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ORDERING UNICYCLIC GRAPHS WITH RESPECT TO F-INDEX

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Abstract. F-index of a graph is the sum of the cube of the degrees of the vertices. Thus, for a graph G with vertex set $V(G)$ and edge set $E(G)$, the degree based topological index F-index is defined as

$$F(G) = \sum_{v\in V(G)} d_G(v)^3 = \sum_{uv\in E(G)} [d_G(u)^2 + d_G(v)^2],$$

where $d_G(v)$ denotes the degree of the vertex v. In this paper, we investigate the F-indices of unicyclic graphs by introducing some transformation, and characterize the unicyclic graphs with the first five largest F-indices and the unicyclic graphs with the first two smallest F-indices, respectively.

1. Introduction

A topological index is a numerical value associated with the graph representation of a molecule for correlation of the chemical structure of a molecule with various physical properties, chemical reactivity, or biological activity. Let G be a simple graph. As usual, we denote the vertex set of G as $V(G)$ and the edge set of G as $E(G)$. The first Zagreb index, introduced in 1972 [13], is one of the oldest topological indices. It is defined as

$$M_1(G) = \sum_{v\in V(G)} d^2(v) = \sum_{uv\in E(G)} [d(u) + d(v)].$$

In the same study, where the first Zagreb index was introduced by Gutman and Trinajstić [14], it was shown that the sum of squares and the sum of the cubes of the vertex degrees of the underlying molecular graph influences the total π-electron energy E. Zagreb indices are the first degree based topological indices, those were initially intended for the study of total π- electron energy [12] . The sum of squares of the vertex degrees, known as the

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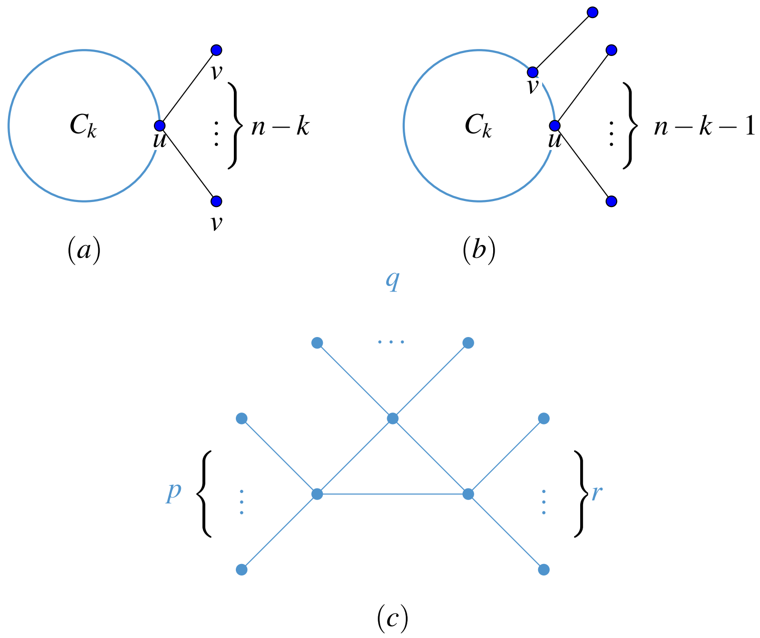

Figure 1. (a) $G_{k,1}^{(n)}$; (b) $G_{k,2}^{(n)}$; (c) $S_{p,q,r}$.

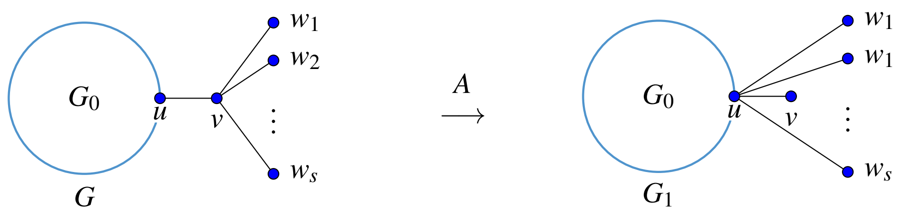

Figure 2. Transformation A.

first Zagreb index, has been studied in hundreds of research papers, but the sum of cubes of the vertex degrees has remained unstudied for a long time by scholars doing research on degree–based topological indices. Furtula and Gutman, restudied this index recently and named it as "forgotten" topological index, or F-index [10]. Thus, F-index is defined as

$$F(G) = \sum_{v \in V(G)} d_G(v)^3 = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2].$$

A leaf is a vertex of degree one, pendant edges are edges incident on a leaf, and a stem is a vertex adjacent to at least one leaf. P_n, C_n and $K_{1,n-1}$ denote paths, cycles, and stars with n vertices respectively. $\mathscr{U}_n$ and $\mathscr{U}_n^k$ denote the set of all unicyclic graphs with n vertices and the set of all unicyclic graphs with n vertices and cycles of length k respectively. We

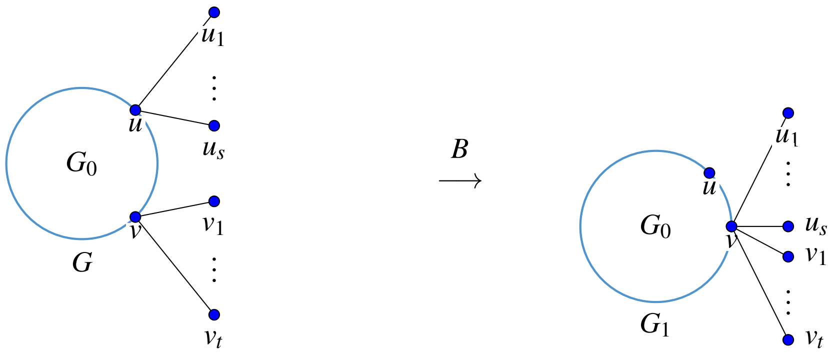

Figure 3. Transformation B.

