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On Zagreb Indices of Graphs

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Abstract

Let $\mathcal{G}_n$ be the set of class of graphs of order n. The first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices, and the second Zagreb index $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices of the underlying molecular graph G. The three set of graphs are as follows:

$$A = \left\{ G \in \mathcal{G}_n : \, \frac{M_1(G)}{n} > \frac{M_2(G)}{m} \right\}, \; B = \left\{ G \in \mathcal{G}_n : \, \frac{M_1(G)}{n} = \frac{M_2(G)}{m} \right\}$$

and

$$C = \left\{ G \in \mathcal{G}_n : \, \frac{M_1(G)}{n} < \frac{M_2(G)}{m} \right\}.$$

In this paper we prove that $|A| + |B| < |C|$. Finally, we give a conjecture $|A| < |B|$.

1 Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let $\overline{G}$ be the complement of G. We denote by $d_i = d_G(v_i)$ the degree of vertex v_i for $i = 1, 2, \ldots, n$. Let $\mathcal{G}_n$ be the set of class of graphs of order n. For $S \subseteq \mathcal{G}_n$, let $|S|$ be the number of graphs in the set S. For any two nonadjacent vertices v_i and v_j in graph G, we use $G + v_iv_j$ to denote the graph obtained

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from adding a new edge v_iv_j to graph G. Similarly, for $v_iv_j \in E(G)$, we use $G - v_iv_j$ to denote the graph obtained from deleting an edge v_iv_j to graph G. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ is defined as follows:

$$M_1(G) = \sum_{v_i \in V} d_i^2 \quad \text{and} \quad M_2(G) = \sum_{v_iv_j \in E(G)} d_i\, d_j.$$

The Zagreb indices M_1 and M_2 were first introduced by Gutman and Trinajstić in 1972, the quantities of the Zagreb indices were found to occur within certain approximate expressions for the total π-electron energy [12]. For more details of the mathematical theory and chemical applications of the Zagreb indices, see [1, 4, 6, 10, 11, 15, 20–22, 28, 29].

Let us consider the three sets A, B and C be as follows:

$$A = \left\{ G \in \mathcal{G}_n : \frac{M_1(G)}{n} > \frac{M_2(G)}{m} \right\},\ B = \left\{ G \in \mathcal{G}_n : \frac{M_1(G)}{n} = \frac{M_2(G)}{m} \right\}$$

and

$$C = \left\{ G \in \mathcal{G}_n : \frac{M_1(G)}{n} < \frac{M_2(G)}{m} \right\}.$$

Thus we have $|A| + |B| + |C| = |\mathcal{G}_n|$ as $A \cap B = \emptyset$, $B \cap C = \emptyset$ and $C \cap A = \emptyset$.

Caporossi and Hansen [2] conjectured that $A = \emptyset$. Although this conjecture is disproved for general graphs [13], it was the beginning of a long series of studies to characterize the graphs G for which $G \in A$ or $G \in B$ or $G \in C$, see [3, 5, 7, 9, 16–19, 23–27] and the references cited therein. For a more detailed discussion of the comparison between the classical Zagreb indices we refer to the monograph [14].

In this paper, we prove that $|A| + |B| < |C|$. Finally, we give a conjecture $|A| < |B|$.

2 Main result

In this section we compare three classes of graphs. For this we need the following results.

Lemma 1. *Let G be a graph of order $n > 1$ and size m.*

(i) If $G \in A$, then $\overline{G} \in C$.

(ii) If G is irregular and $G \in B$, then $\overline{G} \in C$.

Proof. From the results in [6, 8], we have

$$M_2(\overline{G}) = \frac{n(n-1)^3}{2} - 3m(n-1)^2 + 2m^2 + \left(n - \frac{3}{2}\right) M_1(G) - M_2(G) \tag{1}$$

and

$$M_1(\overline{G}) = n(n-1)^2 - 4m(n-1) + M_1(G). \tag{2}$$

On the other hand, it is well known that

$$M_1(G) \geq \frac{4m^2}{n} \tag{3}$$

with equality if and only if G is a regular graph. Clearly, $\mid V(\overline{G}) \mid = n$ and $\mid E(\overline{G}) \mid = n(n-1)/2 - m$. Using (3), from (1) and (2), we obtain

$$\begin{aligned} |V(\overline{G})|M_2(\overline{G}) - |E(\overline{G})|M_1(\overline{G}) &= nM_2(\overline{G}) - (n(n-1)/2 - m)M_1(\overline{G}) \\ &= (n-2)\left(\frac{n}{2}M_1(G) - 2m^2\right) - nM_2(G) + mM_1(G) \\ &\geq mM_1(G) - nM_2(G) \end{aligned} \tag{4}$$

with equality if and only if G is regular.

(i) If $G \in A$, then $mM_1(G) - nM_2(G) > 0$. From (4), we have $|V(\overline{G})|M_2(\overline{G}) - |E(\overline{G})|M_1(\overline{G}) > 0$, that is, $\overline{G} \in C$.

(ii) Similarly, if G is irregular and $G \in B$, then $\overline{G} \in C$ from the definition of B and (4). ■

Lemma 2. *Let G be a regular graph of order $n > 3$. Then*

(i) $G - e \in C$, where $e = v_i v_j \in E(G)$,

(ii) $G + e \in C$, where $e = v_i v_j \notin E(G)$.

Proof. Let r be the degree of the regular graph G. Then $\mid E(G) \mid = nr/2$.

