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EXTREMAL F-INDICES FOR BICYCLIC GRAPHS WITH k PENDANT VERTICES

Ruhul Amin [a] and Sk. Md. Abu Nayeem [b,*]

Abstract. Long back in 1972, it was shown that the sum of the squares of vertex degrees and the sum of cubes of vertex degrees of a molecular graph both have large correlations with total π-electron energy of the molecule. Later on, the sum of squares of vertex degrees was named as first Zagreb index and became one of the most studied molecular graph parameter in the field of chemical graph theory. Whereas, the other sum remained almost unnoticed until recently except for a few occasions. Thus it got the name "forgotten" index or F-index. This paper investigates extremal graphs with respect to F-index among the class of bicyclic graphs with n vertices and k pendant vertices, $0 \leq k \leq n-4$. As consequences, we obtain the bicyclic graphs with largest and smallest F-indices.

1. Introduction

A topological index (or molecular structure descriptor) is a numerical value associated with chemical constitution of some molecule for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. By "molecular graph", we understand a simple graph, representing the carbon atom skeleton of an organic molecule (usually, of a hydrocarbon). Thus the vertices of a molecular graph represent the carbon atoms and its edges the carbon-carbon bonds. Degree based topological indices have been studied extensively by mathematician and chemist since the introduction of Randic index in 1975 [13]. Although Zagreb indices are the first degree based topological indices, those were initially intended for the study of total π- electron energy [9] and were included among the topological indices much later. In the paper where Zagreb indices were introduced first time by Gutman and Trinajstić [12], a series of approximate formulas for total π-electron

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*Corresponding author.

energy E were deduced. By means of these formulas, several structural details have been identified, on which E depends. Among these were the sum of squares and sum of the cubes of the vertex degrees of the underlying molecular graph. Eventually, the sum of squares, became known as the first Zagreb index, but the latter term remained unnoticed by researchers until a recent work of Furtula and Gutman, where they named it as "forgotten" topological index, or F-index [8].

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. The set of vertices adjacent to a vertex v in G is denoted by $N_G(v)$ and $d_G(v) = |N_G(v)|$ denotes the degree of the vertex v in G. Two vertices u and v are of almost equal degree if $|d_G(u) - d_G(v)| \leq 1$. Let $V = \{v_1, v_2, \ldots, v_n\}$ and $d_i = d_G(v_i), 1 \leq i \leq n$. Then $\{d_1, d_2, \ldots, d_n\}$ is called the degree sequence of G. In a degree sequence, we use the symbol $d_i^{t_i}$ if the degree d_i is repeated t_i times.

The first Zagreb index and the F-index are defined by

$$M_1(G) = \sum_{v \in V(G)} [d_G(v)]^2, \text{and } F(G) = \sum_{v \in V(G)} [d_G(v)]^3.$$

It is easy to follow that

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)], \text{and } F(G) = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2].$$

Finding the extremal values or bounds for the degree based topological indices of graphs, as well as related problems of characterizing the extremal graphs, have recently attracted the attention of researchers and many results are obtained. Gutman and Das [10] have shown that the trees with the smallest and largest first Zagreb indices are the path and the star, respectively. It has also been shown that the trees with the smallest and largest second Zagreb indices are the path and the star, respectively [4]. Extremal trees with respect to F-index have been studied by Abdo et al. [1]. A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs have been studied by Deng [6]. F-index for graph operations are found in [5]. Some lower and upper bounds for F-index are found in [3, 7].

Zhang et al. [14] introduced the first general Zagreb index as

$$M_1^\alpha(G) = \sum_{v \in V(G)} [d_G(v)]^\alpha,$$

where α is an arbitrary real number. It is clear that $M_1^3(G)$ coincides with $F(G)$. In [14], they have obtained the bicyclic graphs with the first three smallest and greatest M_1^α when $\alpha > 1$ among all the n-vertex bicyclic graphs, $n \geq 5$.

Recently, 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 paper, we investigate the bicyclic graphs with the largest and smallest F-indices among all the bicyclic graphs with n vertices and k pendant vertices, $0 \leq k \leq n - 4$. As consequences, we have also obtained the bicyclic graphs with largest and smallest F-indices. Those are in agreement with the results in [11] and [14].

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. Let v be a pendant vertex and u be a non-pendant vertex of G. A u-v path is said to be a *pendant path* attached to u if $d_G(u) \geq 3, d_G(v) = 1$ and every other vertex on the path has degree 2. The vertex w adjacent to the vertex u in the u-v pendant path is said to be the *lead vertex* of the pendant path.