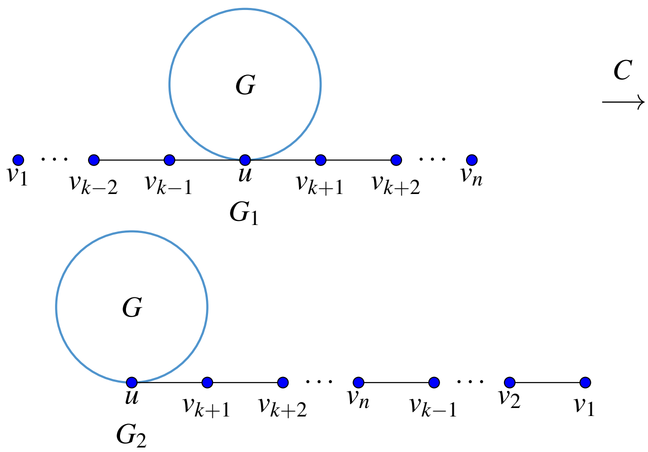

Figure 4. Transformation C.

denote the unicyclic graph constructed by identifying the center of $K_{1,n-k-1}$ with a vertex of C_k as $G^{(n)}_{k,1}$ as shown in Figure 1(a). $G^{(n)}_{k,2}$ is the unicyclic graph constructed by identifying the center of $K_{1,n-k-2}$ with the vertex u of the cycle C_k and identifying a vertex of K_2 with a adjacent vertex of u as shown in Figure 1(b). We denote by $S_{p,q,r}$ the unicyclic graph constructed by identifying the centers of $K_{1,p}, K_{1,q}$ and $K_{1,r}$ to the vertices of $C_3, (p,q,r \geq 0, p+q+r = n-3)$ as shown in Figure 1(c).

The ordering of unicyclic graphs with respect to Zagreb indices was studied by Xia [9]. Unicyclic graphs with the first three smallest and largest first general Zagreb indices were studied by Zhang [20]. A unified approach to extremal Zagreb indices for trees, unicyclic graphs, and bicyclic graphs was proposed by Deng [7]. Extremal trees with respect to the F-index was found by Abdo et al. [1]. F-index of some graph operations has been

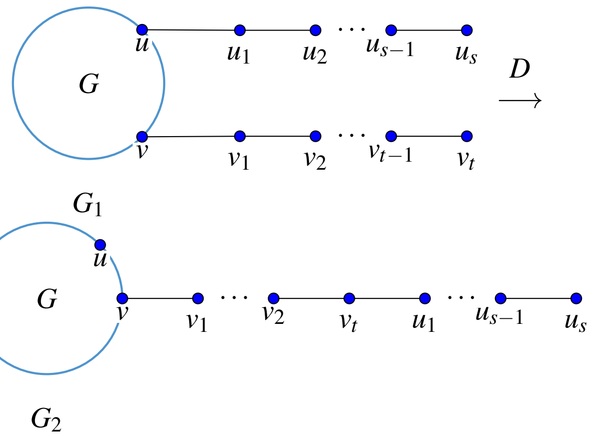

Figure 5. Transformation D.

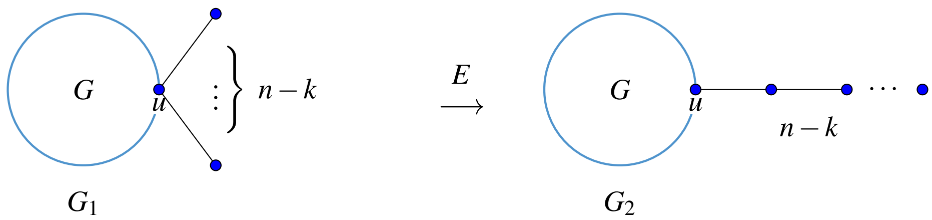

Figure 6. Transformation E.

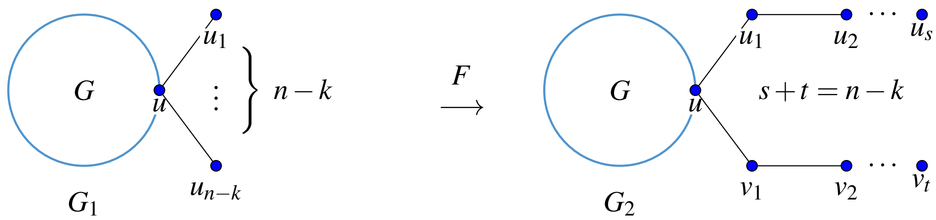

Figure 7. Transformation F.

studied by De et al. [6]. Some lower and upper bounds for F-index are found in [5, 8]. Recently, extremal F-indices for bicyclic graphs with k pendant vertices and extremal F-index of a graph with k cut edges was found by Amin et al. [3, 4]. Topological indices for new classes of benes network, algebraic invariants of edge ideals of some bristled circulant graphs and *ev* and *ve*-degree based topological indices of silicon carbides was found in [15, 18, 19]. Applications of symmetric conic domains to a subclass of q-starlike functions

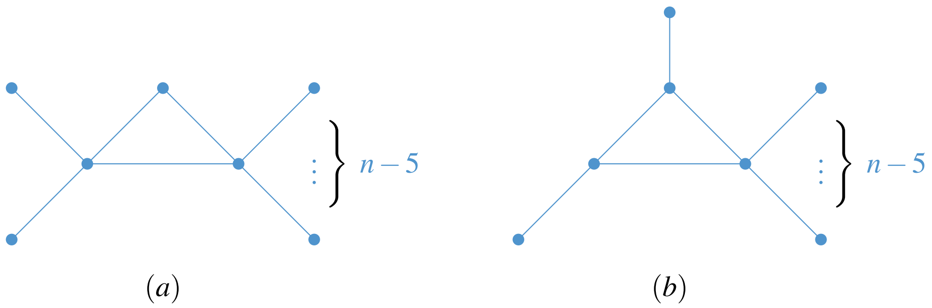

Figure 8. (a) $G_{3,3}^{(n)}$; (b) $G_{3,3}^{(n)}$.

