Extremal Zagreb Indices of Graphs with a Given Number of Cut Edges

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Abstract For a graph, the first Zagreb index M_1 is equal to the sum of the squares of the degrees of the vertices, and the second Zagreb index M_2 is equal to the sum of the products of the degrees of pairs of adjacent vertices. Denote by $\mathcal{G}_{n,k}$ the set of graphs with n vertices and k cut edges. In this paper, we showed the types of graphs with the largest and the second largest M_1 and M_2 among $\mathcal{G}_{n,k}$.

Keywords Zagreb index · Cut edges · Grafting transformation

Mathematics Subject Classification (2000) 05C05 · 92E10 · 05C35

1 Introduction

We use Bondy and Murty [1] for terminology and notions not defined here. Let $G = (V, E)$ be a simple connected graph with n vertices and m edges. For any $v \in V$, $N(v)$ denotes the neighbors of v , and $N_G[v] = \{v\} \cup \{u | uv \in E(G)\}$, $d_G(v) = |N(v)|$ is the degree of v . A leaf is a vertex of degree one and a stem is a vertex adjacent to at least one leaf, pendant edges are edges incident to a leaf and stem, denote it simply as K_2 . The distance $d(x, y)$ from a vertex x to another vertex y is the minimum number of edges in a x – y path. The distance $d_G(x, S)$ from a vertex x to the set S is $\min_{y \in S} d(x, y)$. Let P_n ,

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C_n and $K_{1,n-1}$ be the path, cycle and the star on n vertices. The cyclomatic number of a connected graph G is defined as $c(G) = m - n + 1$. A graph G with $c(G) = k$ is called a k cyclic graph, for $c(G) = 0, 1$ and 2 , we named G as tree, unicyclic graph and bicyclic graph, resp. For any two graphs G_1 and G_2 , if there exists a common vertex v between them, we denote this graph as $G_1 v G_2$, i.e., the vertex set of $G_1 v G_2$ is $V(G_1) \cup V(G_2)$, $V(G_1) \cap V(G_2) = \{v\}$, and $E(G_1 v G_2) = E(G_1) \cup E(G_2)$. If there are l copies of graphs $G_1, G_2, \dots, G_l (l \geq 2)$ with all graphs sharing one common vertex v , then, we denote this graph as $G_1 v G_2 v \dots v G_l$. If there exists a bridge uv between them such that $u \in V(G_1)$ and $v \in V(G_2)$, we denote this graph as $G_1 uv G_2$. Let $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E' . $W \subseteq V(G)$, $G - W$ denotes the subgraph of G obtained by deleting the vertices of W and the edges incident with them.

The first Zagreb index M_1 and the second Zagreb index M_2 of G are defined as

$$M_1(G) = \sum_{x \in V(G)} (d_G(x))^2$$

$$M_2(G) = \sum_{xy \in E(G)} d_G(x) d_G(y)$$

The Zagreb indices M_1 and M_2 were introduced in [2] and elaborated in [3]. The main properties of M_1 and M_2 were summarized in [4,5]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [5,6].

Recently, finding the extremal values or bounds for the topological indices of graphs, as well as related problems of characterizing the extremal graphs, attracted the attention of many researchers and many results are obtained (see [3–11]). Nikolić et al. [4] showed that the trees with the smallest and largest M_1 are the path and the star, respectively. Gutman and Das [7] also showed that the trees with the smallest and largest M_2 are the path and the star, respectively. In [8] the authors ordered the unicyclic graphs with respect to M_1 and M_2 . Zhang and Zhang [9] gave the unicyclic graphs with the first three smallest and largest M_1 . Chen and Deng [10] gave the bicyclic graph with the largest M_1 . Deng [11] presented a unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs. More results in this direction can be found in Refs. [12–23].

Let $\mathcal{G}_{n,k}$ is the set of graphs with n vertices and k cut edges. Let $E' = \{e_1, e_2, \dots, e_k\}$ is the set of cut edge of G , then E' can be classified into two kinds, i.e., the pendant edges and non-pendant edges, the number of them are k' , $k - k'$ resp. The components of $G - \{e_1, e_2, \dots, e_k\}$ are 2-edge-connected graphs and isolated vertices. The connected graphs with k cut edges(or vertices) have been considered in many mathematical literatures [24–31]. It is natural to think that, for the n vertex tree, $k = n - 1$, and trees with extremal Zagreb indices had been obtained long time ago. For a connected graph on n vertices having the cyclomatic number at least one, the number of its cut edges is most $n - 3$, therefore, in our following discussion, we always assume that G has k cut edges with $1 \leq k \leq n - 3$. In this paper, we shall investigate the Zagreb indices of $\mathcal{G}_{n,k}$ by introducing some graph grafting operations, and determine the graphs in $\mathcal{G}_{n,k}$ with the largest and the second largest Zagreb indices.

