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A Simple Proof On The Extremal Zagreb Indices Of Graphs With Cut Edges*

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Abstract

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a (molecular) graph G are $M_1(G) = \sum_{u\in V(G)} (d(u))^2$ and $M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$ respectively, where $d(u)$ denotes the degree of a vertex u in G. In [3] and [4], Feng *et al.* obtained the sharp bounds of $M_1(G)$ and $M_2(G)$ on the graphs with cut edges and characterized the extremal graphs. However, the proof in [3] was rather complicated. In this paper, we give a simple proof on these results.

1 Introduction

A *molecular graph* is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. For a (molecular) graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined in [5] as

$$M_1(G) = \sum_{u\in V(G)} (d(u))^2, \quad M_2(G) = \sum_{uv\in E(G)} d(u)d(v),$$

where $d(u)$ denotes the degree of the vertex u of G.

A *cut edge* in a connected graph is an edge whose deletion breaks the graph into two components. Denote by $\mathcal{G}_n^k$ the set of graphs with n vertices and k cut edges. The graph K_n^k is a graph obtained by joining k independent vertices to one vertex of K_{n-k}. The graph P_n^k is a graph obtained by attaching a pendent chain P_{k+1} to one vertex of C_{n-k}. For example, graphs K_7^3 and P_7^3 are shown in Fig.1.

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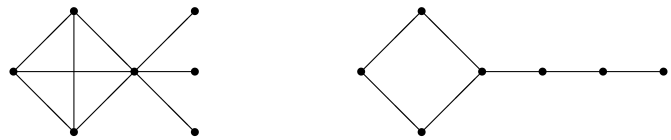

Fig.1 Graphs K_7^3 and P_7^3

If $G \in \mathcal{G}_n^k$ and $n = k+1$, then G is a tree. The sharp bounds of $M_1(G)$ and $M_2(G)$ on trees has been studied in [2]. Therefore, from now on, we may assume $n > k+1$.

In [3] and [4], Feng *et al.* obtained the following results:

THEOREM 1. Let $G \in \mathcal{G}_n^k$, then

$$4n+2 \leq M_1(G) \leq (n-k-1)^3 + (n-1)^2 + k,$$

with the left equality if and only if $G \cong P_n^k$, with the right equality if and only if $G \cong K_n^k$.

THEOREM 2. Let $G \in \mathcal{G}_n^k$, then

$$4n+4 \leq M_2(G) \leq \frac{1}{2}(n-k-1)^3(n-k-2) + [(n-k-1)^2 + k](n-1),$$

the left equality holds if and only if $G \cong P_n^k$ and the right equality holds if and only if $G \cong K_n^k$.

The proof of the above results was rather complicated in [3]. In this paper, we give a simple proof of the results.

First we introduce some graph notations used in this paper. We denote the minimum degrees of vertices of G by $\delta(G)$. A *tree* is a connected acyclic graph. The *star* S_n is a tree on n vertices with one vertex having degree $n-1$ and the other vertices having degree 1. The vertex with degree one is called a *leaf*.

A connected graph that has no cut vertices is called a *block*. If a block is an unique vertex, then it is called *trivial block*. Every block with at least three vertices is 2-connected. A *block of a graph* is a subgraph that is a block and is maximal with respect to this property. An edge e of G is said to be *contracted* if it is deleted and its ends are identified. If G has blocks $B_1, B_2, \ldots, B_r$, all the edges in the blocks are contracted, then the resulting graph is called *block graph* of G, in which a vertex corresponds to a block of G and an edge corresponds to a cut edge of G, denoted by $B(G)$. It is easy to see that $B(G)$ is a tree. Therefore, if $G \in \mathcal{G}_n^k$, then $B(G)$ is a tree with k edges. In $B(G)$, if each neighbor of a block is not a trivial block, then the block is called *naked block*; if a block is both naked block and a leaf in $B(G)$, we call the block *leaf block*.

Remark: Note that the vertex in each block which is incident with a cut edge is a cut vertex of G, *i.e.*, each block contains at least one cut vertex of G.

2 Proof of Theorem 1

Denote

$$\overline{\mathcal{G}_n^k} = \{G \in \mathcal{G}_n^k : M_1(G) \text{ is maximum}\}$$

$$\underline{\mathcal{G}_n^k} = \{G \in \mathcal{G}_n^k : M_1(G) \text{ is minimum}\}$$

LEMMA 1. If $G \in \overline{\mathcal{G}_n^k}$, then each block of G is either a vertex or a complete graph with at least three vertices.