(i) By the definition of the Zagreb indices, we have

$$M_1(G-e) = (n-2)r^2 + 2(r-1)^2 = nr^2 - 4r + 2$$

and

$$M_2(G-e) = 2(r-1)r(r-1) + \left(\frac{nr}{2} - 2r + 1\right) r^2 = \frac{nr^3}{2} - 3r^2 + 2r.$$

Then from the above, we get

$$nM_2(G-e) - (nr/2 - 1)M_1(G-e) = (n-4)r + 2 > 0$$

as $n > 3$. Therefore $G - e \in C$ because $\mid E(G-e) \mid = nr/2 - 1$.

(ii) For $e = v_i v_j \notin E(G)$, by the definition of the Zagreb indices, we have

$$M_1(G+e) = (n-2)r^2 + 2(r+1)^2 = nr^2 + 4r + 2$$

and

$$M_2(G+e) = 2r(r+1)r + \left(\frac{nr}{2} - 2r\right) r^2 + (r+1)^2 = \frac{nr^3}{2} + 3r^2 + 2r + 1.$$

Then from the above, we get

$$nM_2(G+e) - (nr/2+1)M_1(G+e) = (n-4)(r+1) + 2 > 0$$

as $n > 3$. Therefore $G + e \in C$ because $\mid E(G+e) \mid = nr/2 + 1$. ■

We now give our main result as follows:

Theorem 1. *Let $\mathcal{G}_n$ be the set of class of graphs of order $n > 3$. Let the three sets A, B, $C \subseteq \mathcal{G}_n$ be defined before. Then $|A| + |B| < |C|$.*

Proof. First we assume that G is an irregular graph. If $G \in A \cup B$, then by Lemma 1, $\overline{G} \in C$. Next we assume that G is a regular graph. Then by Lemma 2, we obtain $G - e \in C$ ($e \in E(G)$) and $G + e \in C$ ($e \notin E(G)$). Thus we conclude that if any graph G in $A \cup B$ then there exists a graph H ($\cong \overline{G}$ or $G - e$ or $G + e$) in C, that is, $G \in A \cup B$ implies that $H \in C$.

Let G_1 and G_2 ($G_1 \ncong G_2$) be any two graphs in $A \cup B$. Again let H_1 and H_2 be the graphs in C such that G_1 corresponds to H_1 and G_2 corresponds to H_2. We have to prove that H_1 and H_2 are not isomorphic. When G_1 and G_2 are both irregular, then by Lemma 1, we obtain

$$H_1 \cong \overline{G_1} \ncong \overline{G_2} \cong H_2.$$

When G_1 and G_2 are both regular, then by Lemma 2, H_1 and H_2 are not isomorphic. Otherwise, one of them (G_1 or G_2) is regular and the other one is irregular. Without loss of generality, we can assume that G_1 is regular and G_2 is irregular. Then $H_1 \cong G_1 - e$ for some $e \in E(G_1)$ and $H_2 \cong \overline{G_2}$. On the contrary, suppose that H_1 and H_2 are isomorphic. Then $\overline{G_2} \cong G_1 - e$ and it follows that

$$G_2 \cong \overline{G_1 - e} \cong \overline{G_1} + e.$$

Therefore by Lemma 2 (ii), we have $G_2 \in C$ since $\overline{G_1}$ is regular. This contradicts the fact that $G_2 \in A \cup B$. Therefore H_1 and H_2 are not isomorphic. Hence we conclude that $|A| + |B| \leq |C|$.

We now prove that the inequality is strict. For this let $H \cong K_n - e$ (e is an edge in K_n),

$n > 3$. Then $\overline{H} \cong K_2 \cup (n-2)\, K_1$. Thus we have

$$M_1(H) = (n-2)(n-1)^2 + 2(n-2)^2, \quad M_2(H) = \frac{n(n-1)^3}{2} - (n-1)(3n-5),$$

and

$$M_1(\overline{H}) = 2, \quad M_2(\overline{H}) = 1.$$

One can easily check that

$$\frac{M_1(H)}{n} < \frac{M_2(H)}{m} \quad \text{and} \quad \frac{M_1(\overline{H})}{n} < \frac{M_2(\overline{H})}{\frac{n(n-1)}{2} - m}$$

as $m = \frac{n(n-1)}{2} - 1$. Hence $H, \overline{H} \in C$. If there is no graph in $A \cup B$ correspondence to H in C, then we have $|A| + |B| < |C|$. Otherwise, there is a graph G in $A \cup B$ corresponds to H in C. Then by Lemma 1, we have $\overline{G} \cong H$, that is, $G \cong \overline{H} \in C$, a contradiction as $G \in A \cup B$. This completes the proof. ■

Corollary 3. *Let $\mathcal{G}_n$ be the set of class of graphs of order $n > 3$. Also let the three sets A, B, $C \subseteq \mathcal{G}_n$ be defined before. Then $|A| < |C|$ and $|B| < |C|$.*

Corollary 4. *Let $\mathcal{G}_n$ be the set of class of graphs of order $n > 3$. Also let C be the set defined before. Then $|C| > \frac{|\mathcal{G}_n|}{2}$.*

Proof. From the definitions of A, B and C, we have $|A| + |B| + |C| = |\mathcal{G}_n|$. By Theorem 1 with the above result, we obtain

$$2|C| > |\mathcal{G}_n|, \quad \text{that is, } |C| > \frac{|\mathcal{G}_n|}{2}.$$

■

Now we would like to end this paper with the following relevant conjecture.

Conjecture 5. *Let A and B be the two sets defined before. Then $|A| < |B|$.*

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