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

Transformation A. *Let $u_0 - u_1 - \cdots - u_p, p \geq 1$ be a path in the graph G, where $d_G(u_0) \geq 3, d_G(u_p) \geq 3$ and $d_G(u_i) = 2$ for $i \in \{0, 1, \ldots, p\} \setminus \{0, p\}$. Let $N_G(u_p) = \{u_{p-1}, w_1, w_2, \ldots, w_s\}, s \geq 2$, and $w_1, w_2, \ldots, w_s$ be either pendant vertices or lead*

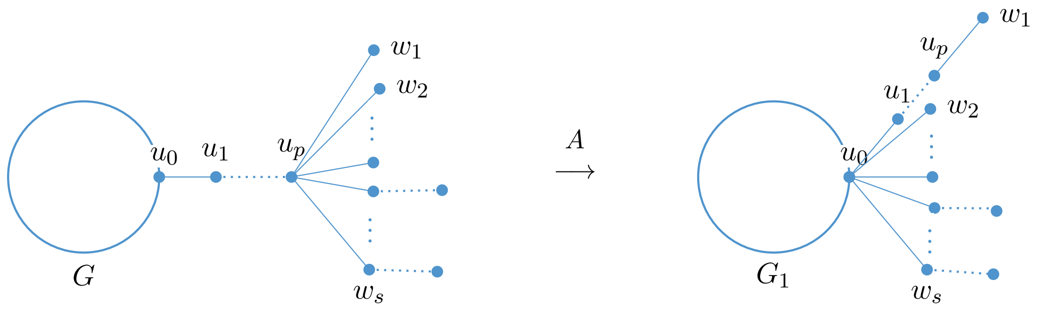

Figure 1. Transformation A.

vertices of some pendant paths attached to u_p. Then $G_1 = G - \{u_pw_2, \ldots, u_pw_s\} + \{u_0w_2, \ldots, u_0w_s\}$, as shown in Figure 1, 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. Since degree of each vertex except u_0 and u_p in G and G_1 are same, we have

$$\begin{aligned} F(G_1) - F(G) &= d^3_{G_1}(u_0) - d^3_G(u_0) + d^3_{G_1}(u_p) - d^3_G(u_p) \\ &= (d_G(u_0) + s - 1)^3 - d^3_G(u_0) + 2^3 - (s+1)^3 \\ &= 3(s-1)(d_G(u_0) - 2)(d_G(u_0) + s + 1) \\ &> 0, \text{ since } d_G(u_0) > 2 \text{ and } s > 1. \end{aligned}$$

Hence, $F(G_1) > F(G)$. □

Remark 2.2. By repeated application of Transformation A, any bicyclic graph can be transformed into such a bicyclic graph that every edge is either an edge of a cycle or an edge of a pendant path and the F-index increases for each such repetition.

Transformation B. *Let u and v be two vertices in G. Also let $u_1, u_2, \ldots, u_s, s > 0$ are the lead vertices of the pendant paths attached to u; $v_1, v_2, \ldots, v_t, t > 0$ are the lead vertices of the pendant paths attached to v 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 $F(G_1) > F(G)$.*

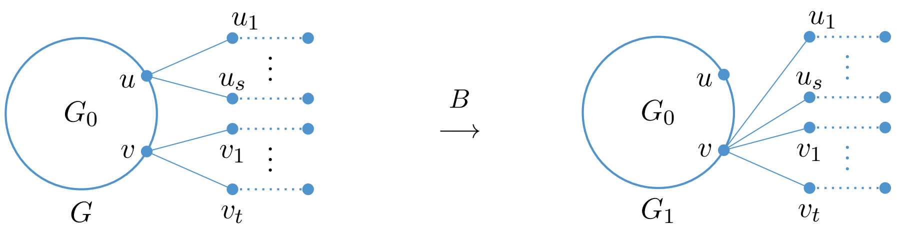

Figure 2. Transformation B.

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 $d_G(u) \le d_G(v)$, we have

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

Hence, $F(G_1) > F(G)$. □

Remark 2.4. Using Transformation B repeatedly, any bicyclic graph can be transformed into such a bicyclic graph that all the pendant paths are attached to the same vertex, and the F-index increases at such repetition.

3. The Graphs with the Largest F-indices

In this section we obtain the bicyclic graph with the largest F-index.

Let us consider the set of all n vertex bicyclic graphs with k pendant vertices and denote it by $\mathbf{B}^k_n$. Clearly, each of the graphs in $\mathbf{B}^k_n$ with two cycles of lengths p and q lies into either of the following three classes.

(1) The set of all $G \in \mathbf{B}^k_n$ in which the cycle C_p and C_q have only one common vertex. This is denoted by $\mathcal{A}(p,q)$. Clearly, $0 \le k \le n-5$ for all $G \in \mathcal{A}(p,q)$.