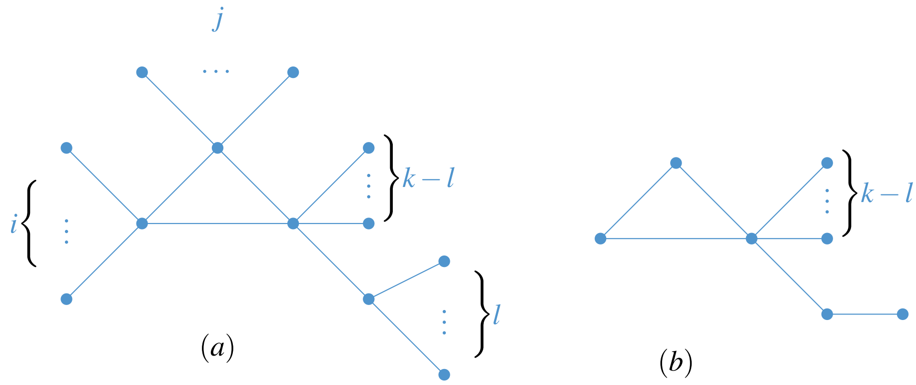

Figure 9. (a) $R_{i,j,k,l}$; (b) $R_{0,0,k,l}$.

and properties of certain subclasses of analytic functions involving q-Poisson distribution was found in [16, 17].

Akhter et al. [2] have determined the extremal graph with respect to F-index among the classes of connected unicyclic and bicyclic graphs. They have considered seven subclasses of bicyclic graphs having equal number of pendant edges attached to given number of vertices, and ordered those subclasses with respect to F-index. But, in their study, all the graphs across the different subclasses do not have equal number of vertices. Not all those have equal number of pendant vertices also. If a graph G has n vertices, m edges and p components, then $\gamma = n - m + p$ is called the cyclomatic number of G. Gutman et al. [11] have determined the first through the sixth smallest F-indices among all trees, the first through the third smallest F-indices among all connected graph with cyclomatic number $\gamma = 1, 2$, the first through the fourth smallest F-indices among all connected graph with cyclomatic number $\gamma = 3$, and the first and the second smallest F-indices among all connected graph with cyclomatic number $\gamma = 4,5$.

In this study, we investigate the F-index of unicyclic graphs by introducing some transformations, and characterize the unicyclic graphs for the first five maximal F-indices and the unicyclic graphs with the first two minimal F-indices.

2. TWO TRANSFORMATIONS WHICH INCREASE THE F-INDICES

Let $E_1 \subseteq E(G)$. We denote by $G - E_1$ the subgraph of G obtained by deleting the edges in E_1. Let $W \subseteq V(G)$. $G - W$ denotes the subgraph of G obtained by deleting the vertices in W and the edges incident with them. Again let, $E_2 \subseteq E(\overline{G})$, where $\overline{G}$ is the complement of G. Then by $G + E_2$ we mean the graph obtained by adding the edges in E_2 to G.

We give two transformations which increase the F-index as follows.

Transformation A. Let uv be an edge of the graph G, $d_G(u) \geq 2, N_G(v) = \{u, w_1, w_2, \ldots, w_s\}$, and $w_1, w_2, \ldots, w_s$ are leaves. Then $G_1 = G - \{vw_1, vw_2, \ldots, vw_s\} + \{uw_1, uw_2, \ldots, uw_s\}$, as shown in Figure 2, is said to be the graph obtained from G by Transformation A.

Lemma 2.1. *Let G_1 be obtained from G by Transformation A, then $F(G_1) > F(G)$.*

Proof. Let $G_0 = G - \{v, w_1, w_2, \ldots, w_s\}$. Clearly, the degree of each vertex of G_1 except u and v is same as that of the corresponding vertex of G and is also equal to the degree of the corresponding vertex in G_0, i.e., $d_G(i) = d_{G_1}(i) = d_{G_0}(i)$ for all $i \in V(G_0)$. For the vertices u and v, we have $d_{G_1}(u) = d_G(u) + s, d_{G_1}(v) = 1, d_G(v) = s + 1$.

By the definition of F-index, we have

$$\begin{aligned} F(G_1) - F(G) &= [d^3_{G_1}(u) + d^3_{G_1}(v)] - [d^3_G(u) + d^3_G(v)] \\ &= [(d_G(u) + s)^3 + 1^3] - [d^3_G(u) + (s+1)^3] \\ &= 3s(d^2_G(u) - s + s d_G(u) - 1) \\ &= 3s(d_G(u) - 1)(d_G(u) + 1 + s) \\ &> 0 \text{ (since } d_G(u) > 1). \end{aligned}$$

Hence, $F(G_1) > F(G)$. □

Remark 2.2. Using Transformation A repeatedly, any unicyclic graph can be transformed into such a unicyclic graph that all the edges not on the cycle are pendant edges.

Transformation B. Let u and v be two vertices in G. Also let $u_1, u_2, \ldots, u_s$ are the leaves adjacent to u and $d_G(u) \leq d_G(v)$. Then $G_1 = G - \{uu_1, uu_2, \ldots, uu_s\} + \{vu_1, vu_2, \ldots, vu_s\}$, as shown in Figure 2, is said to be the graph obtained from G by Transformation B.

Lemma 2.3. *Let G_1 be obtained from G by Transformation B. Then $F(G_1) > F(G)$.*

Proof. Since the degrees of all the vertices in G_1 and those of all the vertices in G are same, except for the vertices u and v, where $d_G(u) \leq d_G(v)$, we have

$$\begin{aligned} F(G_1) - F(G) &= d^3_{G_1}(v) - d^3_G(v) + d^3_{G_1}(u) - d^3_G(u) \\ &= (d_G(v) + s)^3 - d^3_G(v) + (d_G(u) - s)^3 - d^3_G(u) \\ &= 3s(d_G(v) + d_G(u))(d_G(v) - d_G(u) + s) > 0. \end{aligned}$$

Hence, $F(G_1) > F(G)$. □

Remark 2.4. Using Transformation B repeatedly, any unicyclic graph can be transformed into such a unicyclic graph that all the pendant edges are attached to the same vertex.