PROOF. Let B_i be a block of G. If $|B_i| = 1$, then B_i is a vertex. If $|B_i| > 1$, since B_i is block, we have $\delta(B_i) \geq 2$. So we have $|B_i| \geq 3$. Since $M_1(G)$ is maximum, we have that B_i is a complete graph.

LEMMA 2. If $G \in \overline{\mathcal{G}_n^k}$, then G has an unique block which is a complete graph with at least three vertices.

PROOF. By Lemma 1, we have that each block of G is either a vertex or a complete graph with at least three vertices. If G has blocks $B_1, B_2, \ldots, B_p$ $(p \geq 2)$ which are complete vertices with at least three vertices.

If there exists two blocks in $\{B_1, B_2, \ldots, B_p\}$ are not naked block, without loss of generality, we may assume that B_1 and B_2 are not naked block. Then there exist a leaf x adjacent to B_1 and a leaf y adjacent to B_2. Let $V(B_1) = \{u_1, u_2, \ldots, u_s\}$, $V(B_2) = \{v_1, v_2, \ldots, v_t\}$ $(s, t \geq 3)$. Without loss of generality, we may assume that u_1 and v_1 are vertices adjacent to x and y respectively in G and $d_G(u_1) \geq d_G(v_1)$. Let $G' = G - yv_1 + yu_1$. We have $G' \in \mathcal{G}_n^k$. However,

$$\begin{aligned}
M_1(G') - M_1(G) &= d_{G'}^2(u_1) + d_{G'}^2(v_1) - d_G^2(u_1) - d_G^2(v_1) \\
&= [d_G(u_1) + 1]^2 + [d_G(v_1) - 1]^2 - d_G^2(u_1) - d_G^2(v_1) \\
&= 2(d_G(u_1) - d_G(v_1)) + 2 \\
&> 0,
\end{aligned}$$

a contradiction.

Otherwise at most one of $\{B_1, B_2, \ldots, B_p\}$ is not naked block. Then there exists leaf block in $\{B_1, B_2, \ldots, B_p\}$. Without loss of generality, we may assume that B_p is leaf block. Let $V(B_p) = \{w_1, w_2, \ldots, w_\ell\}$, $V(B_{p-1}) = \{z_1, z_2, \ldots, z_q\}$ $(\ell, q \geq 3)$, w_1 be the unique cut vertex of G in $V(B_p)$ (Note that $d_G(w_1) = \ell$).

We delete the edges $\{w_1w_2, w_1w_3, \ldots, w_1w_\ell\}$ in B_p and let $\{z_1, z_2, \ldots, z_q, w_2, w_3, \ldots, w_\ell\}$ be a complete graph; the resulting graph is denoted by G''. It is easy to have

$G'' \in \mathcal{G}_n^k$. However,

$$\begin{aligned}
M_1(G'') - M_1(G) &= \sum_{i=1}^{\ell} d^2_{G''}(w_i) + \sum_{j=1}^{q} d^2_{G''}(z_j) - \sum_{i=1}^{\ell} d^2_G(w_i) - \sum_{j=1}^{q} d^2_G(z_j) \\
&= 1 + \sum_{i=2}^{\ell} [d_G(w_i) - 1 + q]^2 + \sum_{j=1}^{q} [d_G(z_j) + \ell - 1]^2 \\
&\quad - \sum_{i=1}^{\ell} d^2_G(w_i) - \sum_{j=1}^{q} d^2_G(z_j) \\
&= 1 + (\ell - 1)(q-1)^2 + 2(q-1)\sum_{i=2}^{\ell} d_G(w_i) + q(\ell-1)^2 \\
&\quad + 2(\ell - 1)\sum_{j=1}^{q} d(v_j) - \ell^2 \quad (\ell, q \geq 3) \\
&> 0,
\end{aligned}$$

a contradiction. This completes the proof.

LEMMA 3. If $G \in \overline{\mathcal{G}_n^k}$, then $B(G)$ is a star and the maximum vertex corresponds to the unique block, which is a complete graph with at least three vertices.