(2) The set of all $G \in \mathbf{B}^k_n$ in which the cycle C_p and C_q have no common vertex. This is denoted by $\mathcal{B}(p,q)$. For all $G \in \mathcal{B}(p,q), 0 \le k \le n-6$.

(3) The set of all $G \in \mathbf{B}^k_n$ in which the cycle C_p and C_q have a common path of length l. This is denoted by $\mathcal{C}(p,q,l)$. For all $G \in \mathcal{C}(p,q,l), 0 \le k \le n-4$.

We also note that, $\mathcal{C}(p,q,l) = \mathcal{C}(p,p+q-2l,p-l) = \mathcal{C}(p+q-2l,q,q-l)$.

First, we find the bicyclic graph with the largest F-index in $\mathcal{A}(p,q)$.

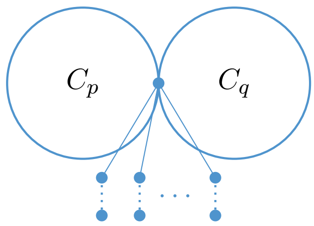

Figure 3. $S_n(p, q)$.

Let $S_n(p, q)$ be a graph in $\mathcal{A}(p, q)$ such that k pendant paths are attached to the common vertex of C_p and C_q, as shown in Figure 3.

Lemma 3.1. *A graph with the largest F-index in $\mathcal{A}(p, q)$ is of the form $S_n(p, q)$.*

Proof. Using the Transformation A and B repeatedly on graph G we can get a graph G_1 such that all the edges not on the cycles are edges on the pendant paths attached to the same vertex u. By Lemma 2.1 and Lemma 2.3, we have $F(G) \leq F(G_1)$ with the equality if and only if all the edges not on the cycles are edges on the pendant paths attached to the same vertex in G. If G_1 is not of the form $S_n(p, q)$, then $u \neq v$, where v is the common vertex of C_p and C_q.

Without loss of generality, we assume that u is on the cycle C_p. Since the degree of all the vertices of $S_n(p, q)$ and those of G_1 are same except for the vertices u and v, we have

$$\begin{aligned} F(S_n(p, q)) - F(G_1) &= \{(k+4)^3 + 2^3\} - \{(k+2)^3 + 4^3\} \\ &= 6k(k+6) \geq 0 \text{ since } k \geq 0. \end{aligned}$$

Equality holds if and only if $k = 0$, or G_1 is of the form $S_n(p, q)$.

Thus the proof is complete. □

Remark 3.2. Degree sequence of every graph of the form $S_n(p, q)$ is $\{1^k, 2^{n-k-1}, k+4\}$ and so, the F-index of every graph of the form $S_n(p, q)$ is $k^3 + 12k^2 + 41k + 56 + 8n, 0 \leq k \leq n - 5$. Clearly, it does not depend on the lengths of the pendant paths or the cycles.

Next we find the bicyclic graph with the largest F-index in $\mathcal{B}(p, q)$.

The bicyclic graph obtained by connecting C_p and C_q by a path P_{r+1} of length r and attaching k pendant paths to the common vertex of C_p and P_r is denoted by $T_n^r(p, q)$, (see Figure 4(a)). Similarly, we have $T_n^r(q, p)$, see Figure 4(b).