3. SOME TRANSFORMATIONS WHICH DECREASE THE F-INDICES

Transformation C. Let $G \neq P_1$ be a connected graph and we choose $u \in V(G)$ and G_1 denotes the graph that results from identifying u with the vertex v_k of a simple path $v_1 v_2 \ldots v_n$, $1 < k < n$. The graph G_2 obtained from G_1 by deleting $v_{k-1}v_k$ and adding $v_{k-1}v_n$, as shown in Figure 4, is said to be the graph obtained by applying Transformation C to the graph G_1.

Lemma 3.1. *Let G_2 be the graph obtained by Transformation C to G_1, as shown in Figure 4. Then $F(G_1) > F(G_2)$.*

Proof. Let $G = G_1 - \{v_1, v_2, \ldots, v_{k-1}, v_{k+1}, \ldots, v_n\}$. Clearly, the degree of each vertex of G_2 except $v_k = u$ and v_n is same as that of the corresponding vertex of G_1 and is also equal to the degree of the corresponding vertex in G, i.e., $d_{G_1}(i) = d_{G_2}(i) = d_G(i)$ for all $i \in V(G)$. For the vertices v_k and v_n, we have $d_{G_1}(v_k) = d_{G_1}(u) = d_G(u) + 2, d_{G_2}(v_k) = d_{G_2}(u) = d_G(u) + 1, d_{G_1}(v_n) = 1, d_{G_2}(v_n) = 2$.

So, by the definition of F-index, we have

$$\begin{aligned} F(G_1) - F(G_2) &= (d_G(u) + 2)^3 + 1 - (d_G(u) + 1)^3 - 8 \\ &= 3d_G(u)(d_G(u) + 3) > 0. \end{aligned}$$

Hence, $F(G_1) > F(G_2)$. □

Remark 3.2. By repeated applications of Transformation C, any tree T attached to a graph G can be transformed into a path attached to G and F-index decreases at each step of applying Transformation C.

Transformation D. Let u and v be two vertices in a graph G. G_1 denotes the graph that results from identifying u with the vertex u_0 of a path $u_0u_1u_2...u_s$ and identifying v with the vertex v_0 of a path $v_0v_1v_2...v_t$. The graph G_2 obtained from G_1 by deleting uu_1 and adding v_tu_1, as shown in Figure 5, is the graph obtained by applying Transformation D from G_1 to G_2.

Lemma 3.3. *Let G_2 be the graph obtained from G_1, by Transformation D, as shown in Figure 5, where $d_G(u) \geq d_G(v) > 1, s \geq 1$ and $t \geq 0$.*
(i) If $t > 0$, then $F(G_1) > F(G_2)$.
(ii) If $t = 0$, and $d_G(u) > d_G(v)$, then $F(G_1) > F(G_2)$.

Proof. (i) Since $d_G(u) > 1$ and $t > 0$, we have

$$\begin{aligned} F(G_1) - F(G_2) &= d^3_{G_1}(u) + d^3_{G_1}(v_t) - d^3_{G_2}(u) - d^3_{G_2}(v_t) \\ &= (d_G(u)+1)^3 + 1 - d^3_G(u) - 8 \\ &= 3d^2_G(u) + 3d_G(u) - 6 > 0. \end{aligned}$$

Hence, $F(G_1) > F(G_2)$.
(ii) If $t = 0$ and $d_G(u) > d_G(v)$ then

$$\begin{aligned} F(G_1) - F(G_2) &= d^3_{G_1}(u) + d^3_{G_1}(v_t) - d^3_{G_2}(u) - d^3_{G_2}(v_t) \\ &= (d_G(u)+1)^3 + d^3_G(v) - d^3_G(u) - d^3_G(v) \\ &= 3d^2_G(u) + 3d_G(u) + 1 > 0. \end{aligned}$$

Hence, $F(G_1) > F(G_2)$. □

Remark 3.4. After repeated applications of Transformation D, any tree attached to a unicyclic graph can be transformed into such a unicyclic graph that a path is attached to a cycle, and F-indices decrease in each application of Transformation D.

Transformation E. Let G_1 be the unicyclic graph constructed by identifying the center of $S_{1,n-k}$ with a vertex u of a unicyclic graph G. Also let G_2 be the graph obtained from G by identifying a pendant vertex of P_{n-k+1} with a vertex u of G, as shown in Figure 6. The graph G_2 is said to be the graph obtained from G_1 by Transformation E.

Lemma 3.5. *Let the graph G_2 is obtained from G_1 by Transformation E. Then $F(G_2) \leq F(G_1)$.*

Proof. Let G be the graph from which G_1 is obtained by identifying the center of $S_{1,n-k}$ with the vertex u of G. Also let $v_1, v_2, \ldots, v_{n-k}$ be the pendant vertices of $S_{1,n-k}$. Then except for the vertex u, the degree of each vertex of G_2 which is also a vertex of G is same as that of the corresponding vertex of G_1 and is also equal to the degree of the corresponding vertex in G, i.e., $d_{G_1}(i) = d_{G_2}(i) = d_G(i)$ for all $i \in V(G) \setminus \{u\}$. For the vertices u and $v_1, v_2, \ldots, v_{n-k}$, we have $d_{G_1}(u) = d_G(u) + n - k, d_{G_1}(v_1) = d_{G_1}(v_2) = \ldots = d_{G_1}(v_{n-k}) = 1, d_{G_2}(u) = d_G(u) + 1, d_{G_2}(v_1) = d_{G_2}(v_2) = \ldots = d_{G_2}(v_{n-k-1}) = 2, d_{G_2}(v_{n-k}) = 1$.

So, by the definition of F-index, we have
$F(G_1) - F(G_2) = (d_G(u) + n - k)^3 + (n-k) \cdot 1^3 - (d_G(u) + 1)^3 - (n-k-1) \cdot 2^3 - 1^3$
$= 3d_G^2(u)(n-k-1) + 3d_G(u)\{(n-k)^2 - 1\} + (n-k)\{(n-k)^2 - 7\} + 6 \geq 0$
since $(n-k) \geq 1$. Hence, $F(G_2) \leq F(G_1)$. □

Transformation F. Let G_1 be a unicyclic graph constructed by attaching $n-k$ leaves to a vertex u on a cycle of length k. By Transformation F, the graph G_2 is obtained from G_1 by attaching two paths of length s and t, where $s+t = n-k$, at the vertex u, as shown in Figure 7.