PROOF. Let $B_1, B_2, \ldots, B_r$ be the blocks of G and $b_1, b_2, \ldots, b_r$ be the corresponding vertices in $B(G)$. By Lemma 1 and Lemma 2, only one of $B_1, B_2, \ldots, B_r$ is a complete graph with at least three vertices. Without loss of generality, let B_r be the block which is a complete graph, $V(B_r) = \{u_1, u_2, \ldots, u_s\}$ $(s \geq 3)$. Then B_i $(i = 1, 2, \ldots, r-1)$ is a vertex, *i.e.*, $b_i = B_i$ $(i = 1, 2, \ldots, r-1)$ in $B(G)$.

Without loss of generality, we may assume that u_1 is an arbitrary cut vertex of G in B_r and $u_1 b_1 \in E(G)$ (Note that $d_G(u_1) \geq 3$). If b_1 is not an isolated vertex in $B(G)$, then let $N_G(b_1) = \{u_1, b_2, \ldots, b_t\}$ $(t \geq 2)$. Let $G' = G - \{b_1 b_2, \ldots, b_1 b_t\} + \{u_1 b_2, \ldots, u_1 b_t\}$. It is easy to see $G' \in \mathcal{G}_n^k$. However,

$$\begin{aligned}
M_1(G') - M_1(G) &= d^2_{G'}(u_1) + d^2_{G'}(b_1) - d^2_G(u_1) - d^2_G(b_1) \\
&= [d_G(u_1) + t - 1]^2 + 1 - d^2_G(u_1) - t^2 \\
&= 2(t-1)[d_G(u_1) - 1] \\
&> 0,
\end{aligned}$$

a contradiction. Therefore, b_1 is an isolated vertex in $B(G)$.

Since u_1 is an arbitrary cut vertex of G in B_r, we have that all the vertices adjacent to b_r are isolated vertices in $B(G)$. Therefore, $B(G)$ is a star and the maximum vertex corresponds to the unique block, which is a complete graph with at least three vertices.

LEMMA 4. If $G \in \overline{\mathcal{G}_n^k}$, then $G \cong K_n^k$.

PROOF. By Lemma 3, $B(G)$ is a star and the maximum vertex corresponds to the unique block, which is a complete graph with at least three vertices. Let $V(B(G)) = \{b_1, b_2, \ldots, b_r\}$ and b_r be the vertex with maximum degrees. Let u_1, u_2 be the neighbors of b_1, b_2 in G, respectively, and $d_G(u_1) \geq d_G(u_2)$.

If $u_1 \neq u_2$, let $G' = G - u_2b_2 + u_1b_2$. Then $G' \in \mathcal{G}_n^k$. However,

$$\begin{aligned} M_1(G') - M_1(G) &= d^2_{G'}(u_1) + d^2_{G'}(u_2) - d^2_G(u_1) - d^2_G(u_2) \\ &= [d_G(u_1)+1]^2 + [d_G(u_2)-1]^2 - d^2_G(u_1) - d^2_G(u_2) \\ &= 2[d_G(u_1) - d_G(u_2)] + 2 \\ &> 0, \end{aligned}$$

a contradiction. Therefore, $u_1 = u_2$.

Since b_1 and b_2 are arbitrary, we have that the neighbors of $\{b_1, b_2, \ldots, b_{r-1}\}$ are the same. Therefore, $G \cong K_n^k$.

LEMMA 5. If $G \in \underline{\mathcal{G}_n^k}$, then each block of G is either a vertex or a cycle with at least three vertices.

PROOF. Let B_i be a block of G. If $|B_i| = 1$, then B_i is a vertex. If $|B_i| > 1$, since B_i is block, we have $\delta(B_i) \geq 2$. So we have $|B_i| \geq 3$. Since $M_1(G)$ is minimum, we have that B_i is a cycle.

LEMMA 6. If $G \in \underline{\mathcal{G}_n^k}$, then G has an unique block which is a cycle with at least three vertices.

PROOF. By Lemma 5, we have that each block of G is either a vertex or a cycle with at least three vertices. If G has blocks B_1 and B_2 which are cycles with at least three vertices, let $V(B_1) = \{u_1, u_2, \ldots, u_s\}$, $V(B_2) = \{v_1, v_2, \ldots, v_t\}$ $(s, t \geq 3)$, u_1 and v_1 be cut vertices in G (Note that $d_G(u_1) \geq 3$). We delete all the edges in B_1, B_2 and let $\{v_1, v_2, \ldots, v_t, u_2, u_3, \ldots, u_s\}$ be a cycle; the resulting graph is denoted by G'. It is easy to see $G' \in \mathcal{G}_n^k$. However,

$$\begin{aligned} M_1(G') - M_1(G) &= d^2_{G'}(u_1) - d^2_G(u_1) \\ &= [d_G(u_1) - 2]^2 - d^2_G(u_1) \\ &< 0, \end{aligned}$$

a contradiction.