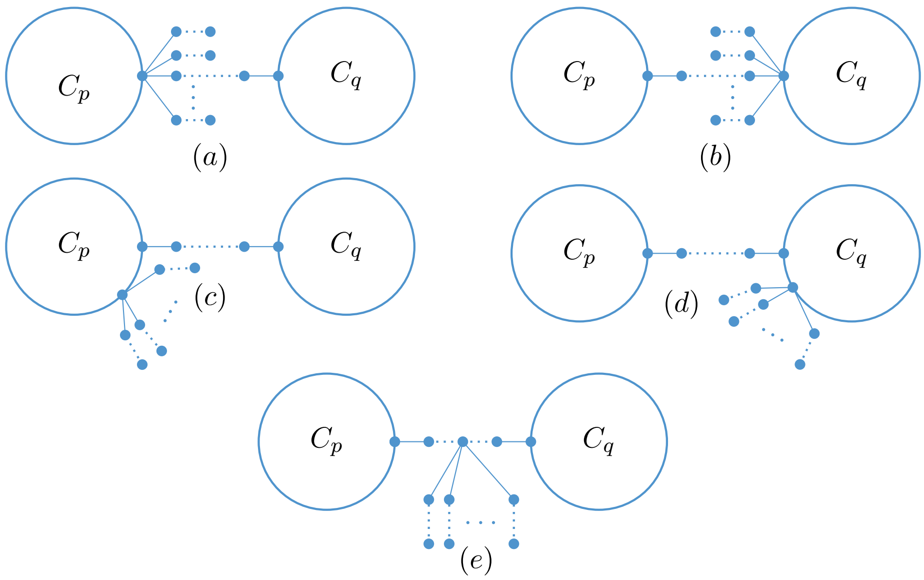

Figure 4. (a) $T_n^r(p,q)$; (b) $T_n^r(q,p)$; (c) Pendant paths are attached to a vertex of C_p which is not common with P_{r+1}; (d) Pendant paths are attached to a vertex of C_q which is not common with P_{r+1}; (e) Pendant paths are attached to a vertex of P_{r+1} which is neither on C_p nor on C_q.

Lemma 3.3. *Let G be a graph in $\mathcal{B}(p,q)$ and C_p and C_q in G are connected by a path of length $r > 0$ and pendant paths are attached to a vertex of C_p which is not common with the path or pendant paths are attached to a vertex of C_q which is not common with the path or pendant paths are attached to a vertex of path which is neither on C_p nor on C_q. Then either*

(i) $F(G) \leq F(T_n^r(p,q))$ with the equality if and only if $G \cong T_n^r(p,q)$;

or

(ii) $F(G) \leq F(T_n^r(q,p))$ with the equality if and only if $G \cong T_n^r(q,p)$.

Proof. Let $W = v_1v_2...v_rv_{r+1}$ be the path connecting C_p and C_q in G, and v_1 be the common vertex of W and C_p, v_{r+1} be the common vertex of W and C_q.

Using the Transformation A and B on the graph G, we can get a graph G_1 such that all the edges not on the cycles are the edges on pendant paths attached to the same vertex v. By Lemma 2.1 and Lemma 2.3, we have $F(G) \leq F(G_1)$ with the equality if and only if all the edges not on the cycles are edges on pendant paths attached to the same vertex in G.

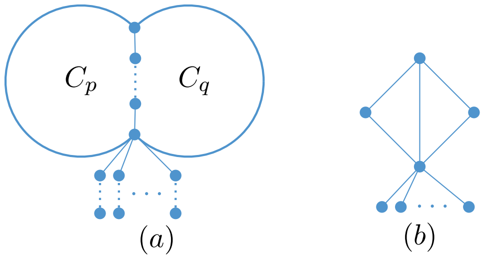

Figure 5. (a) $\theta_n(p,q)$; (b) $\theta_n^*(3,3)$.

Case I. Let v be on the cycle C_p, as shown in Figure 4(c). Since the degree of the vertices of $T_n^r(p,q)$ and those of G_1 are same except for the vertices to which the pendant paths are attached, we have

$$\begin{aligned} F(T_n^r(p,q)) - F(G_1) &= \{(k+3)^3 + 2^3\} - \{(k+2)^3 + 3^3\} \\ &= 3k(k+5) \geq 0 \text{ since } k \geq 0, \end{aligned}$$

with equality if and only if $k = 0$ or G_1 is of the form $T_n^r(p,q)$.
Case II. If v is on the cycle C_q, as shown in figure 4(d). The proof is the same as in Case I.
Case III. Let v be on the path W, as shown in Figure 4(e), then $d_{G_1}(v) = k+2$ and it can be shown in a similar fashion that either $F(T_n^r(p,q)) > F(G_1)$ or $F(T_n^r(q,p)) > F(G_1)$. □

Remark 3.4. Every graph of the form $T_n^r(p,q)$ or $T_n^r(p,q)$ has the degree sequence $\{1^k, 2^{n-k-2}, 3^1, k+3\}$, and thus each of them has the F-index $k^3 + 9k^2 + 20k + 38 + 8n, 0 \leq k \leq n-6$. Clearly, it does not depend on the lengths of the pendant paths or the cycles.

Lastly, we find the bicyclic graph with the largest F-index in $\mathcal{C}(p,q,l)$.

Let $\theta_n(p,q)$ be a graph in $\mathcal{C}(p,q,l)$ such that k pendant paths are attached to a common vertex of C_p and C_q and their common path, as shown in Figure 5(a). In particular, $\theta_n^*(3,3)$ denotes the graph where k pendant edges are attached to a common vertex of two triangles having a common edge.

Lemma 3.5. *A graph with the largest F-index in $\mathcal{C}(p,q,l)$ is of the form $\theta_n(p,q)$.*

Proof. Using the Transformation A and B on graph G, we can get a graph G_1 such that all the edges not on the cycles are on the pendant paths attached to the same vertex v in G. By Lemma 2.1 and Lemma 2.3, we have $F(G_1) \geq F(G)$ with the equality if and only if all the edges not on the cycles are the edges on the pendant paths attached to the same vertex in G.