Fig. 1 The grafting transformation A of non-end cut edge uv

2 Grafting Transformations on Graphs with Cut Edges Related to Zagreb Indices

Before our discussion, we introduce a known proposition, which is useful to our main results.

Proposition 1 Let $G = (V, E)$ is a simple connected graph,

- (i) If $e = uv \notin E(G)$, $u, v \in V(G)$. Then, $M_i(G) < M_i(G + uv)$ ($i = 1, 2$);
- (ii) If $e \in E(G)$, then, $M_i(G) > M_i(G - e)$ ($i = 1, 2$).

For convenience, we provide some grafting transformations on graphs with cut edges which will increase the Zagreb indices in the following:

Lemma 1 Let uv is a non-pendent cut edge of G_1uvG_2 , G_1 and G_2 are 2-edge connected graphs, G_1uvG_2 and $G_1uG_2uK_2$ are two graphs with $|V(G_1)|, |V(G_2)| \geq 2$, depicted in Fig. 1. Then $M_1(G_1uG_2uK_2) > M_1(G_1uvG_2)$, $M_2(G_1uG_2uK_2) > M_2(G_1uvG_2)$.

Proof Let $G = G_1uvG_2$, $G^* = G_1uG_2uK_2$. By the definition of Zagreb indices, we have

$$\begin{aligned} M_1(G^*) - M_1(G) &= d_{G^*}^2(u) + 1 - d_G^2(u) - d_G^2(v) \\ &= [d_G(u) + d_G(v) - 1]^2 + 1 - d_G^2(u) - d_G^2(v) \\ &= 2(d_G(u) - 1)(d_G(v) - 1) > 0 \end{aligned} \quad (1)$$

Let $N_G(u) \setminus v = \{u_1, u_2, \dots, u_r\}$ ($r \geq 2$), $N_G(v) \setminus u = \{v_1, v_2, \dots, v_s\}$ ($s \geq 2$). Then, $d_G(u) = r + 1$, $d_G(v) = s + 1$, $d_{G^*}(u) = r + s + 1$. From the assume, we know that $\{u_1, u_2, \dots, u_r\} \in V(G_1)$, $\{v_1, v_2, \dots, v_s\} \in V(G_2)$.

$$\begin{aligned} M_2(G^*) - M_2(G) &= \sum_{x \in N_{G^*}(u)} d_{G^*}(x)d_{G^*}(u) - \sum_{x \in N_G(u)} d_G(x)d_G(u) - \sum_{x \in N_G(v) \setminus u} d_G(x)d_G(v) \\ &= (r + s + 1) + \sum_{x \in N_G(u) \setminus v} d_G(x)(r + s + 1) + \sum_{x \in N_G(v) \setminus u} d_G(x)(r + s + 1) \\ &\quad - \sum_{x \in N_G(u) \setminus v} d_G(x)(r + 1) - \sum_{x \in N_G(u) \setminus v} d_G(x)(s + 1) - (r + 1)(s + 1) \\ &= \sum_{i=1}^r d_G(u_i)s + \sum_{j=1}^s d_G(v_j)r + r + s + 1 - (r + 1)(s + 1) \\ &\geq rs > 0 \quad (\text{since } d_G(u_i) \geq 1(d_G(v_j) \geq 1 \text{ resp.})) \end{aligned} \quad (2)$$

Fig. 2 Grafting transformation B

Fig. 3 The graph $G_{k''}^*$

Fig. 4 Grafting transformation C

The proof is completed. $\square$

Note that the graphs $G_1uG_2uK_2$ has k cut edges, and the pendant vertex increase one, i.e., w . G_1, G_2 are 2-edge-connected graphs as well.

