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EXTREMAL F-INDEX OF A GRAPH WITH k CUT EDGES

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Abstract. The so called forgotten index or F-index is defined as the sum of cubes of vertex degrees of a molecular graph. In this paper, we have obtained the upper and lower bounds of F-index for the graphs with k cut edges and also we have characterized the extremal graphs.

1. Introduction

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. If an end vertex of an edge is of degree one, then the edge is called a pendant edge. A cut-edge is an edge of G which when removed from G, leaves it disconnected. The path, cycle and star of n vertices are denoted by P_n, C_n and $K_{1,n-1}$ respectively. If two simple connected graphs G_1 and G_2 are concatenated at a common vertex v, we denote the new graph as G_1vG_2. The vertex set of G_1vG_2 is $V(G_1) \cup V(G_2)$, where $V(G_1) \cap V(G_2) = \{v\}$, and edge set of G_1vG_2 is $E(G_1) \cup E(G_2)$. Similarly, the concatenation of the graphs G_1 and G_2 by adding an edge uv between the graphs G_1 and G_2 such that $u \in V(G_1)$ and $v \in V(G_2)$ is denoted by G_1uvG_2.

The first Zagreb index being one of the oldest degree based topological index, is defined as

$$M_1(G) = \sum_{v \in V(G)} [d_G(v)]^2.$$

In the paper where Zagreb indices were introduced for the first time by Gutman and Trinajstić [4], it was shown that total π-electron energy has correlation with both the sum of squares and sum of cubes of the vertex degrees of the underlying molecular graph. Eventually, the sum of squares of vertex degrees became known as the first Zagreb index, but the sum of cubes of vertex degrees remained unnoticed

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by researchers until a recent work of Furtula and Gutman, where they have named it "forgotten" topological index, or F-index [3]. Formally, F-index is defined as $F(G) = \sum_{v\in V(G)}[d_G(v)]^3$. It is easy to follow that $M_1(G) = \sum_{uv\in E(G)}[d_G(u)+d_G(v)]$ and $F(G) = \sum_{uv\in E(G)}[d_G(u)^2 + d_G(v)^2]$.

Finding the extremal values or bounds for the topological indices of graphs, as well as related problems of characterizing the extremal graphs are among the most studied research topics in mathematical chemistry during last few decades. Extremal trees with respect to F-index have been found by Abdo et al. [1]. Ordering of unicyclic graphs with respect to F-index have also been done [6]. Extremal Zagreb indices of graphs with a given number of cut edges have been studied by Chen [2].

Let $\mathcal{G}_{n,k}$ be the set of graphs with n vertices and k cut edges. Let $\{e_1, e_2, \ldots, e_k\}$ be the set of cut edges of G. The connected graphs with k cut edges have been considered by many researchers while finding extremal topological indices [2, 5, 7, 8]. If an edge e of G is on a cycle in G, e cannot be a cut-edge. Every edge of G is a cut-edge if and only if G is a tree. Since the extremal trees with respect to F-index have already been studied, we assume that G contains at least one cycle. Thus the number of its cut edges is at most $n - 3$. Therefore, in the following discussion we consider $1 \leq k \leq n - 3$.

In this paper, we investigate the graphs in $\mathcal{G}_{n,k}$ and determine the graphs with the largest and smallest F-indices among them.

2. Some transformations which increase the F-index

Since addition of an edge e to G increases the degrees of each of the end vertices of e by one, and deletion of an edge e from G reduces the degrees of each of the end vertices of e by one, the following proposition is obvious. By $G+e$ we mean the graph obtained by adding an edge $e = uv \notin E(G), u, v \in V(G)$ to G. Similarly, by $G-e$ we mean the graph obtained by deleting the edge e from G.

Proposition 2.1. *Let $G = (V, E)$ is a simple connected graph.*
(i) If $e = uv \notin E(G), u, v \in V(G)$, then $F(G) < F(G + e)$;

(ii) If $e \in E(G)$, then $F(G) > F(G - e)$.

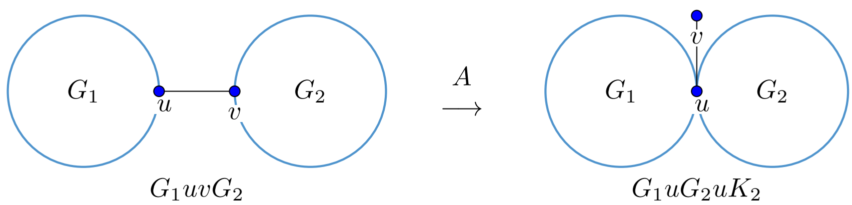

Figure 1: Transformation A.