Lemma 3.6. *Let the graph G_2 be obtained from G_1 by Transformation F. Then $F(G_2) \leq F(G_1)$.*

*Proof.*Let G be the graph from which G_1 is obtained by identifying the center of $S_{1,n-k}$ with the vertex u of G. Also let $v_1, v_2, \ldots, v_{n-k}$ be the pendant vertices of $S_{1,n-k}$. Now we divide $(n-k)$ pendant vertices into two parts. One part contains s vertices and another part contains t vertices. The graph G_2 is obtained by identifying the vertex u of G with the vertex u of the paths uu_s and uw_t. Then except for the vertex u, the degree of each vertex of G_2 which is also a vertex of G is same as that of the corresponding vertex of G_1 and is also equal to the degree of the corresponding vertex in G, i.e., $d_{G_1}(i) = d_{G_2}(i) = d_G(i)$ for all $i \in V(G) \setminus \{u\}$. For the vertices u and $v_1, v_2, \ldots, v_{n-k}$, we have $d_{G_1}(u) = d_G(u) + n - k, d_{G_1}(v_1) = d_{G_1}(v_2) = \ldots = d_{G_1}(v_{n-k}) = 1, d_{G_2}(u) = d_G(u) + 2, d_{G_2}(u_1) = d_{G_2}(u_2) = \ldots = d_{G_2}(u_{s-1}) = 2, d_{G_2}(w_1) = d_{G_2}(w_2) = \ldots = d_{G_2}(w_{t-1}) = 2, d_{G_2}(u_s) = 1, d_{G_2}(w_t) = 1$. So,by the definition of F-index, we have
$F(G_1) - F(G_2) = (d_G(u) + n - k)^3 + (n-k) \cdot 1^3 - (d_G(u) + 2)^3 - (s-1) \cdot 2^3 - (t-1) \cdot 2^3 - 2 \cdot 1^3 = 3d_G^2(u)(n-k-2) + 3d_G(u)\{(n-k)^2 - 4\} + (n-k)\{(n-k)^2 - 7\} + 6 \geq 0$,
since $(n-k) \geq 2$. Hence, $F(G_2) \leq F(G_1)$. □

4. UNICYCLIC GRAPHS WITH LARGER F-INDICES

In this section, we obtain some upper bounds of the unicyclic graphs with respect to their F-indices.

Lemma 4.1. *Let $G \in \mathscr{U}_n^k$. Then $F(G) \leq F(G_{k,1}^{(n)})$, the equality holds if and only if $G \cong G_{k,1}^{(n)}$.*

Proof. Using Lemma 2.1 to Lemma 3.6, we have $F(G) \leq F(G_{k,1}^{(n)})$ and equality holds if and only if $G \cong G_{k,1}^{(n)}$. □

Lemma 4.2. *Let $G \in \mathscr{U}_n$. Then*
(i) $F(G) \leq F(G_{3,1}^{(n)})$, with equality if and only if $G \cong G_{3,1}^{(n)}$.
(ii) If G is not isomorphic to $G_{3,1}^{(n)}$, then $F(G) \leq F(G_{3,2}^{(n)})$ the equality holds if and only if $G \cong G_{3,2}^{(n)}$.

Proof. (i) By Lemma 4.1, we have $F(G) \leq F(G_{k,1}^{(n)})$.

Next we prove that $F(G_{k,1}^{(n)}) \leq F(G_{3,1}^{(n)})$.

By definition of F-index, we have

$$\begin{aligned} F(G_{3,1}^{(n)}) - F(G_{k,1}^{(n)}) &= (n-1)^3 - (n-k+2)^3 + 2.2^3 - 2^3.(k-1) + (n-3) - (n-k) \\ &= (k-3)\{(n-1)^2 + (n-1)(n-k+2) + (n-k+2)^2 - 7\} \geq 0 \\ &\quad \text{since } n-k \geq 1 \text{ and } k \geq 3. \end{aligned}$$

Hence, $F(G_{k,1}^{(n)}) \leq F(G_{3,1}^{(n)})$. Therefore, $F(G) \leq F(G_{3,1}^{(n)})$, the equality holds if and only if $G \cong G_{3,1}^{(n)}$.

(ii) By Lemma 4.1, we have, $F(G) \leq F(G_{k,1}^{(n)})$.

Next we prove that if G is not isomorphic to $G_{3,1}^{(n)}$, then $G_{k,1}^{(n)} \leq G_{3,2}^{(n)}$.

By definition of F-index, we have

$$\begin{aligned} F(G_{3,2}^{(n)}) - F(G_{k,1}^{(n)}) &= (n-2)^3 + 3^3 + 2^3 + (n-3) - (n-k+2)^3 - (k-1)\cdot 2^3 - (n-k) \\ &= (k-4)\{3n(n-k) + (k-2)^2\} - 8(k-4) + 8 > 0 \; if \; k \geq 4. \end{aligned}$$

If $k = 3$ and $G_{k,1}^{(n)}$ is not isomorphic to $G_{3,1}^{(n)}$, then obviously $G_{k,1}^{(n)} \leq G_{3,2}^{(n)}$.

