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THE ZAGREB INDICES OF BIPARTITE GRAPHS WITH MORE EDGES†

KEXIANG XU*, KECHAO TANG, HONGSHUANG LIU, JINLAN WANG

Abstract. For a (molecular) graph, the first and second Zagreb indices (M_1 and M_2) are two well-known topological indices, first introduced in 1972 by Gutman and Trinajstić. 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. Let $K^p_{n_1,n_2}$ with $n_1 \le n_2$, $n_1 + n_2 = n$ and $p < n_1$ be the set of bipartite graphs obtained by deleting p edges from complete bipartite graph K_{n_1,n_2}. In this paper, we determine sharp upper and lower bounds on Zagreb indices of graphs from $K^p_{n_1,n_2}$ and characterize the corresponding extremal graphs at which the upper and lower bounds on Zagreb indices are attained. As a corollary, we determine the extremal graph from $K^p_{n_1,n_2}$ with respect to Zagreb coindices. Moreover a problem has been proposed on the first and second Zagreb indices.

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1. Introduction

We only consider finite, undirected and simple graphs throughout this paper. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For any vertex $v \in V(G)$, we denote by $N_G(v)$ the set of its neighbors in G. The *degree* of $v \in V(G)$, denoted by $d_G(v)$, is the cardinality of $N_G(v)$, i.e., the number of vertices in G adjacent to v. For a subset W of $V(G)$, let $G-W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, for a subset E' of $E(G)$, we denote by $G-E'$ the subgraph of G obtained by deleting the edges of E'. If $W=\{v\}$ and $E'=\{xy\}$, the subgraphs $G-W$ and $G-E'$ will be written as $G-v$ and $G-xy$ for short, respectively.

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*Corresponding author.
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K_{n_1,n_2} is a complete bipartite graph of order $n = n_1 + n_2$ and two bipartite sets V_1 and V_2 with $|V_i| = n_i$ for $i = 1, 2$. Other undefined notations and terminology on the graph theory can be found in [4].

A graphical invariant is a number related to a graph which is a structural invariant, in other words, it is a fixed number under graph automorphisms. In chemical graph theory, these invariants are also known as the topological indices. Two of the oldest graph invariants are the well-known Zagreb indices first introduced in [17] where Gutman and Trinajstić examined the dependence of total π-electron energy on molecular structure and elaborated in [18]. For a (molecular) graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are, respectively, defined as follows:

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

Another well-known version of first Zagreb index is in the following:

$$M_1(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v)) \tag{1}$$

These two classical topological indices reflect the extent of branching of the molecular carbon-atom skeleton [3, 22, 25]. The main properties of M_1 and M_2 were summarized in [5, 7–9, 14–16, 20, 24, 26, 28]. In particular, Deng [9] gave a unified approach to determine extremal values of Zagreb indices for trees, unicyclic, and bicyclic graphs, respectively. For some newest applications of Zagreb indices of graphs, please see [6, 13, 14, 19, 23]. In recent years, some novel variants of ordinary Zagreb indices have been introduced and studied, such as Zagreb coindices [1, 2, 10], multiplicative Zagreb indices [12, 24, 30], multiplicative sum Zagreb index [11, 27] and multiplicative Zagreb coindices [29]. Especially the first and second Zagreb coindices of graph G are defined [1, 10] in what follows:

$$\overline{M}_1 = \overline{M}_1(G) = \sum_{u\neq v, uv\notin E(G)} (d_G(u) + d_G(v)),$$
$$\overline{M}_2 = \overline{M}_2(G) = \sum_{u\neq v, uv\notin E(G)} d_G(u)d_G(v).$$

Hereafter we always assume that n_1, n_2, p are three positive integers such that $n_1 \leq n_2$, $n_1 + n_2 = n$ and $p < n_1$. We denote by $K^p_{n_1,n_2}$ the set of bipartite graphs obtained by deleting p edges from the complete bipartite graph K_{n_1,n_2}. In this paper we present sharp upper and lower bounds on the Zagreb indices of graphs from $K^p_{n_1,n_2}$ and characterize the extremal graphs at which the upper or lower bounds are attained. As a corollary, we also determine the extremal graph from $K^p_{n_1,n_2}$ with respect to Zagreb coindices. Finally an open problem is proposed on the Zagreb indices.