Lemma 2.2. *Let G_1uvG_2 and $G_1uG_2uK_2$ be two graphs as shown in Figure 1, with $|V(G_1)|, |V(G_2)| \geq 2$, where G_1, G_2 have no cut-edges and uv is a non-pendant cut edge of G_1uvG_2. Then $F(G_1uG_2uK_2) > F(G_1uvG_2)$.*

Proof. Let G^*=G_1uvG_2 and G^{**}=$G_1uG_2uK_2$. By the definition of F-index, we have

$$\begin{aligned}F(G^{**}) - F(G^*) &= d^3_{G^{**}}(u) + 1^3 - d^3_{G^*}(u) - d^3_{G^*}(v)\\ &= [d_{G^*}(u) + d_{G^*}(v) - 1]^3 + 1 - d^3_{G^*}(u) - d^3_{G^*}(v)\\ &= 3d^2_{G^*}(u)[d_{G^*}(v) - 1] + 3d_{G^*}(u)[d_{G^*}(v) - 1]^2 - 3d^2_{G^*}(v) + 3d_{G^*}(v)\\ &= 3[d_{G^*}(u) + d_{G^*}(v)][d_{G^*}(u)d_{G^*}(v) - d_{G^*}(u) - d_{G^*}(v) + 1] > 0.\end{aligned}$$

Hence, $F(G_1uG_2uK_2) > F(G_1uvG_2)$. □

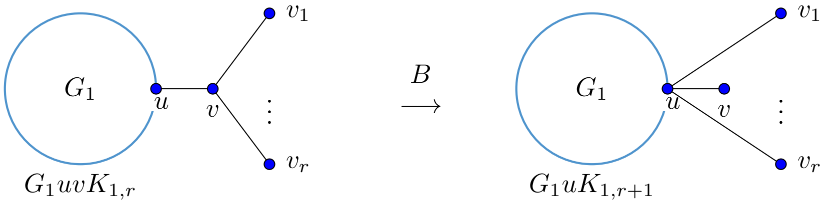

Figure 2: Transformation B.

Lemma 2.3. *Let $G_1uvK_{1,r}$ and $G_1uK_{1,r+1}$ be two graphs as shown in Figure 2, with $|V(G_1)| \geq 2$, where G_1 is a 2-edge connected graph and uv is a non pendant cut edge of $G_1uvK_{1,r}$. Then $F(G_1uK_{1,r+1}) > G_1uvK_{1,r}$.*

Proof. Let G^*=$G_1uvK_{1,r}$ and G^{**}=$G_1uK_{1,r+1}$. By the definition of F-index, we have

$$\begin{aligned}F(G^{**}) - F(G^*) &= d^3_{G^{**}}(u) + 1 - d^3_{G^*}(u) - d^3_{G^*}(v)\\ &= [d_{G^*}(u) + d_{G^*}(v) - 1]^3 + 1 - d^3_{G^*}(u) - d^3_{G^*}(v)\\ &= 3d^2_{G^*}(u)[d_{G^*}(v) - 1] + 3d_{G^*}(u)[d_{G^*}(v) - 1]^2 - 3d^2_{G^*}(v) + 3d_{G^*}(v)\\ &= 3[d_{G^*}(u) + d_{G^*}(v)][d_{G^*}(u)d_{G^*}(v) - d_{G^*}(u) - d_{G^*}(v) + 1] > 0.\end{aligned}$$

Hence, $F(G_1uK_{1,r+1}) > F(G_1uvK_{1,r})$. □

Lemma 2.4. *Let G be a graph and u, v be two vertices of G such that $u_1, u_2, \ldots, u_s$ are the pendant edges adjacent to u and $v_1, v_2, \ldots, v_t$ are pendant edges adjacent to v. $G^{'} = G - \{uu_1, uu_2, \ldots, uu_s\} + \{vu_1, vu_2, \ldots, vu_s\}, G^{''} = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \ldots, uv_t\}$ and $|V(G_0)| \geq 3$, as shown in Figure 3. Then either $F(G^{'}) > F(G)$ or $F(G^{''}) > F(G)$.*

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

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

$$\begin{aligned} F(G^{''}) - F(G) &= d^3_{G''}(v) + d^3_{G''}(u) - d^3_G(v) - d^3_G(u) \\ &= [d_G(v) - t]^3 + [d_G(u) + t]^3 - d^3_G(v) - d^3_G(u) \\ &= 3t[d_G(u) + d_G(v)][d_G(u) - d_G(v) + t]. \end{aligned}$$