If the vertex v is different from either of the common vertex of C_p, C_q and their common path, then we have

$$\begin{aligned} F(\theta_n(p,q)) - F(G_1) &= \{(k+3)^3 + 2^3\} - \{(k+2)^3 + 3^3\} \\ &= 3k(k+5) \geq 0 \text{ since } k \geq 0, \end{aligned}$$

with equality if and only if $k = 0$ or G_1 is of the form $\theta_n(p,q)$. □

Remark 3.6. Degree sequence of every graph of the form $\theta_n(p,q)$ being $\{1^k, 2^{n-k-2}, k+3, 3^1\}$, F-index of every graph of that form is $k^3+9k^2+20k+38+8n, 0 \leq k \leq n-4$. Clearly, it does not depend on the lengths of the pendant paths or the cycles.

Finally we have the following theorem.

Theorem 3.7. *The graph with largest F-index in $\mathbf{B}_n^k$ is of the form $S_n(p,q)$ if $0 \leq k \leq n-5$, and is the unique graph $\theta_n^*(3,3)$ if $k = n-4$.*

Proof. Let G be the graph with largest F-index among all bicyclic graphs with n vertices and k pendant vertices. From Lemma 3.1, Lemma 3.3, and Lemma 3.5, it is clear that G is of the form $S_n(p,q)$, $T_n^r(p,q)$ or $\theta_n(p,q)$. Comparing the corresponding F-indices, we have

$$\begin{aligned} F(G) &= \begin{cases} k^3 + 12k^2 + 41k + 56 + 8n, & 0 \leq k \leq n-5 \\ k^3 + 9k^2 + 20k + 38 + 8n, & k = n-4 \end{cases} \\ &= \begin{cases} k^3 + 12k^2 + 41k + 56 + 8n, & 0 \leq k \leq n-5 \\ n^3 - 3n^2 + 4n + 38, & k = n-4. \end{cases} \end{aligned}$$

It is easy to follow that if $k = n-4$, $\theta_n^*(3,3)$ is the only graph of the form $\theta_n(p,q)$. □

Theorem 3.8. *The graph with largest F-index among all bicyclic graphs with n vertices is $\theta_n^*(3,3)$.*

Proof. Let $f(n,k) = k^3 + 12k^2 + 41k + 56 + 8n, 0 \leq k \leq n-5$. Then $\frac{\partial f}{\partial k} = 3k^2 + 24k + 41 > 0$ for $k \geq 0$. Thus $f(n,k)$ is a monotonic increasing function of k. Hence $f(n,0) \leq f(n,k) \leq f(n,n-5)$ for $0 \leq k \leq n-5$, i.e., $8n + 56 \leq f(n,k) \leq n^3 - 3n^2 + 4n + 28$ for $0 \leq k \leq n-5$. Thus the result follows from the above theorem. □

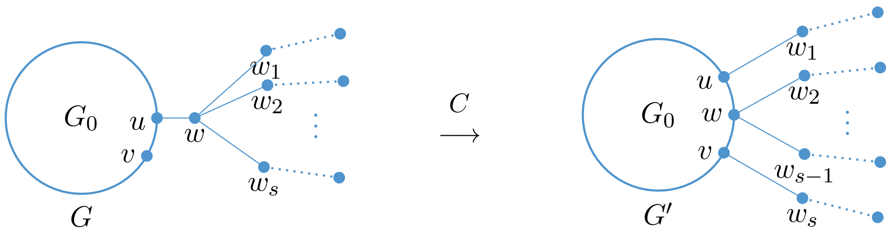

Figure 6. Transformation C.

4. Two Transformations which decrease the F-index

The following transformations decrease the F-index of a graph.

Transformation C. *Let u be a vertex of G and $d_G(u) \geq 2$. Also let $\{v, w\} \subseteq N_G(u)$ be such that $vw \notin E(G), d_G(w) > d_G(v)$, and $w_1, w_2, \ldots, w_s, s \geq 2$ be the lead vertices of pendant paths attached to w. Then $G' = G - \{uv, ww_1, ww_s\} + \{uw_1, vw, vw_s\}$, as shown in Figure 6, is said to be the graph obtained from G by Transformation C.*

Lemma 4.1. *Let G' be obtained from G by Transformation C. Then $F(G') \leq F(G)$.*