2. Preliminaries

In this section we list or prove some lemmas as preliminaries, which will be further used .

Lemma 2.1 ([1,2])**.** Let G be a connected graph of order n and with m edges. Then we have

(1) $\overline{M}_1(G) = 2m(n-1) - M_1(G)$;
(2) $\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G)$.

Lemma 2.2. Let G be a connected graph with $e = uv \in E(G)$ and $G' = G - uv$. Then we have $M_1(G') = M_1(G) - 2 - 2(d_{G'}(u) + d_{G'}(v))$.

Proof. By the definition of first Zagreb index, we have

$$\begin{aligned} M_1(G) - M_1(G') &= d_G(u)^2 - d_{G'}(u)^2 + d_G(v)^2 - d_{G'}(v)^2 \\ &= (d_{G'}(u)+1)^2 - d_{G'}(u)^2 + (d_{G'}(v)+1)^2 - d^2_{G'}(v) \\ &= 2 + 2(d_{G'}(u) + d_{G'}(v)), \end{aligned}$$

which completes the proof. □

Lemma 2.3. Let G be a connected graph with $uv \in E(G)$ and $N_G(u) \setminus \{v\} = \{v_1, v_2, \cdots, v_\alpha\}$ and $N_G(v) \setminus \{u\} = \{u_1, u_2, \cdots, u_\beta\}$. Suppose that $G' = G - uv$. Then we have

$$M_2(G') = M_2(G) - \Big[d_G(u)d_G(v) + \sum_{i=1}^{\alpha} d_G(v_i) + \sum_{j=1}^{\beta} d_G(u_j)\Big].$$

Proof. From the definition of second Zagreb index, we have

$$\begin{aligned} M_2(G') - M_2(G) &= d_{G'}(u)\sum_{i=1}^{\alpha} d_{G'}(v_i) + d_{G'}(v)\sum_{j=1}^{\beta} d_{G'}(u_j) \\ &\quad - \Big[d_G(u)\sum_{i=1}^{\alpha} d_G(v_i) + d_G(v)\sum_{j=1}^{\beta} d_G(u_j)\Big] - d_G(u)d_G(v) \\ &= (d_G(u)-1)\sum_{i=1}^{\alpha} d_G(v_i) + (d_G(v)-1)\sum_{j=1}^{\beta} d_G(u_j) \\ &\quad - \Big[d_G(u)\sum_{i=1}^{\alpha} d_G(v_i) + d_G(v)\sum_{j=1}^{\beta} d_G(u_j)\Big] - d_G(u)d_G(v) \\ &= -\Big[d_G(u)d_G(v) + \sum_{i=1}^{\alpha} d_G(v_i) + \sum_{j=1}^{\beta} d_G(u_j)\Big]. \end{aligned}$$

Thus the proof this lemma was completed. □

3. Extremal graphs from $K^p_{n_1,n_2}$ w. r. t. Zagreb indices

In this section we will consider the extremal graphs from $K^p_{n_1,n_2}$ with respect to Zagreb indices. Before presenting the main results, we first introduce some special graphs in $K^p_{n_1,n_2}$. Let $K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p)$ be a bipartite graph obtained by deleting p edges $e_1, e_2, \cdots, e_p$ from K_{n_1,n_2} where all $e_1, e_2, \cdots, e_p$ are pairwise independent. And we denote by $K^{1,1}_{n_1,n_2}(e_1, e_2, \cdots, e_p)$ the bipartite graph obtained by deleting p edges $e_1, e_2, \cdots, e_p$ from K_{n_1,n_2} where $e_1, e_2, \cdots, e_p$ have a common vertex in the partite set of size n_1 in it. Similarly, $K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_p)$ is a bipartite graph obtained by deleting p edges $e_1, e_2, \cdots, e_p$ from K_{n_1,n_2} where all $e_1, e_2, \cdots, e_p$ have a common vertex in the partite set of size n_2 in it. As three examples, $K^0_{3,4}(e_1, e_2)$, $K^{1,1}_{3,4}(e_1, e_2)$ and $K^{1,2}_{3,4}(e_1, e_2)$ are shown in Figure 1.