Since either $d_G(v) \geq d_G(u)$ or $d_G(u) \geq d_G(v)$, we have therefore either $F(G^{'}) > F(G)$ or $F(G^{''}) > F(G)$. □

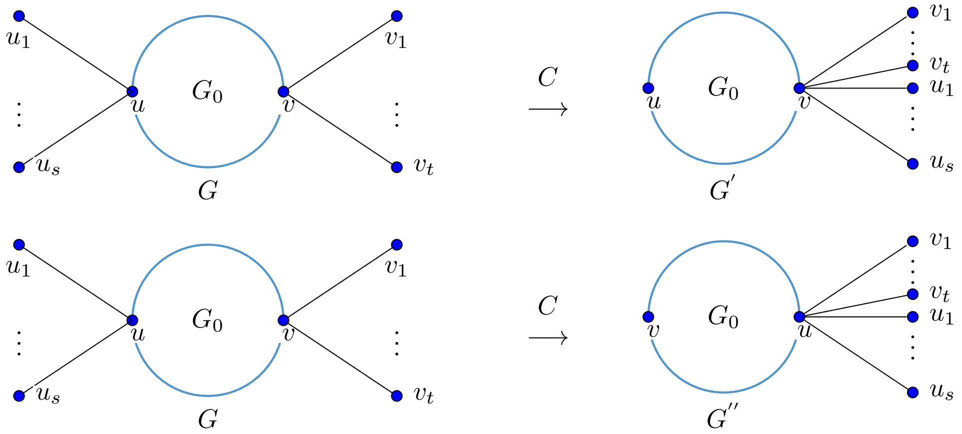

Figure 3: Transformation C.

LEMMA 2.5. *Let $G \in \mathcal{G}_{n,k}$. Any non-pendant cut edge of G can be transformed to a pendant cut-edge by applying the transformation A and Transformation B repeatedly, so that we obtain a graph $G^* = S_1uS_2u\ldots uS_l$ as shown in Figure 4, where each $S_i, 1 \leq i \leq l$ has no non-pendant cut-edges. Clearly, the F-index increases at each application of the Transformation A and Transformation B.*

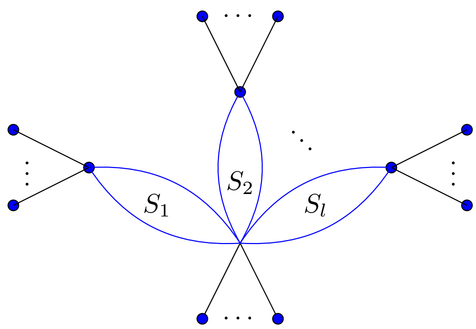

Figure 4: The graph G^*.

LEMMA 2.6. *By repeating Transformation C, we can attach all the pendant edges at the same vertex to get a graph of the form H_1, H_2 or H_3 as shown in Figure 5, so that F-index increases at each application of Transformation C.*

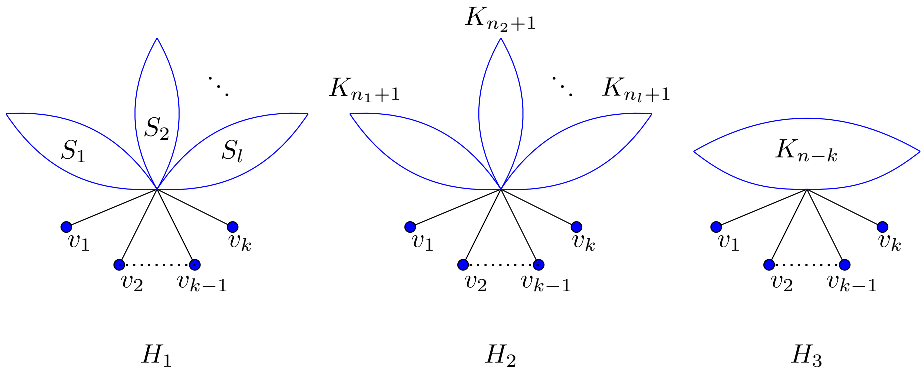

Figure 5: The graphs H_1, H_2, H_3.

3. Upper bound of F-index for the graphs in $\mathcal{G}_{n,k}$

THEOREM 3.1. *For all connected graphs G in $\mathcal{G}_{n,k}$, $F(G) \leq (n-k-1)^4 + (n-k)^3 + k$, and the maximum F-index is achieved uniquely at K_n^k, where K_n^k is the graph obtained by joining k pendent vertices to one vertex of K_{n-k}.*

Proof. From Lemma 2.6, it follows that we have three candidate graphs H_1, H_2 and H_3 in $\mathcal{G}_{n,k}$, as shown in Figure 5, for the upper bound of F-index.