If uv is a non-pendant cut edge of $G_1uvK_{1,k}$, as shown in Fig. 2. We shall have

Lemma 2 *Let uv is a non-pendant cut edge of $G_1uvK_{1,r}$, G_1 is a 2-edge connected graphs, $G_1uvK_{1,r}$ and $G_1uK_{1,r+1}$ are two graphs with $|V(G_1)| \geq 2$, depicted in Fig. 2. Then $M_1(G_1uK_{1,r+1}) > M_1(G_1uvK_{1,r})$, $M_2(G_1uK_{1,r+1}) > M_2(G_1uvK_{1,r})$.*

Proof It follows from the proof of Lemma 1, the results is obviously. $\square$

Remark 1 Repeating the grafting transformation A or B, any cut(non-pendant cut) edge can be changed into pendant edge. The graph is shown in Fig. 3, where $S_i (1 \leq i \leq l)$ are 2-edge-connected graphs.

Lemma 3 [11] *Let u and v be two vertices in G . $u_1, u_2, \dots, u_s$ are the leaves adjacent to u , $v_1, v_2, \dots, v_t$ are the leaves adjacent to v . $G' = G - \{uu_1, uu_2, \dots, uu_s\} + \{vu_1, vu_2, \dots, vu_s\}$, $G'' = G - \{vv_1, vv_2, \dots, vv_t\} + \{uv_1, uv_2, \dots, uv_t\}$ and $|V(G_0)| \geq 3$, as shown in Fig. 4. Then, either $M_i(G') > M_i(G)$ or $M_i(G'') > M_i(G)$, $i = 1, 2$.*

Remark 2 Repeating grafting transformation C, all the pendant edges are attached to the same vertex.

Fig. 5 Three simple graphs with k cut edges

3 Graphs in $\mathcal{G}_{n,k}$ with the Largest, the Second Largest Zagreb Indices

In this section we shall get graphs in $\mathcal{G}_{n,k}$ with the largest, the second largest Zagreb indices.

3.1 Graphs in $\mathcal{G}_{n,k}$ with the Largest Zagreb Indices

In this section, we discuss graphs in $\mathcal{G}_{n,k}$ with the largest M_1 , M_2 .

Theorem 1 *Of all the connected graphs in $\mathcal{G}_{n,k}$ ($1 \leq k \leq n-3$), the maximum M_1 , M_2 values are obtained uniquely at K_n^k . Where K_n^k is a graph obtained by joining k independent vertices to one vertex of K_{n-k} .*

Proof Firstly, from above Lemmas we present the graphs in $\mathcal{G}_{n,k}$ the upper bounds, respectively, for M_1 , M_2 . As described above, we obtained graphs in the following (see Fig. 5) will achieve the upper bounds with respect to M_1 , M_2 .

Nextly, we consider three Claim as follows.

Claim 1 *If a graph $G \in \mathcal{G}_{n,k}$, then $M_i(G) \leq M_i(G^*)$ for $i = 1, 2$.*

Proof of Claim 1 Suppose that $G \in \mathcal{G}_{n,k}$ and $G \not\cong G^*$, then by the proof of Lemma 1, Lemma 2 and Lemma 3, we know $M_i(G) < M_i(G^*)$ for $i = 1, 2$. Obviously, when $G \cong G^*$, $M_i(G) = M_i(G^*)$ for $i = 1, 2$, which completes the proof.

Claim 2 *For the graph G^* , we have $M_i(G^*) \leq M_i(H)$ ($i = 1, 2$), and the equalities hold if and only $G^* \cong H$.*

Proof of Claim 2 Let $\{e_1, e_2, \dots, e_k\}$ be the set of the cut edges of $G \in \mathcal{G}_{n,k}$. Note that by Proposition 1, if we add an edge not belong to G , then, we have $M_i(G + e) > M_i(G)$ for $i = 1, 2$. For the 2-edge-connected graph S_i ($i = 1, 2, \dots, l$), we add edges in them, changing them into complete sub-graphs K_{n_i+1} ($i = 1, 2, \dots, l$), thus the graphs G^* is changed into the graph H , and H is still possesses k cut edges, i.e., $H \in \mathcal{G}_{n,k}$, $G^* \leq H$. By the Proposition, if $G^* < H$, then $M_i(G^*) < M_i(H)$ ($i = 1, 2$), else, $M_i(G^*) = M_i(H)$ ($i = 1, 2$) iff $G^* \cong H$.

This completes the proof of Claim 2.