Proof. Since the degrees of all the vertices in G' and those of all the vertices in G are same, except for the vertices v and w, we have

$$\begin{aligned} F(G') - F(G) &= d^3_{G'}(v) - d^3_G(v) + d^3_{G'}(w) - d^3_G(w) \\ &= (d_G(v)+1)^3 - d^3_G(v) + (d_G(w)-1)^3 - d^3_G(w) \\ &= 3(d_G(v)+d_G(w))(d_G(v)-d_G(w)+1) \leq 0 \text{ since } d_G(v) < d_G(w). \end{aligned}$$

Hence, $F(G') \leq F(G)$. □

Transformation D. *Let u and v be two vertices in G. Also let $uu_1, uu_2, \ldots, uu_s$ be the pendant edges attached to u, $vv_1, vv_2, \ldots, vv_t$ be the pendant edges attached to v and $d_G(v) - d_G(u) > 1$. Then $G' = G - \{vv_1\} + \{uv_1\}$, as shown in Figure 7, is said to be the graph obtained from G by Transformation D.*

Lemma 4.2. *Let G' be obtained from G by Transformation D. Then $F(G') < F(G)$.*

Proof. Since the degrees of all the vertices in G' 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

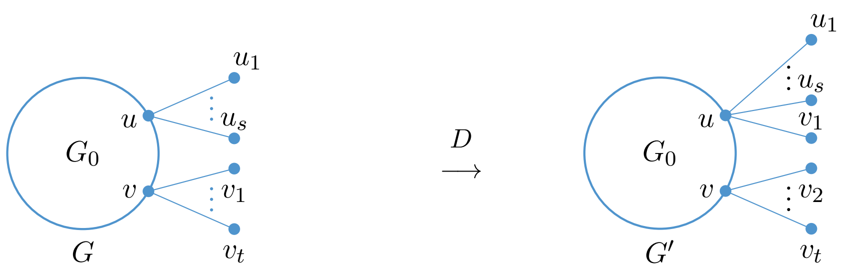

Figure 7. Transformation D.

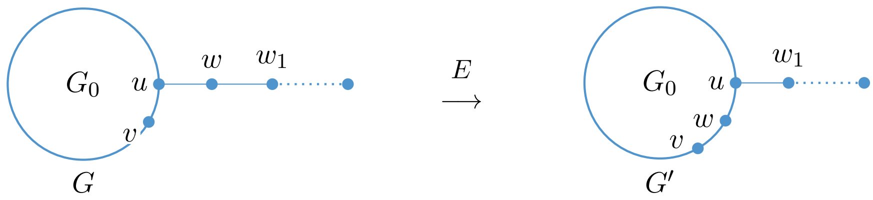

Figure 8. Transformation E.

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

Hence, $F(G') < F(G)$. □

5. Graphs with Smallest F-indices

It is clear from the definition of F-index that it depends on the degree sequence only. There may be several graphs with same F-index if they have same degree sequences. To understand easily the structure of a class of graphs having smallest F-indices, we define the following transformation which does not change the degree sequence of the graph and hence the F-index.

Transformation E. *Let uv be an edge of a cycle in G. Also let w be the lead vertex of a pendant path attached to u. Then $G' = G - \{uv, ww_1\} + \{wv, uw_1\}$, as shown in Figure 8, is said to be the graph obtained from G by Transformation E.*

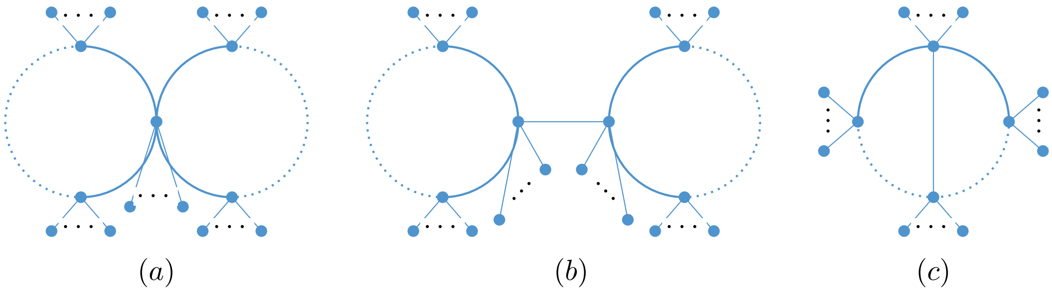

Figure 9. (a) F_1; (b) F_2; (c) F_3.

Since degree of each vertex of G remains unaltered under Transformation E, it is clear that $F(G') = F(G)$ if G' is obtained from G by Transformation E.