Hence, $F(G) \leq F(G_{3,2}^{(n)})$, the equality holds if and only if $G \cong G_{3,2}^{(n)}$. □

Theorem 4.3. *Let $G \in \mathscr{U}_n^k (k \geq 3)$. Then $F(G_{k,1}^{(n)}) > F(G_{k,2}^{(n)})$.*

Proof. From the definition of F-index, we have

$$\begin{aligned} F(G_{k,1}^{(n)}) - F(G_{k,2}^{(n)}) &= (n-k-2)^3 + 2^3 - 3^3 - (n-k+1)^3 \\ &= 3(n-k)^2 + 9(n-k) - 2 > 0 \text{ since } n-k > 0. \end{aligned}$$

Hence, $F(G_{k,1}^{(n)}) > F(G_{k,2}^{(n)})$. □

Theorem 4.4. *Let $G \in \mathscr{U}_n^k$ be an arbitrary unicyclic graph. Then $F(G_{k,2}^{(n)}) > F(G_{k+1,2}^{(n)})$.*

Proof. From the definition of F-index, we have

$$\begin{aligned} F(G_{k,2}^{(n)}) - F(G_{k+1,2}^{(n)}) &= (n-k+1)^3 + 1^3 - 2^3 - (n-k)^3 \\ &= 3(n-k)^2 + 3(n-k) - 7 > 0 \text{ since } n-k \geq 2. \end{aligned}$$

Hence, $F(G_{k,2}^{(n)}) > F(G_{k+1,2}^{(n)})$. □

Theorem 4.5. *Let $p \geq q \geq r \geq 0$, and $p+q+r = n-3$. Then*
(i) $F(S_{p,q,r}) < F(S_{p+1,q-1,r})$, and (ii) $F(S_{p,q,r}) < F(S_{p,q+1,r-1})$.

Proof. (i) By the definition of F-index, we have

$$\begin{aligned} F(S_{p,q,r}) - F(S_{p+1,q-1,r}) &= (p+2)^3(q+2)^3(r+2)^3 - (p+3)^3 - (q+1)^3 - (r+2)^3 \\ &= (q-p-1)(3p+3q+12) < 0. \end{aligned}$$

Hence, $F(S_{p,q,r}) < F(S_{p+1,q-1,r})$.
(ii)

$$\begin{aligned} & F(S_{p,q,r}) - F(S_{p,q+1,r-1}) \\ = & (p+2)^3 + (q+2)^3 + (r+2)^3 - (p+2)^3 - (q+3)^3 - (r+1)^3 \\ = & (r-q-1)(3r+3q+12) < 0. \end{aligned}$$

Hence, $F(S_{p,q,r}) < F(S_{p,q+1,r-1})$. □

By attaching $K_{1,n-5}$ and $K_{1,2}$ to the adjacent vertices of C_3, respectively, we have the graph $G_{3,3}^{(n)}$. Also by attaching $K_{1,n-5}$ to one vertex of C_3 and $K_{1,2}$ to another two vertices of C_3, respectively, we have the graph $G_{3,4}^{(n)}$. See Figure 8(a) and 8(b) for illustrations. Now, $F(G_{3,3}^{(n)}) = (n-3)^3 + 2^3 + 4^3 + (n-2)1^3 = n^3 - 9n^2 + 28n + 43$, and $F(G_{3,4}^{(n)}) = (n-3)^3 + 3^3 + 3^3 + (n-2)1^3 = n^3 - 9n^2 + 28n + 25$.

By Lemma 3.5, Lemma 3.6, Theorem 4.5 and above calculations, we have the following theorem.

Theorem 4.6. *For $n \geq 6$, we have $F(G_{3,3}^{(n)}) > F(G_{3,4}^{(n)}) > \ldots$*

Let $\mathscr{S}$ denote the set of graphs $S_{p,q,r}$. Then by Lemma 3.5, Lemma 3.6, Theorem 4.5, and Theorem 4.6 we have the following theorem.

Theorem 4.7. *For $n \geq 6$, the order in $\mathscr{S}$ with respect to the F-indices is $F(G_{3,1}^{(n)}) > F(G_{3,2}^{(n)}) > F(G_{3,3}^{(n)}) > F(G_{3,4}^{(n)}) > \ldots$*

Let $\mathscr{U}_n^{'3}$ be the set of unicyclic graphs with C_3 being the only cycle and there is at least one vertex in the graph, which is at distant ≥ 2 from C_3. Obviously, $\mathscr{U}_n^{'3} = \mathscr{U}_n^3 - \mathscr{S}$. By Lemma 2.1 and Lemma 2.3, it is clear that the graphs with the largest F-indices in $\mathscr{U}_n^{'3}$ must be made by attaching $K_{1,l}(l \geq 1)$ to one of the pendent vertices of $S_{i,j,k}(i,j \geq 0, k \geq 1)$. Denote the graph as $R_{i,j,k,l}$, as shown in Figure 9. Similar to Theorem 4.5, we have the following theorem.

Theorem 4.8. *Let $i \geq j \geq 1, i+j+k+l = n-3$. Then, $F(R_{i+1,j-1,k,l}) > F(R_{i,j,k,l})$. In particular, $F(R_{i+j,0,k,l}) > F(R_{i,j,k,l})$.*

Proof. From the definition of F-index, we have

$F(R_{i+1,j-1,k,l}) = (i+3)^3 + (j+1)^3 + (k+2)^3 + (l+1)^3 + (n-4)$, and $F(R_{i,j,k,l}) = (i+2)^3 + (j+2)^3 + (k+2)^3 + (l+1)^3 + n - 4$.

So, $F(R_{i+1,j-1,k,l}) - F(R_{i,j,k,l}) = (i+3)^3 + (j+1)^3 - (i+2)^3 - (j+2)^3 = 3(i^2 - j^2 + 5i - 3j + 4) > 0$. Hence, $F(R_{i+1,j-1,k,l}) > F(R_{i,j,k,l})$.

In particular, $F(R_{i+j,0,k,l}) > F(R_{i,j,k,l})$. □

Theorem 4.9. *Let $i \geq 1$. Then, $F(R_{i,0,k,l}) < F(R_{0,0,i+k,l})$.*

Proof. From definition of F-index, we have

$F(R_{i,0,k,l}) = (i+2)^3 + (k+2)^3 + (l+2)^3 + (l+k+i-1)1^3$,

and $F(R_{0,0,i+k,l}) = 2^3 + 2^3 + (i+k+2)^3 + (l+2)^3 + (l+k+i-1)$.