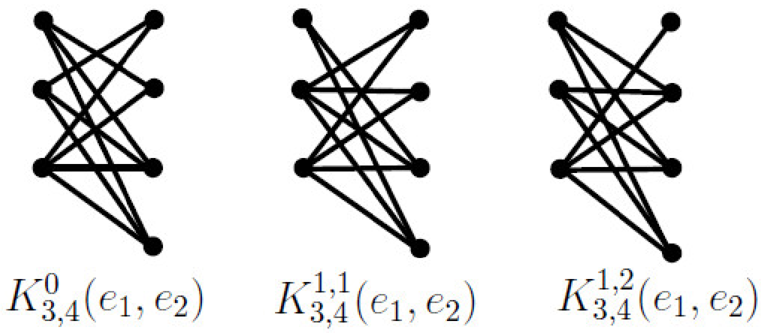

FIGURE 1. The graphs $K^0_{3,4}(e_1, e_2)$, $K^{1,1}_{3,4}(e_1, e_2)$ and $K^{1,2}_{3,4}(e_1, e_2)$

When $p = 1$, there is only one graph in $K^p_{n_1,n_2}$, and there is nothing to deal with for our main problem. So in what follows, we always assume that $p \geq 2$. In the following theorem we will determine the extremal graphs from $K^p_{n_1,n_2}$ with respect to the first Zagreb index.

Theorem 3.1. For any graph $G \in K^p_{n_1,n_2}$, we have

$$nn_1n_2 - 2np + 2p \leq M_1(G) \leq nn_1n_2 - 2np + p^2 + p \tag{2}$$

with left equality holding if and only if $G \cong K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p)$ and right equality holding if and only if $G \cong K^{1,i}_{n_1,n_2}(e_1, e_2, \cdots, e_p)$ for $i = 1, 2$.

Proof. We prove this result by induction on p, i.e., the number of edges deleted from K_{n_1,n_2}. When $p = 2$, there exist exactly three graphs in the set $G \in K^p_{n_1,n_2}$, which are just $K^0_{n_1,n_2}(e_1, e_2)$, $K^{1,1}_{n_1,n_2}(e_1, e_2)$ and $K^{1,2}_{n_1,n_2}(e_1, e_2)$. From the definition of first Zagreb index, we have

$$\begin{aligned} M_1(K^0_{n_1,n_2}(e_1,e_2)) &= nn_1n_2 - 4n + 4, \\ M_1(K^{1,1}_{n_1,n_2}(e_1,e_2)) &= M_1(K^{1,2}_{n_1,n_2}(e_1,e_2)) \\ &= nn_1n_2 - 4n + 6. \end{aligned}$$

Therefore the results in this theorem hold immediately.

Assume that the results hold for $p = k-1$. Now we consider the case when $p = k$. For any graph $G \in K^k_{n_1,n_2}$, there exists a graph $G^* \in K^{k-1}_{n_1,n_2}$ with $uv \in E(G^*)$ and $G^* - uv = G$. By Lemma 2.2, we have

$$M_1(G) = M_1(G^*) - 2 - 2(d_G(u) + d_G(v)) \tag{3}$$

Now we assume that, at vertices $u \in V_1$ and $v \in V_2$ in G^*, there are k_1, k_2 edges, respectively, deleted from K_{n_1,n_2}. Then we claim that $0 \le k_1 + k_2 \le k-1$ and $d_{G^*}(u) + d_{G^*}(v) = n - k_1 - k_2$. Considering the facts that $d_G(u) = d_{G^*}(u) - 1$ and $d_G(v) = d_{G^*}(v) - 1$, we have

$$d_G(u) + d_G(v) = n - 2 - k_1 - k_2 \tag{4}$$

Combining these two equalities (3) and (4), we arrive at the following:

$$M_1(G) = M_1(G^*) - 2(n-1) + 2(k_1 + k_2) \tag{5}$$

Next it suffices to deal with the equality (5). For the left part in (2), by the induction hypothesis and equality (5), we have

$$\begin{aligned} M_1(G) &= M_1(G^*) - 2(n-1) + 2(k_1 + k_2) \\ &\ge nn_1n_2 - 2n(k-1) + 2(k-1) - 2(n-1) \\ &= nn_1n_2 - 2nk + 2k \\ &= M_1(K^0_{n_1,n_2}(e_1, e_2, \cdots, e_k)) \end{aligned}$$

The above equality holds if and only if $G^* \in K^{k-1}_{n_1,n_2}$ with $G^* \cong K^0_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$ and $k_1 = 0, k_2 = 0$. Equivalently, $G^* \cong K^0_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$ and $e_k = uv$ is independent of any one edge from $\{e_1, e_2, \cdots, e_{k-1}\}$. Therefore we have $G \cong K^0_{n_1,n_2}(e_1, e_2, \cdots, e_k)$. Then the proof of the left part in (2) is completed.

Now we turn to the right part of (2). By the induction hypothesis and equality (5), we have

$$\begin{aligned} M_1(G) &= M_1(G^*) - 2(n-1) + 2(k_1 + k_2) \\ &\le nn_1n_2 - 2n(k-1) + (k-1)^2 + (k-1) - 2(n-1) + 2(k-1) \\ &= nn_1n_2 - 2nk + k^2 + k \\ &= M_1(K^{1,i}_{n_1,n_2}(e_1, e_2, \cdots, e_k)) \quad for\ i = 1, 2. \end{aligned}$$

The above equality holds if and only if $G^* \in K^{k-1}_{n_1,n_2}$ with $G^* \cong K^{1,i}_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$ for $i = 1, 2$ and $k_1 + k_2 = k-1$, i.e., $G^* \cong K^{1,1}_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$ and $k_1 = k-1$, $k_2 = 0$ or $G^* \cong K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$ and $k_1 = 0$, $k_2 = k-1$.

Thus we find that, either in $G^* \cong K^{1,1}_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$, there are $k-1$ edges deleted from the vertex $u \in V_1$ of K_{n_1,n_2}; or in $G^* \cong K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$, there are $k-1$ edges from $v \in V_2$ of K_{n_1,n_2}. Therefore, we conclude that $G \cong K^{1,1}_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1}, e_k)$ or $\cong K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1}, e_k)$. This completes the proof of this theorem. □

In the theorem below we characterize the extremal graphs from $K^p_{n_1,n_2}$ with respect to the second Zagreb index.

Theorem 3.2. For any graph $G \in K^p_{n_1,n_2}$ with $n_1 < n_2$, we have

$$n_1^2n_2^2 - 3pn_1n_2 + np + p^2 - p \le M_2(G) \le n_1^2n_2^2 - 3pn_1n_2 + np + n_2(p^2 - p) \quad (6)$$

with left equality holding if and only if $G \cong K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p)$ and right equality holding if and only if $G \cong K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_p)$.

Proof. We prove this result by induction on p. When $p = 2$, there exist exactly three graphs in the set $K^p_{n_1,n_2}$, which are just $K^0_{n_1,n_2}(e_1, e_2)$, $K^{1,1}_{n_1,n_2}(e_1, e_2)$ and $K^{1,2}_{n_1,n_2}(e_1, e_2)$. From the definition of second Zagreb index, we have

$$\begin{aligned}
M_2(K^0_{n_1,n_2}(e_1, e_2)) &= n_1^2n_2^2 - 6n_1n_2 + 2n + 2,\\
M_2(K^{1,1}_{n_1,n_2}(e_1, e_2)) &= n_1^2n_2^2 - 6n_1n_2 + 2n + 2n_1,\\
M_2(K^{1,2}_{n_1,n_2}(e_1, e_2)) &= n_1^2n_2^2 - 6n_1n_2 + 2n + 2n_2.
\end{aligned}$$

Obviously, $M_2(K^0_{n_1,n_2}(e_1, e_2)) < M_2(K^{1,1}_{n_1,n_2}(e_1, e_2)) < M_2(K^{1,2}_{n_1,n_2}(e_1, e_2))$. Thus our results hold as desired.