Lemma 5.1. *Any bicyclic graph G can be transformed to a graph G' with either of the forms F_1, F_2 or F_3 as shown in Figure 9, so that the $F(G') \leq F(G)$.*

Proof. By repeated applications of Transformation C on G, we get a graph $G^{\#}$ whose each edge is either on a cycle or on a pendant path and $F(G^{\#}) \leq F(G)$. Now, if we repeat Transformation E on $G^{\#}$ successively, we get a graph G' whose each edge is either an edge of a cycle or a pendant edge, and $F(G^{\#}) = F(G')$. Clearly, G' will have either of the forms F_1, F_2 or F_3, if G is in $\mathcal{A}(p,q), \mathcal{B}(p,q)$ or $\mathcal{C}(p,q,l)$ respectively. □

Theorem 5.2. *A graph of the form F_2 or F_3 has smallest F-index in $\mathbf{B}_n^k$ if $0 \leq k < (n-1)/2$. A graph with either of the forms F_1, F_2 or F_3 has smallest F-index in $\mathbf{B}_n^k$ if $(n-1)/2 \leq k \leq n-6$. A graph of the form F_1 or F_3 has smallest F-index in $\mathbf{B}_n^k$ if $(n-1)/2 \leq k = n-5$ and a graph of the form F_3 has minimum F-index in $\mathbf{B}_n^k$ if $(n-1)/2 \leq k = n-4$. In each case, every non-pendant vertex is of almost equal degree.*

Proof. Transformation D can be applied repeatedly to reduce the F-index of a graph G having the form F_1, F_2 or F_3 until every non-pendant vertex is of almost equal degree except when $k < (n-1)/2$ and $G \in \mathcal{A}(p,q)$. When $k < (n-1)/2$, the F-index of G can be reduced by repeated applications of Transformation D until the degree sequence becomes $\{1^k, 2^{n-2k-1}, 3^k, 4\}$ if $G \in \mathcal{A}(p,q)$, and $\{1^k, 2^{n-2k-2}, 3^{k+2}\}$ if $G \in \mathcal{B}(p,q)$ or $G \in \mathcal{C}(p,q,l)$. Now, the F-indices of two graphs with degree sequences $\{1^k, 2^{n-2k-1}, 3^k, 4\}$ and $\{1^k, 2^{n-2k-2}, 3^{k+2}\}$ are $8n + 12k + 58$ and $8n + 12k + 38$ respectively.

For $k = n-5$, no graph of the form F_2 exists, and for $k = n-4$, no graph of the form F_1 or F_2 is possible. Hence the theorem follows. □

Theorem 5.3. *A bicyclic graph with smallest F-index has the degree sequence* $\{2^{n-2}, 3^2\}$.

Proof. From Theorem 5.2, it is evident that the degree sequence of a graph with smallest F-index in $\mathbf{B}_n^k$ is $\{1^k, q^{n-k-r}, (q+1)^r\}$, where

$$2(n+1) - k = (n-k)q + r, 0 \leq r < n-k.$$

The F-index of such a graph is

$$k.1^3 + (n-k-r)q^3 + r(q+1)^3 = g(k) \quad \text{(say)}.$$

We shall show that $g(k)$ is a monotonic increasing function of k.

With the above values of q and r, the degree sequence of a graph with smallest F-index in $\mathbf{B}_n^{k+1}$ is

$$\{1^{k+1}, q^{(n-k)-(q+r)}, (q+1)^{q+r-1}\}$$

if $1 \leq q+r < n-k$, and

$$\{1^{k+1}, (q+1)^{2(n-k)-(q+r)-1}, (q+2)^{(q+r)-(n-k)}\}$$

if $q+r \geq n-k$ since

$$2(n+1)-(k+1) = \begin{cases} (n-k-1)q + (q+r-1), \text{when } 0 \leq q+r-1 < n-k-1, \\ (n-k-1)(q+1) + (q+r) - (n-k), \text{otherwise.} \end{cases}$$

So,

$$g(k+1) = \begin{cases} (k+1)1^3 + \{(n-k)-(q+r)\}q^3 + (q+r-1)(q+1)^3, \text{when} \\ 1 \leq q+r < n-k, \\ (k+1)1^3 + \{2(n-k)-(q+r)-1\}(q+1)^3 + \{(q+r)-(n-k)\} \\ (q+2)^3, \text{ when } q+r \geq n-k. \end{cases}$$

Case I. $(1 \leq q+r < n-k)$

Here, $g(k) < g(k+1)$ if

$$\begin{aligned} 0 &< 1 - q.q^3 + (q-1)(q+1)^3 \\ \text{i.e., if } q^4 &< 1 + (q-1)(q+1)^3 \\ \text{i.e., if } q^4 &< 1 + (q^2-1)(q^2+2q+1) \\ \text{i.e., if } q^4 &< 1 + q^4 + 2q^3 + q^2 - q^2 - 2q - 1 \\ \text{i.e., if } 0 &< 2q(q^2-1). \end{aligned}$$

Since $q \geq 2$, the last inequality is true indeed. Hence, $g(k) < g(k+1)$.