Then $F(R_{0,0,i+k,l}) - F(R_{0,0,k,l}) = 16 + (i+k+2)^3 - (i+2)^3 - (k+2)^3 - 2^3 = 3ik(i+k+4) > 0$. Hence, $F(R_{i,0,k,l}) < F(R_{0,0,i+k,l})$. □

We shall denote $R_{0,0,k,1}$ simply as $R_{k,1}$ and also by $G_{3,1}^{'(n)}$.

Theorem 4.10. *For $n \geq 9$, we have $F(G_{3,3}^{(n)}) < F(R_{k,1}) < F(G_{3,2}^{(n)})$.*

Proof. By the definition of F-index, we have

$$F(G_{3,3}^{(n)}) = n^3 - 9n^2 + 28n + 43,$$
$$F(G_{3,2}^{(n)}) = n^3 - 6n^2 + 13n + 24,$$
$$\text{and } F(R_{k,1}) = n^3 - 6n^2 + 13n + 12.$$

Therefore, $F(R_{k,1}) - F(G_{3,3}^{(n)}) = 3n^2 - 15n - 13 > 0$, and $F(G_{3,2}^{(n)}) - F(R_{k,1}) = 12 > 0$. Hence, $F(G_{3,3}^{(n)}) < F(R_{k,1}) < F(G_{3,2}^{(n)})$. □

Theorem 4.11. *For $n \geq 6$, $l \geq 2$, $k+l+3=n$, we have $F(G_{3,4}^{(n)}) > F(R_{k,l})$.*

Proof. From the definition of $R_{k,l}$ and since $k+l+3=n$, we have

$$\begin{aligned} F(R_{k,l}) &= 2^3+2^3+(k+2)^3+2^3+k \\ &= 24+(n-l-1)^3+(n-3-l) \\ &= n^3-3n^2+4n+12+3nl^2+(6n-3n^2)l. \end{aligned}$$

Let $f(l)=n^3-3n^2+4n+12+3nl^2+(6n-3n^2)l$, $l \in [2,n-4]$.
Then $\max f(l)=\{f(2), f(n-4)\}=n^3-9n^2+28n+12$, (since $f(2)=f(n-4)$).
Therefore, $F(G_{3,4}^{(n)}) > F(R_{k,l})$. □

Theorem 4.12. *Let $n \geq 9$. Then F-indices order in $\mathscr{U}_n^3$ is*
$F(G_{3,1}^{(n)}) > F(G_{3,2}^{(n)}) > F(G_{3,1}^{'(n)}) > F(G_{3,3}^{(n)}) > F(G_{3,4}^{(n)}) > F(R_{k,l}) > \ldots$

Let $G_{4,3}^{(n)}$ be the graph obtained from a C_4 by attaching $n-5$ leaves to one of its vertices and another leaf to the vertex which is at a distance 2 from the $n-3$ degree vertex of C_4.

By the definition of F-index, we have $F(G_{4,3}^{(n)})=n^3-9n^2+28n+12$, and $F(G_{4,2}^{(n)})=n^3-9n^2+28n+12$.

Similar to Theorem 4.12, we have the following theorem.

Theorem 4.13. *Let $n \geq 6$. Then F-index order in $\mathscr{U}_n^4$ is*
$F(G_{4,1}^{(n)}) > F(G_{4,2}^{(n)}) = F(G_{4,3}^{(n)}) > F(G_{4,1}^{'(n)}) > \ldots$, where $G_{4,1}^{'(n)}$ is obtained from $G_{4,1}^{(n-1)}$ by attaching K_2 to one pendant edges of $G_{4,1}^{(n-1)}$.

Theorem 4.14. *Let $n \geq 6$. Then we have*
(i) $F(G_{4,1}^{(n)}) = F(G_{3,1}^{'(n)})$, and
(ii) $F(G_{3,4}^{(n)}) > F(G_{4,2}^{(n)})$.

Proof. (i) By the definition of F-index, we have
$F(G_{4,1}^{(n)}) = 2^3+2^3+2^3+(n-2)^3+(n-4) = n^3-6n^2+13n+12 = F(G_{3,1}^{'(n)})$.
(ii) $F(G_{3,4}^{(n)}) - F(G_{4,2}^{(n)}) = (n^3-9n^2+28n+25)-(n^3-9n^2+28n+12) = 13$.
Hence, $F(G_{3,4}^{(n)}) > F(G_{4,2}^{(n)})$. □

Combining all the above results, we have the upper bounds of unicyclic graphs with respect to F-indices.

Theorem 4.15. *For $n \geq 6$, we have*
$F(G_{3,1}^{(n)}) > F(G_{3,2}^{(n)}) > F(G_{3,1}^{'(n)}) = F(G_{4,1}^{(n)}) > F(G_{3,3}^{(n)}) > F(G_{3,4}^{(n)}) > \ldots$

5. THE LOWER BOUNDS OF THE UNICYCLIC GRAPHS WITH RESPECT TO F-INDICES

Given integers n and k with $3 \leq k \leq n-1$, 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 end vertex of P_{n-k}.

Theorem 5.1. *The graph C_n is the unique graph with the smallest F-index among all unicyclic graphs with n vertices.*

Proof. First we shall prove that if G is a unicyclic graph with $n \geq 7$ vertices, then $F(G)$ attains the smallest value only if degree sequence of G is $[2^n]$. Suppose $F(G)$ attains the smallest value and degree sequence of G is not equal to $[2^n]$. Let $C = u_1u_2...u_ku_1$ be the unique cycle in G. Then $k < n$ and there is at least one vertex u_i with $d(u_i) \geq 3$. Without loss of generality, we assume $d(u_1) \geq 3$. Choose a maximal $C-$path $P[u_1, v_1]$ in G. Clearly $d(v_1) = 1$. Let $G^{'} = G - u_1u_2 + u_2v_1$. Then we have, $F(G) - F(G^{'}) = [d^3(u_1) + d^3(v_1)] - [(d^3(u_1)-1)^3 + (d^3(v_1)+1)^3] = 3(d(u_1)+d(v_1))(d(u_1)-d(v_1)-1) > 0$. Therefore $F(G) > F(G^{'})$, a contradiction. Hence degree sequence of G is $[2^n]$.