We consider three claims as follows.

Claim 1. For the graphs H_1 and H_2, we have $F(H_1) \leq F(H_2)$.

If we add an edge $e \notin E(G)$ to G, then by Proposition 2.1 we have $F(G+e) > F(G)$. The sub-graphs K_{n_i+1} $(i = 1, 2, \ldots, l)$ are obtained by adding some edges to the

2-edge connected graphs S_i $(i = 1, 2, \ldots, l)$. Thus the graph H_2 is obtained by adding some edges to the graph H_1. Hence $F(H_1) \leq F(H_2)$. Equality holds if and only if $H_1 \cong H_2$.

Claim 2. For the graphs H_2 and H_3, we have $F(H_2) \leq F(H_3)$.

If we add edges between every two vertices of the sub-graphs K_{n_i+1} $(i = 1, 2, \ldots, l)$ of H_2, H_2 will be changed into the graph H_3. Thus the graph H_3 is obtained by adding some edges to the graph H_2. Therefore by Proposition 2.1 we have $F(H_2) \leq F(H_3)$. Equality holds if and only if $H_2 \cong H_3$.

Claim 3. For any graph $G \in \mathcal{G}_{n,k}$, $F(G) \leq F(H_3)$.

Suppose that $G \in \mathcal{G}_{n,k}$ and G is not isomorphic to H_3. Then by Lemma 2.6, Claim 1. and Claim 2., we have $F(G) \leq F(H_3)$. Clearly, $F(G) = F(H_3)$, only when G isomorphic to H_3.

Combining the above three claims we have, $H_3 \cong K_n^k$ has maximum F-index $F(K_n^k) = (n-k-1)^4 + (n-k)^3 + k$, and the theorem follows. $\square$

4. Two transformations which decrease the F-index

Lemma 4.1. *Let G be a graph and u, v be two vertices of G such that $u_1, u_2, \ldots, u_s$ are the pendant vertices adjacent to u and $v_1, v_2, \ldots, v_t$ are pendant vertices adjacent to v. Let $G_3 = G - vv_1 + v_2v_1$, as shown in Figure 6. Then $F(G_3) < F(G)$.*

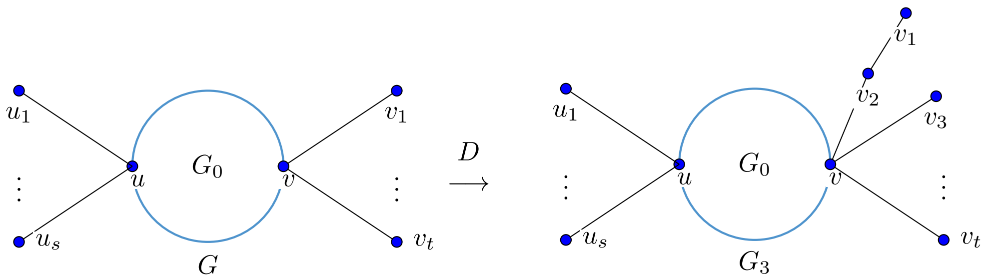

Figure 6: Transformation D.

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

$$\begin{aligned} F(G) - F(G_3) &= d_G^3(v) + d_G^3(v_2) - d_{G_3}^3(v) - d_{G_3}^3(v_2) \\ &= d_G^3(v) + 1 - (d_G(v) - 1)^3 - 2^3 = 3d_G^2(v) - 3d_G(v) - 6 \\ &= 3d_G(v)(d_G(v) - 1) - 6 > 0 \quad (\text{since } d_G(v) \geq 3)\,. \end{aligned}$$

Hence $F(G) > F(G_3)$. □

Lemma 4.2. *Let G be a graph and u, v be two vertices of G such that $u_1, u_2, \ldots, u_s$ are the pendant vertices adjacent to u and $v_1, v_2, \ldots, v_t$ are pendant vertices adjacent to v. Let $G_4 = G - uu_1 + v_1u_1$, as shown in Figure 7. Then $F(G_4) < F(G)$.*