Now we assume that the results in (6) hold for $p = k-1$. Then we consider the case when $p = k$. For any graph $G \in K^k_{n_1,n_2}$, there exists a graph $G^* \in K^{k-1}_{n_1,n_2}$ with $u \in V_1$, $v \in V_2$, $uv \in E(G^*)$ and $G^* - uv = G$. The structure of G^* is shown in Fig. 2 where the polygonal lines denote the deleted edges from K_{n_1,n_2}. Suppose that $N_{G^*}(u) \setminus \{v\} = \{v_1, v_2, \cdots, v_\alpha\} \triangleq X_1$ and $N_{G^*}(v) \setminus \{u\} = \{u_1, u_2, \cdots, u_\beta\} \triangleq X_4$. Let $V_1 \setminus (X_4 \cup \{u\}) = X_3$ and $V_2 \setminus (X_1 \cup \{v\}) = X_2$. By Lemma 2.3, we have

$$M_2(G) = M_2(G^*) - \Big[d_{G^*}(u)d_{G^*}(v) + \sum_{i=1}^{\alpha} d_{G^*}(v_i) + \sum_{j=1}^{\beta} d_{G^*}(u_j)\Big]. \quad (7)$$

As introduced in [8], for any vertex v in a graph G, we denote by $m_G(v)$ the average of the degrees of all vertices adjacent to vertex v in G. Again we assume that, at vertices $u \in V_1$ and $v \in V_2$ in G^*, there are k_1, k_2 edges, respectively, deleted from K_{n_1,n_2}. Let the number of edges deleted between the two subsets X_1, X_3 in G^* and between the two subsets X_1, X_4 be x_1 and y_1, respectively, the edges deleted between the two subsets X_2, X_3 and between the two subsets X_2, X_4 be x_2 and y_2, respectively. Moreover we have $x_1 + x_2 + y_1 + y_2 = k - 1 - k_1 - k_2$. Then we claim that

$$d_{G^*}(v_1) + \cdots + d_{G^*}(v_\alpha) = d_{G^*}(u)m_{G^*}(u) - d_{G^*}(v) \ \textit{with}\ \alpha = n_2 - k_1 - 1,$$

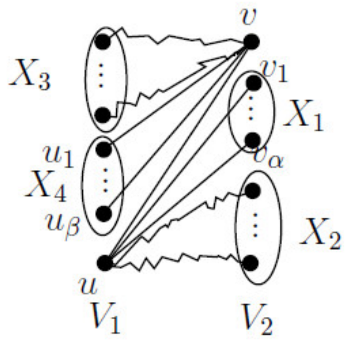

FIGURE 2. The structure of graph G^*

$d_{G^*}(u_1) + \cdots + d_{G^*}(u_\beta) = d_{G^*}(v)m_{G^*}(v) - d_{G^*}(u)$ *with* $\beta = n_1 - k_2 - 1$.

From the definition of $m_{G^*}(u)$, we arrive at:

$$\begin{aligned} m_{G^*}(u) &= \frac{d_{G^*}(v_1) + \cdots + d_{G^*}(v_\alpha) + d_{G^*}(v)}{n_2 - k_1} \\ &= \frac{(n_2 - k_1)n_1 - (x_1 + y_1 + k_2)}{n_2 - k_1}. \end{aligned}$$

Similarly, we have

$$\begin{aligned} m_{G^*}(v) &= \frac{d_{G^*}(u_1) + \cdots + d_{G^*}(u_\beta) + d_{G^*}(u)}{n_1 - k_2} \\ &= \frac{(n_1 - k_2)n_2 - (k_1 + y_1 + y_2)}{n_1 - k_2}. \end{aligned}$$