Claim 3 *$M_i(H) \leq M_i(G_0)$ ($i = 1, 2$), the equalities hold if and only $H \cong G_0$, i.e., $l = 1$.*

Proof of Claim 3

If we add edges between the every two vertices of completed sub-graphs K_{n_i+1} ($i = 1, 2, \dots, l$) of H , H will be changed into the graph G_0 , and G_0 is still possesses

Fig. 6 Three simple connected graphs with cut edges

k cut edges, i.e., $G_0 \in G \in \mathcal{G}_{n,k}$, and $H < G_0$. Thus, by Proposition 1, we have $M_i(H) \leq M_i(G_0)$ ($i = 1, 2$), the equalities hold if and only if $H \cong G_0$, i.e., $l = 1$.

This completes the proof of Claim 3.

Combine above Claims, theorem holds.

3.2 Graphs in $\mathcal{G}_{n,k}$ with the Second Largest Zagreb Indices

In this section, we shall determine graphs in $\mathcal{G}_{n,k}$ with the second largest M_1, M_2 , respectively.

Firstly, we characterize the three graphs will achieve the upper bounds on M_1, M_2 .

Theorem 2 For an arbitrary graph $G \in \mathcal{G}_{n,k}$ ($1 \leq k \leq n-3$), and $G \not\cong G_0$, we have

- (i) If $1 \leq k \leq 4$, then $M_1(G) \leq M_1(G_1)$, the equalities hold if and only if $G \cong G_1$;
- (ii) If $k > 4$, and $n \leq [\frac{3}{2}k + 1]$, then $M_1(G) \leq M_1(G_1)$, the equalities hold if and only if $G \cong G_2$;
- (iii) If $k > 4$, and $n > [\frac{3}{2}k + 1]$, then $M_1(G) < M_1(G_1)$;
- (iv) $M_2(G) \leq M_2(G_1)$, the equalities hold if and only if $G \cong G_1$.

Proof Firstly, we shall prove that the graph $G \in \mathcal{G}_{n,k}$ ($1 \leq k \leq n-3$), and $G \not\cong G_0$ attain the maximum $M_i(G)$ ($i = 1, 2$), then G must be one of the graph G_1, G_2 and G_3 depicted in Fig. 6.

Follows the remark 1, we get the graph $G_{k''}^*$, and $M_i(G_{k''}^*) \geq M_i(G)$ ($i = 1, 2$), where k'' is the number of non-pendant vertices connected the cut edges. From the structure of $G_{k''}^*$, we divide our discussion into two cases according to parameters l and k'' . $\square$

Case 1 When $l = 1$, there are two subcases in the following:

Subcase 1.1 If $k'' = 1$.

In this case, we adding edges to the vertices of the 2-edge-connected subgraph S_1 , thus, S_1 can be changed into the graph G_2 or G_3 , see Fig. 7. Adding one edge again to G_2 or G_3 , they can be changed into G_0 . By the proposition 1, we have

- (i) $M_i(G) \leq M_i(G_{k''}^*) \leq M_i(G_2) \leq M_i(G_0)$ ($i = 1, 2$); or
- (ii) $M_i(G) \leq M_i(G_{k''}^*) \leq M_i(G_3) \leq M_i(G_0)$ ($i = 1, 2$).

Subcase 1.2 If $k'' \geq 2$.

In this case, at first, we adding edges to the vertices of the 2-edge-connected subgraph S_1 , thus, S_1 can be changed into the graph K_{n-k} , see Fig. 8, denote the

Fig. 7 The transformation of graph $G_{k''}^*$ when $l=1, k''=1$

Fig. 8 The transformation of graph $G_{k''}^*$ when $l=1, k'' \geq 2$

Fig. 9 The transformation of $G_{k''}^*$ when $l \geq 2, k''=1$

graph as H_1 . By the proposition 1, we have $M_i(H) \geq M_i(G_{k''}^*)(i = 1, 2)$. In the next, repeating graft transformation C on H , we can get the graph G_1 . Obviously, we only graft one edge of G_1 , G_1 will change into G_0 . By Lemma 3, we have $M_i(G) \leq M_i(H_1) \leq M_i(G_1) \leq M_i(G_0)(i = 1, 2)$.

Case 2 When $l \geq 2$, similar to the Case 1, there are two subcases in the following:

Subcase 2.1

If $k''=1$.