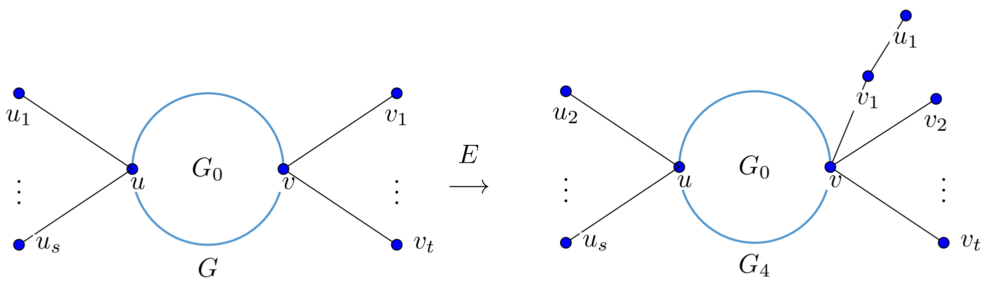

Figure 7: Transformation E.

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

$$\begin{aligned} F(G) - F(G_4) &= d_G^3(u) + d_G^3(v_1) - d_{G_4}^3(u) - d_{G_4}^3(v_1) = d_G^3(u) + 1 - (d_G(u) - 1)^3 - 2^3 \\ &= 3d_G(u)(d_G(u) - 1) - 6 > 0 \quad (\text{since } d_G(u) \geq 3)\,. \end{aligned}$$

Hence $F(G) > F(G_4)$. □

5. Lower bound of F-index for the graphs in $\mathcal{G}_{n,k}$

THEOREM 5.1. *For the connected graphs G in $\mathcal{G}_{n,k}$, $F(G) \geq 4(2n+3)$, and the minimum F-index is obtained uniquely at C_n^k, where C_n^k is a graph obtained by joining a path of length k to one vertex of C_{n-k}.*

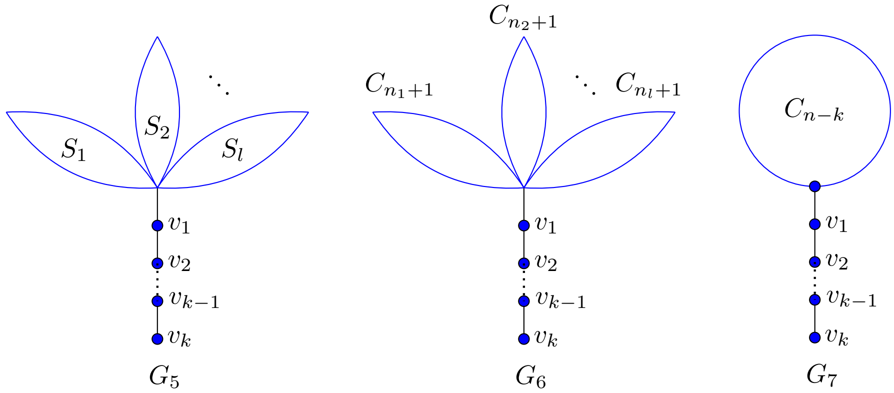

Figure 8: The graphs G_5, G_6 and G_7.

Proof. From Lemma 4.1 and Lemma 4.2, we have three graphs in $\mathcal{G}_{n,k}$, namely G_5, G_6 and G_7 as shown in Figure 8, for the lower bound of F-index.

We consider three claims as follows.

Claim 1. For the graphs G_5 and G_6, we have $F(G_5) \geq F(G_6)$.

The graphs C_{n_i+1} $(i = 1, 2, \ldots, l)$ are obtained by deleting some edges from the 2-edge connected graphs S_i $(i = 1, 2, \ldots, l)$. Thus the graph G_6 is obtained by deleting some edges from the graph G_5. Therefore by Proposition 2.1, we have $F(G_5) \geq F(G_6)$. Equality holds if and only if $G_5 \cong G_6$.

Claim 2. For the graphs G_6 and G_7, we have $F(G_6) \geq F(G_7)$.

By the definition of F-index we have,

$$F(G_6)-F(G_7) = \{(n-2)2^3+(2l+1)^3+1^3\} - \{(n-2)2^3+3^3+1^3\} \geq 0 \text{ (since } l \geq 1).$$

Hence, $F(G_6) \geq F(G_7)$. Equality holds if and only if $G_6 \cong G_7$.

Claim 3. For a graph $G \in \mathcal{G}_{n,k}$, $F(G) \geq F(G_7)$.

The proof folows directly from Lemma 4.1, Lemma 4.2, Claim 1. and Claim 2. Combining the above three claims, we have $G_7 \cong C_n^k$ has minimum F-index $F(C_n^k) = (n-2)2^3 + 3^3 + 1^3 = 4(2n+3)$ and the theorem follows. □

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