-2)}) \\ &= i(xK_1 \cup P_{n',n'-(k-2)}). \end{aligned}$$

Note that $P_{n',n'-(k-2)}$ contains $(n' - k + 1)K_1 \cup P_{k-1}$ as a proper spanning subgraph. Thus, $xK_1 \cup P_{n',n'-(k-2)}$ contains $(n - k - 2)K_1 \cup P_{k-1}$ as a proper spanning subgraph. By Lemma 2.3, we have

$$\begin{aligned} i(G_{max} - [v]) &\leq i(xK_1 \cup P_{n',n'-(k-2)}) \\ &< i((n - k - 2)K_1 \cup P_{k-1}) \\ &= 2^{n-k-2} i(P_{k-1}). \end{aligned}$$

So, $i(G_{max}) < i(H_3(n, k))$, a contradiction to our choice of G_{max}.

By discussions above, we conclude that $G_{max} \cong C_3(n, k)$, as claimed. □

4. Connected graph with at least one cycle, given number of cut vertices and the maximal Merrifield-Simmons index

Let $\mathcal{U}_{n,k^+}$ be the set of unicyclic graphs of order n and at least k cut vertices. According to Theorem 3.6, we have the following consequence.

Corollary 4.1. *Let G be a graph in $\mathcal{U}_{n,k^+}$. Then $i(G) \leq i(C_3(n, k))$, with the equality if and only if $G \cong C_3(n, k)$.*

Proof. Let G be a graph in $\mathcal{U}_{n,k'}$ $(1 \leq k' \leq n - 3)$. Then by Theorem 3.6, we have $i(G) \leq i(C_3(n, k'))$, with the equality if and only if $G \cong C_3(n, k')$. We need only to prove that if $k' \geq k$, then $i(C_3(n, k')) \leq i(C_3(n, k))$.

If $k = 1$, the result is obvious. So we may suppose that $k \geq 2$. Then $k' \geq k \geq 2$. For $1 \leq k \leq n - 4$, we have

$$\begin{aligned} i(C_3(n, k + 1)) &= 2^{n-(k+1)-2} F_{(k+1)+2} + 2F_{(k+1)-1} \\ &= 2^{n-k-3} F_{k+3} + 2F_k \\ &< 2^{n-k-2} F_{k+2} + 2F_{k-1} \\ &= i(C_3(n, k)). \end{aligned}$$

Thus, for any $1 \leq k < k' \leq n - 3$, we have

$$i(C_3(n, k')) < \cdots < i(C_3(n, k + 1)) < i(C_3(n, k)),$$

as claimed. □

Theorem 4.2. *Let G be a connected graph, not isomorphic to a tree, of n vertices and k cut vertices. Then $i(G) \leq i(C_3(n, k))$, with the equality if and only if $G \cong C_3(n, k)$.*

Proof. If G is a graph in $\mathcal{U}_{n,k}$, then by Theorem 3.6, we have completed the proof. Now, we may assume that G is a connected graph of n vertices, k cut vertices and at least two cycles.

We can always obtain a connected unicyclic spanning subgraph of G by deleting edges along some cycles of G. Let $USS(G)$ denote a connected unicyclic spanning subgraph of G. Note that $USS(G)$ is a connected unicyclic graph of n vertices and at least k cut vertices. Thus, by Lemma 2.3 and Corollary 4.1, we have

$$i(G) < i(USS(G)) \leq i(C_3(n, k)),$$

as claimed. □

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