Firstly, we add edges in the 2-edge-connected subgraphs $S_i(i = 1, 2, \dots, l)$ of $G_{k''}^*$, and we get complete graphs $K_{i+1}(i = 1, 2, \dots, l)$, which composed the graph H_2 (see Fig. 9). By the proposition 1, we have $M_i(H_2) \geq M_i(G_{k''}^*)(i = 1, 2)$. Then, adding edges between $K_{i+1}(i = 1, 2, \dots, l)$, we shall get the graph G_2 (see Fig. 9), and if we add one edge again to G_2 , it can be changed into the graph G_0 . By proposition 1, we know that $M_i(G_{k''}^*) \leq M_i(H_2) \leq M_i(G_2) \leq M_i(G_0)(i = 1, 2)$.

Fig. 10 The transformation of $G_k^{*''}$ when $l \geq 2, k \geq 2$

Subcase 2.2. If $k'' \geq 2$.

Similar to the method of subcase 2.1, firstly, we add edges in the 2-edge-connected subgraphs $S_i (i = 1, 2, \dots, l)$ of $G_k^{*''}$, and we get complete graphs $K_{i+1} (i = 1, 2, \dots, l)$. Then, adding edges between $K_{i+1} (i = 1, 2, \dots, l)$, we shall get the graph H_3 (see Fig. 10). At last, applying grafting transformation C on H_3 , we shall get the graph G_1 , and if we add one edge again to G_1 , it can be changed into the graph G_0 . By proposition 1 and Lemma 3, we know that $M_i(G_k^{*''}) \leq M_i(H_3) \leq M_i(G_1) \leq M_i(G_0) (i = 1, 2)$.

From above operations, it is sufficient to see that one of the graphs G_1, G_2 and G_3 attains the second largest $M_i (i = 1, 2)$. In our following work, we only need to compare the Zagreb indices $M_i (i = 1, 2)$ of G_1, G_2 and G_3 .

By simple calculation, we have:

$$M_1(G_1) = (n-2)^2 + (n-k)^2 + (n-k-2)(n-k-1)^2 + k \quad (3)$$

$$M_1(G_2) = (n-1)^2 + 2(n-k-2)^2 + (n-k-3)(n-k-1)^2 + k; \quad (4)$$

$$M_1(G_3) = (n-2)^2 + (n-k-2)^2 + (n-k-2)(n-k-1)^2 + k; \quad (5)$$

$$\begin{aligned} M_2(G_1) &= (n-2)[(n-k)^2 - 3n + 4k + 1] + (n+1)(n-k) + (n-k)^3 \\ &\quad - 3(n-k)^2 + (n-k-1)^2 \left[\frac{1}{2}(n-k)^2 - \frac{5}{2}(n-k) + 3 \right]; \end{aligned} \quad (6)$$

$$\begin{aligned} M_2(G_2) &= (n-1)[(n-k)^2 - 2n + 3k - 1] + 2(n-k-1)(n-k-2) \\ &\quad (n-k-3) + (n-k-1)^2 \left[\frac{1}{2}(n-k)^2 - \frac{7}{2}(n-k) + 6 \right]; \end{aligned} \quad (7)$$

$$\begin{aligned} M_2(G_3) &= k(n-2) + (n-k-2)(n-k-1)(2n-k-4) \\ &\quad + (n-k-1)^2 \left[\frac{1}{2}(n-k)^2 - \frac{5}{2}(n-k) + 3 \right]. \end{aligned} \quad (8)$$

Therefore

$$\Delta_1 = M_1(G_1) - M_1(G_2) = 4 \left(n - \frac{3}{2}k - 1 \right) \quad (9)$$

$$\Delta_2 = M_1(G_2) - M_1(G_3) = 2k > 0 \quad (10)$$

$$\Delta_3 = M_2(G_1) - M_2(G_2) = 3(n - k)^2 - 8(n - k) + k + 6 > 0 \quad (11)$$

$$\Delta_4 = M_2(G_2) - M_2(G_3) = k(n - 2 - k) > 0 \quad (12)$$

As pointed out before, we have $1 \leq k \leq n - 3$.

Let $k + 3 = \frac{3}{2}k + 1$, then $k = 4$. Therefore,

- (i) $\Delta_1 \geq 0$, if $1 \leq k \leq 4$. otherwise
- (ii) $\Delta_1 < 0$, if $k > 4$ and $n \leq [\frac{3}{2}k + 1]$, where $[x]$ stands for the integer part of x , or else
- (iii) $\Delta_1 > 0$, if $k > 4$ and $n > [\frac{3}{2}k + 1]$.

The proof of theorem is completed.

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