Combining the above two equalities with equality (7), we get

$$\begin{aligned} M_2(G) = M_2(G^*) &- \Big[d_{G^*}(u)d_{G^*}(v) - d_{G^*}(u) - d_{G^*}(v) \\ &\qquad + d_{G^*}(u)m_{G^*}(u) + d_{G^*}(v)m_{G^*}(v)\Big] \\ = M_2(G^*) &- \Big[(n_2 - k_1)(n_1 - k_2) - (n_2 - k_1) - (n_1 - k_2) \\ &\quad + (n_2 - k_1)n_1 - (x_1 + y_1 + k_2) + (n_1 - k_2)n_2 - (k_1 + y_1 + y_2)\Big] \\ = M_2(G^*) &- \Big[3n_1n_2 - n_2 - n_1 - 2k_1n_1 - 2k_2n_2 \\ &\qquad + k_1k_2 - x_1 - 2y_1 - y_2\Big] \\ = M_2(G^*) &- (3n_1n_2 - n) + 2k_1n_1 + 2k_2n_2 - k_1k_2 + x_1 + 2y_1 + y_2 \qquad (*) \end{aligned}$$

It can be easily checked that the term $2k_1n_1 + 2k_2n_2 - k_1k_2$ reaches its minimum value 0 when $k_1 = k_2 = 0$. For the left part in (6), from equality $(*)$ and the induction hypothesis, we have

$$
\begin{aligned}
M_2(G) &= M_2(G^*) - (3n_1n_2 - n) + 2k_1n_1 + 2k_2n_2 - k_1k_2 + x_1 + 2y_1 + y_2 \\
&\geq n_1^2n_2^2 - 3(k-1)n_1n_2 + n(k-1) + (k-1)^2 - (k-1) \\
&- (3n_1n_2 - n) + x_1 + 2y_1 + y_2 \\
&= n_1^2n_2^2 - 3(k-1)n_1n_2 + n(k-1) + (k-1)^2 - (k-1) \\
&- (3n_1n_2 - n) + 2(k-1) \\
&(\textit{since } k_1 = k_2 = 0 \textit{ implies that } x_1 = y_2 = 0 \textit{ and } y_1 = k-1) \\
&= n_1^2n_2^2 - 3kn_1n_2 + nk + k^2 - k \\
&= M_2(K^0_{n_1,n_2}(e_1, e_2, \cdots, e_k)).
\end{aligned}
$$

The above equality holds if and only if $G^* \cong K^0_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$ and $k_1 = 0, k_2 = 0$. Moreover, from the statement $k_1 = 0, k_2 = 0$ we can deduce that $e_k = uv$ is independent of any edge of $\{e_1, e_2, \cdots, e_{k-1}\}$. Therefore we find that $G \cong K^0_{n_1,n_2}(e_1, e_2, \cdots, e_k)$, which ends the proof of left part in (6).

Now we will turn to the proof for the right part in (6). From the definition of $m_G(v)$ for any vertex v in a graph G and the structure of G^*, we have

$$
\begin{aligned}
m_{G^*}(u) &= \frac{d_{G^*}(v_1) + \cdots + d_{G^*}(v_\alpha) + d_{G^*}(v)}{n_2 - k_1} \\
&\geq \frac{(n_2 - k_1)n_1 - (k - 1 - k_1)}{n_2 - k_1}.
\end{aligned}
$$

Similarly, we have

$$
m_{G^*}(v) \geq \frac{(n_1 - k_2)n_2 - (k - 1 - k_2)}{n_1 - k_2}.
$$

Combining the above two inequalities with equality equality (7), we can obtain

$$
\begin{aligned}
M_2(G) = M_2(G^*) &- \Big[d_{G^*}(u)d_{G^*}(v) - d_{G^*}(u) - d_{G^*}(v) \\
&+ d_{G^*}(u)m_{G^*}(u) + d_{G^*}(v)m_{G^*}(v)\Big] \\
\leq M_2(G^*) &- \Big[(n_2 - k_1)(n_1 - k_2) - (n_2 - k_1) - (n_1 - k_2) \\
&+ (n_2 - k_1)n_1 - (k - 1 - k_1) + (n_1 - k_2)n_2 - (k - 1 - k_2)\Big] \\
= M_2(G^*) &- (3n_1n_2 - n - 2k + 2) + 2(n_2 - 1)k_2 \\
&+ 2(n_1 - 1)k_1 - k_1k_2 \qquad (**)
\end{aligned}
$$