LEMMA 7. If $G \in \underline{\mathcal{G}_n^k}$, then $G \cong P_n^k$.

PROOF. Let $B_1, B_2, \ldots, B_r$ be the blocks of G and $b_1, b_2, \ldots, b_r$ be the corresponding vertices in $B(G)$. By Lemma 5 and Lemma 6, only one of $\{B_1, B_2, \ldots, B_r\}$ is a cycle with at least three vertices. Without loss of generality, let B_1 be the block which is a cycle, $V(B_1) = \{u_1, u_2, \ldots, u_s\}$ $(s \geq 3)$. Then B_i $(i = 2, 3, \ldots, r)$ is a vertex, *i.e.*, $b_i = B_i$ $(i = 2, 3, \ldots, r)$ in $B(G)$. Now we prove $d_{B(G)}(b_1) = 1$ and $d_{B(G)}(b_i) \leq 2$ $(2 \leq i \leq r)$.

If $d_{B(G)}(b_1) \geq 2$, let b_i be a neighbor of b_1 and $B_iu_j \in E(G)$ $(2 \leq i \leq r, 1 \leq j \leq s)$(Note that $d_G(u_j) \geq 3$). Since $B(G)$ is tree, without loss of generality, we may assume that b_t is a leaf of $B(G)$ $(2 \leq t \leq r, t \neq i)$. Let $G' = G - B_iu_j + B_tB_i$, then $G' \in \mathcal{G}_n^k$. However,

$$\begin{aligned} M_1(G') - M_1(G) &= d^2_{G'}(u_j) + d^2_{G'}(B_t) - d^2_G(u_j) - d^2_G(B_t) \\ &= [d_G(u_j) - 1]^2 + 4 - d^2_G(u_j) - 1 \\ &= -2d_G(u_j) + 4 \\ &< 0, \end{aligned}$$

a contradiction. Therefore, $d_{B(G)}(b_1) = 1$.

Since $B(G)$ is a tree and a tree has at least two leaves, without loss of generality, we may assume that b_2 is a leaf of $B(G)$. If there exist b_i such that $d_{B(G)}(b_i) \geq 3$ $(3 \leq i \leq r)$(Note that $d_{B(G)}(b_i) = d_G(B_i)$). Let b_j be a neighbor of b_i in $B(G)$ $(3 \leq j \leq r)$. Let $G'' = G - B_iB_j + B_2B_j$, then $G'' \in \mathcal{G}_n^k$. However,

$$\begin{aligned} M_1(G'') - M_1(G) &= d^2_{G''}(B_i) + d^2_{G''}(B_2) - d^2_G(B_i) - d^2_G(B_2) \\ &= [d_G(B_i) - 1]^2 + 4 - d^2_G(B_i) - 1 \\ &= -2d_G(B_i) + 4 \\ &< 0, \end{aligned}$$

a contradiction. Therefore, $d_{B(G)}(b_i) \leq 2$ $(2 \leq i \leq r)$.

Since $d_{B(G)}(b_1) = 1$ and $d_{B(G)}(b_i) \leq 2$ $(2 \leq i \leq r)$, we have $G \cong P_n^k$.

PROOF of THEOREM 1. By Lemma 4, we have $G \cong K_n^k$ if $G \in \overline{\mathcal{G}_n^k}$. Moreover, $M_1(K_n^k) = (n-k-1)^3 + (n-1)^2 + k$.

By Lemma 7, we have $G \cong P_n^k$ if $G \in \underline{\mathcal{G}_n^k}$. Moreover, $M_1(P_n^k) = 4n + 2$. Therefore,

$$4n + 2 \leq M_1(G) \leq (n-k-1)^3 + (n-1)^2 + k,$$

with the left equality if and only if $G \cong P_n^k$, with the right equality if and only if $G \cong K_n^k$.

REMARK**.** In fact, we can give a simple proof of Theorem 2 in a similar way.

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