Since among all unicyclic graphs, the cycle C_n has only degree sequence $[2^n]$, it has smallest F-index among all unicyclic graphs with n vertices. □

Theorem 5.2. *Let $G \in \mathscr{U}_n^k$, $3 \leq k \leq n-1$ be an arbitrary unicyclic graph. Then $F(G) \geq F(L_{n,k})$, the equality holds if and only if $G \cong L_{n,k}$.*

Proof. By Transformation C, D and Lemma 3.1 and 3.3, the conclusion is obvious. □

Theorem 5.3. *Let $G \in \mathscr{U}_n - C_n$ be an arbitrary unicyclic graph, then $F(G) > F(L_{n,k})$, $k \in \{3, 4, ..., n-1\}$.*

Proof. By the definition of $L_{n,k}$, we have $F(L_{n,k}) = 8n + 14$. Therefore the value of F are functions of n, not related to k, hence $F(L_{n,k}) = F(L_{n,l})$, where $k \in \{3, 4, ..., n-1\}$ and $k \neq l$, i.e., if G is not isomorphic to C_n, then $F(G) > F(L_{n,k})$ for $k \in \{3, 4, ..., n-1\}$. □

In this study, we have found the F-index of unicyclic graphs and characterize the unicyclic graphs for the first five maximal F-indices and the unicyclic graphs with the first two minimal F-indices.

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REFERENCES

1. H. Abdo, D. Dimitrov, I. Gutman: On extremal trees with respect to the F-index, *Kuwait J. Sci.* **44(3)**(2017) 1–8. https://doi.org/10.48550/arXiv.1509.03574
2. S. Akhter, M. Imran and M.R. Farahani: Extremal unicyclic and bicyclic graphs with respect to the F-index, *AKCE Int. J. Graphs Combin.* **14** (2017) 81–90. https://doi.org/10.1016/j.akcej.2016.11.011
3. R. Amin, S.M.A. Nayeem: Extremal F-indices for bicyclic graphs with k pendant vertices, *J. Korean Soc. Math. Educ. Ser. B: Pure Appl. Math.* **27** (2020) 171–186. https://doi.org/https://doi.org/10.7468/jksmeb.2020.27.4.171
4. R. Amin, S.M.A. Nayeem: Extremal F-index of a graph with k cut edges, *Mathematicki Vesnik* **72**(2020) 146–153. https://www.vesnik.math.rs/vol/mv20206.pdf
5. Z. Che, Z. Chen: Lower and upper bounds of the forgotten topological index, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 635–648. https://match.pmf.kg.ac.rs/electronic_versions/Match76/n3/match76n3_635-648.pdf
6. N. De, S.M.A. Nayeem, A. Pal: F-index of some graph operations, *Disc. Math. Alg. Appl.* **8(2)** (2016). https://doi.org/10.1142/S1793830916500257
7. H. Deng: A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs, MATCH Commun. Math. Comput. Chem. **57**(2007) 597–616. https://match.pmf.kg.ac.rs/electronic_versions/Match57/n3/match57n3_597-616.pdf
8. S. Elumalai, T. Mansour, M.A. Rostami: On the bounds of the forgotten topological index. *Turk J. Math.* **41** (2017) 1687–1702. https://doi.org/10.3906/mat-1610-127
9. F. Xia, S. Chen: Ordering unicyclic graphs with respect to Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **58**(2007) 663–673. https://match.pmf.kg.ac.rs/electronic_versions/Match58/n3/match58n3_663-673.pdf
10. B. Furtula, I. Gutman: A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190. https://link.springer.com/article/10.1007/s10910-015-0480-z
11. I. Gutman, A. Ghalavand, T. Dehghan–Zadeh and A. R. Ashrafi: Graphs with smallest forgotten index, *Iranian J. Math. Chem.* **8(3)** (2017) 259 – 273. https://doi.org/10.22052/ijmc.2017.43258
12. I. Gutman: Degree-based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361. http://dx.doi.org/10.5562/cca2294

13. I. Gutman, K. C. Das: The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50**(2004)83–92. `https://match.pmf.kg.ac.rs/electronic_versions/Match50/match50_83-92.pdf`
14. I. Gutman, N. Trinajstić: Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17**(1972), 535–538. `https://doi.org/10.1016/0009-2614(72)85099-1`
15. A. Hussain, M. Numan, N. Naz, S. I. Butt, A. Aslam, A. Fahad: On topological indices for new classes of benes network, *J. Math.* **1**(2021) 6690053. `https://doi.org/10.1155/2021/6690053`
16. S. Khan, N. Khan, A. Hussain, S. Araci, B. Khan, H. H. Ai-Sulami: Applications of symmetric conic domains to a subclass of q-starlike functions, *Symmetry* **14(4)**(2022) 803. `https://doi.org/10.3390/sym14040803`
17. B. Khan, Z. G. Liu, N. Khan, A. Hussain, N. Khan, M. Tahir: Properties of certain subclasses of analytic functions involving p-Poisson distribution, *Com. Modeling. Eng. Sc* **131(3)** (2022) 1465–1477. `https://doi.org/10.32604/cmes.2022.016940`
18. J. R.Lee, A. Hussain, A. Fahad, A. Raza, M. I. Qureshi, A. Mahboob, C. Park: On *ev* and *ve*-degree based topological indices of silicon carbides, *Com. Modeling. Eng. Sc* **130(2)** (2022) 871–885. `https://doi.org/10.32604/cmes.2022.016836`
19. I. Ur. Rehman , M. U. K. Afridi, M. Ishaq, A. Asiri, A. Hussain: Algebraic invariants of edge ideals of some bristled circulant graphs, *AIMS Mathematics* **10(5)**(2025) 11330–11348. `https://doi.org/10.3390/math.2025515`
20. H. Zhang, S. Zhang: Unicyclic graphs with the first three smallest and largest first general Zagreb index, *MATCH Commun. Math. Comput.Chem.* **55**(2006) 427–438. `https://match.pmf.kg.ac.rs/electronic_versions/Match55/n2/match55n2_427-438.pdf`

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