On Zagreb Indices of Graphs

Batmend Horoldagva\textsuperscript{a}, Kinkar Chandra Das\textsuperscript{b,∗}

\textsuperscript{aDepartment of Mathematics, Mongolian National University of Education, Baga toiruu-14, Ulaanbaatar, Mongolia}
horoldagva@msue.edu.mn

\textsuperscript{bDepartment of Mathematics, Sungkyunkwan University, Suwon 16419, Republic of Korea}
kinkardas2003@gmail.com

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Abstract

Let $G_n$ 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:

\begin{align*}
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\}
\end{align*}

and

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

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 $G + v_i v_j$ to denote the graph obtained

\textsuperscript{*}Corresponding author
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 \(\pi\)-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:

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

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

\[
M_2(\overline{G}) = \frac{n(n - 1)^3}{2} - 3m(n - 1)^2 + 2m^2 + \left( n - \frac{3}{2} \right) M_1(G) - M_2(G) \quad (1)
\]
and
\[ M_1(\overline{G}) = n(n - 1)^2 - 4m(n - 1) + M_1(G). \] (2)

On the other hand, it is well known that
\[ M_1(G) \geq \frac{4m^2}{n} \] (3)
with equality if and only if \( G \) is a regular graph. Clearly, \(|V(G)| = n\) and \(|E(G)| = n(n - 1)/2 - m\). Using (3), from (1) and (2), we obtain

\[
|V(\overline{G})|M_2(\overline{G}) - |E(\overline{G})|M_1(\overline{G}) = nM_2(\overline{G}) - (n(n - 1)/2 - m)M_1(\overline{G})
\]

\[
= (n - 2) \left( \frac{n}{2}M_1(G) - 2m^2 \right) - nM_2(G) + mM_1(G)
\]

\[
\geq mM_1(G) - nM_2(G) \] (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).

\[ \square \]

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

(i) \( G - e \in C \), where \( e = v_iv_j \in E(G) \),

(ii) \( G + e \in C \), where \( e = v_iv_j \notin E(G) \).

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

(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

\[
M_2(G - e) = \left( \frac{nr}{2} - 1 \right) M_1(G - e) = (n - 4)r + 2 > 0
\]
as \( n > 3 \). Therefore \( G - e \in C \) because \(|E(G - e)| = nr/2 - 1\).

(ii) For \( e = v_iv_j \notin E(G) \), 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 \( |E(G + e)| = nr/2 + 1 \).

We now give our main result as follows:

**Theorem 1.** Let \( G_n \) be the set of class of graphs of order \( n > 3 \). Let the three sets \( A, B, C \subseteq G_n \) 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, \( G \in C \). 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 \( G_2 \) (\( G_1 \not\cong G_2 \)) 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

\[ H_1 \cong \overline{G_1} \not\cong G_2 \cong H_2. \]

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. 

\textbf{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 $|B| < |C|$.

\textbf{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

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

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

\textbf{Conjecture 5.} Let $A$ and $B$ be the two sets defined before. Then $|A| < |B|$.

References