Case II. $(q + r \geq n - k)$

Here, $g(k) < g(k + 1)$ if

$$\begin{aligned}
(n-k-r)q^3 + r(q+1)^3 &< 1 + \{2(n-k) - (q+r) - 1\}(q+1)^3 + \\
&\quad \{(q+r) - (n-k)\}(q+2)^3 \\
\text{i.e., if } (n-k)q^3 - rq^3 + r(q+1)^3 &< 1 + (n-k)(q+1)^3 + \{(q+r) - (n-k)\} \\
&\quad \{(q+2)^3 - (q+1)^3\} - (q+1)^3 \\
\text{i.e., if } r\{(q+1)^3 - q^3\} &< 1 + (n-k)\{(q+1)^3 - q^3\} + \{(q+r) - \\
&\quad (n-k)\}(3q^2 + 9q + 7) - (q+1)^3 \\
\text{i.e., if } r(3q^2 + 3q + 1) &< 1 + (n-k)(3q^2 + 3q + 1) + \{(q+r) - \\
&\quad (n-k)\}(3q^2 + 9q + 7) - (q+1)^3 \\
\text{i.e., if } r(3q^2 + 3q + 1) &< 1 + (n-k)(3q^2 + 3q + 1 - 3q^2 - 9q - 7) + \\
&\quad (q+r)(3q^2 + 9q + 7) - (q+1)^3 \\
\text{i.e., if } r(3q^2 + 3q + 1) &< 1 - 6(n-k)(q+1) + (q+r)(3q^2 + 9q + 7) \\
&\quad -(q+1)^3 \\
\text{i.e., if } r(3q^2 + 3q + 1) &< -6(n-k)(q+1) + (q+r)(3q^2 + 9q + 7) \\
&\quad -(q^3 + 3q^2 + 3q) \\
\text{i.e., if } 6(n-k)(q+1) &< r(3q^2 + 9q + 7 - 3q^2 - 3q - 1) + \\
&\quad (3q^3 + 9q^2 + 7q) - (q^3 + 3q^2 + 3q) \\
\text{i.e., if } 6(n-k)(q+1) &< 6r(q+1) + 2q^3 + 6q^2 + 4q \\
\text{i.e., if } 6(n-k-r)(q+1) &< 2q(q^2 + 3q + 2) \\
\text{i.e., if } 6(n-k-r)(q+1) &< 2q(q+2)(q+1) \\
\text{i.e., if } 3(n-k-r) &< q(q+2).
\end{aligned}$$

Now, $q + r \geq n - k$ gives $n - k - r \leq q$ and so, $3(n - k - r) \leq 3q < q^2 + 2q$ since $q < q^2$ for all $q > 1$. Therefore, $g(k) < g(k + 1)$.

Thus, in both cases $g(k)$ is monotonic increasing in k, and so $g(k) \geq g(0)$ for $k \geq 0$.

Now, from Theorem 5.2, $g(0) = 8n + 38$ and the corresponding degree sequence is $\{2^{n-2}, 3^2\}$.

Hence the theorem. □

6. Discussion and Conclusion

In this paper, we have obtained the graphs with smallest and largest F-indices among the bicyclic graphs with k pendant vertices. As consequences, we have also obtained the bicyclic graphs with smallest and largest F-indices. In [14], Zhang et al. have obtained the bicyclic graphs with smallest and largest general Zagreb index $M_1^\alpha, \alpha > 1$ as the graphs with degree sequences $\{2^2, 3, n-1, 1^{n-4}\}$ and $\{2^{n-2}, 3^2\}$ respectively. Clearly, M_1^3 is nothing but the F-index. Also in [11], it is found that the bicyclic graph with smallest F-index has the degree sequence $\{2^{n-2}, 3^2\}$. We have obtained those results as corollaries of our main results. Hence, our results generalize some previous works. In [2], Akhter et al. 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. So, the results obtained there are not comparable with our results. Rather, our work is a genaralization of that work also.

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[a]DEPARTMENT OF EDUCATION, ASSAM UNIVERSITY, SILCHAR - 788 011, INDIA.
Email address: aminruhul80@gmail.com

[b]DEPARTMENT OF MATHEMATICS AND STATISTICS, ALIAH UNIVERSITY, KOLKATA - 700 160, INDIA.
Email address: nayeem.math@aliah.ac.in/ nayeemsma@gmail.com