Clearly the term $2(n_2 - 1)k_2 + 2(n_1 - 1)k_1 - k_1k_2$ reaches its maximum value $2(n_2 - 1)(k - 1)$ when $k_1 = 0$ and $k_2 = k - 1$. From the induction hypothesis, it follows that

$$\begin{aligned}M_2(G) &\leq n_1^2n_2^2 - 3(k-1)n_1n_2 + n(k-1) + n_2\Big[(k-1)^2 - (k-1)\Big] \\ &\qquad - (3n_1n_2 - n - 2k + 2) + 2(n_2-1)(k-1) \\ &= n_1^2n_2^2 - 3kn_1n_2 + nk + n_2(k^2 - k) \\ &= M_2(K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_k)).\end{aligned}$$

The above two equalities holds if and only if $G^* \cong K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$ and $k_1 = 0, k_2 = k-1$. That is to say, G is obtained by deleting from $K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_{k-1})$ one more edge which has one common vertex with that one of $\{e_1, e_2, \cdots, e_{k-1}\}$ in it. Therefore we claim that $G \cong K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_k)$, finishing the proof of right part in (6). Thus we complete the proof of this theorem. □

Note that $K^{1,1}_{n_1,n_2}(e_1, e_2, \cdots, e_k) \cong K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_k)$ if $n_1 = n_2$. We denote by $K^{1}_{n_1,n_2}(e_1, e_2, \cdots, e_k)$ this graph when $n_1 = n_2$. By a similar reasoning as that in the proof of Theorem 3.2, the following corollary can be easily obtained.

Corollary 3.1. For any graph $G \in K^p_{t,t}$, we have

$$t^4 - 3pt^2 + 2tp + p^2 - p \leq M_2(G) \leq t^4 - 3pt^2 + 2tp + t(p^2 - p) \tag{8}$$

with left equality holding if and only if $G \cong K^0_{t,t}(e_1, e_2, \cdots, e_p)$ and right equality holding if and only if $G \cong K^1_{t,t}(e_1, e_2, \cdots, e_p)$.

Now we turn to the determination of extremal graphs from $K^p_{n_1,n_2}$ with respect to Zagreb coindices. Based on Lemma 2.1 (1), we have

$$\begin{aligned}\overline{M}_1(K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p)) &= 2(n_1n_2 - p)(n-1) - M_1(K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p)) \\ &= 2(n_1n_2 - p)(n-1) - (nn_1n_2 - 2np + 2p) \\ &= (n-2)n_1n_2 - p,\end{aligned}$$

$$\begin{aligned}\overline{M}_1(K^{1,i}_{n_1,n_2}(e_1, e_2, \cdots, e_p)) &= 2(n_1n_2 - p)(n-1) - M_1(K^{1,i}_{n_1,n_2}(e_1, e_2, \cdots, e_p)) \\ &= 2(n_1n_2 - p)(n-1) - (nn_1n_2 - 2np + p^2 + p) \\ &= (n-2)n_1n_2 - p^2 \ for \ i = 1, 2.\end{aligned}$$

Moreover the following result can be easily obtained.

Corollary 3.2. For any graph $G \in K^p_{n_1,n_2}$, we have

$$(n-2)n_1n_2 - p^2 \leq \overline{M}_1(G) \leq (n-2)n_1n_2 - p \tag{9}$$

with left equality holding if and only if $G \cong K^{1,i}_{n_1,n_2}(e_1, e_2, \cdots, e_p)$ for $i = 1, 2$ and right equality holding if and only if $G \cong K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p)$.

In view of Lemma 2.1 (2), we have

$$\overline{M}_2(K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p)) = 2(n_1n_2 - p)^2 - M_2(K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p))$$

$$
\begin{aligned}
&- \frac{1}{2} M_1(K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p)) \\
&= 2(n_1n_2 - p)^2 - (n_1^2n_2^2 - 3pn_1n_2 + np + p^2 - p) \\
&- \frac{1}{2}(nn_1n_2 - 2np + 2p) \\
&= n_1^2n_2^2 - (p + \frac{1}{2})n_1n_2 + p^2,
\end{aligned}
$$

$$
\begin{aligned}
\overline{M}_2(K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_p)) &= 2(n_1n_2 - p)^2 - M_2(K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_p)) \\
&- \frac{1}{2} M_1(K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_p)) \\
&= 2(n_1n_2 - p)^2 - [n_1^2n_2^2 - 3pn_1n_2 + np + n_2(p^2 - p)] \\
&- \frac{1}{2}(nn_1n_2 - 2np + p^2 + p) \\
&= n_1^2n_2^2 - (p + \frac{1}{2})n_1n_2 - (n_2 - \frac{3}{2})p^2 + (n_2 - \frac{1}{2})p.
\end{aligned}
$$

Corollary 3.3. For any graph $G \in K^p_{n_1,n_2}$, we have

$$
n_1^2n_2^2 - (p + \frac{1}{2})n_1n_2 - (n_2 - \frac{3}{2})p^2 + (n_2 - \frac{1}{2})p \le \overline{M}_2(G) \le n_1^2n_2^2 - (p + \frac{1}{2})n_1n_2 + p^2 \quad (10)
$$

with left equality holding if and only if $G \cong K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_p)$ and right equality holding if and only if $G \cong K^0_{n_1,n_2}(e_1, e_2, \cdots, e_p)$.

Proof. From Lemma 2.1 (2), it suffices to find the extremal graphs from $K^p_{n_1,n_2}$ at which the maximal (or minimal, resp.) first and second Zagreb indices are simultaneously attained. Note that, from Theorems 3.1 and 3.2, the first Zagreb index and second Zagreb index of graphs from $K^p_{n_1,n_2}$ with $n_1 < n_2$ reach the maximum only when $G \cong K^{1,2}_{n_1,n_2}(e_1, e_2, \cdots, e_p)$. Thus our results follow immediately from Theorems 3.1 and 3.2. □

4. A related problem

In this section we propose a problem related to the extremal graphs with respect to Zagreb indices. Based on the alternative formula (1) of the first Zagreb index and the definition of the second Zagreb index, these two indices have very similar versions. Therefore, from the intuition, we think that, in a given set G of connected graphs, the graphs with maximal first Zagreb index are the same as the graphs with maximal second Zagreb index, and vice versa; and the graphs with minimal first Zagreb index are the same as the graphs with minimal second Zagreb index, and vice versa. We say that this set G satisfies extremal identical graph property with respect to Zagreb indices (EIG property w. r. t. Zagreb indices for short). Actually, our statement is true for many known results, such as trees, unicyclic graphs, and bicyclic graphs (see [9]), and so on. Furthermore, our main result in this paper is also a positive example to our statement given above.

Now we would like to propose an interesting problem related to the EIG property as follows:

Problem 1. Characterizing the sets Γ of graphs which satisfy EIG property w. r. t. Zagreb indices?

Moreover, it is reasonable to restrict the consideration to the cases when the set Γ contains connected graphs of the same order.

Obviously, from Lemma 2.1, if a set Γ satisfies EIG property w. r. t. Zagreb indices, then it also satisfies EIG w. r. t. Zagreb coindices. Moreover we can also study the EIG property of any set of graphs with respect to other vertex-degree-based topological indices, which may be of interest to us.

References

1. A.R. Ashrafi, T. Došlić and A. Hamzeh, *The Zagreb coindices of graph operations*, Discrete Appl. Math. **158** (2010), 1571-1578.
2. A.R. Ashrafi, T. Došlić and A. Hamzeh, *Extremal graphs with respect to the Zagreb coindices*, MATCH Commun. Math. Comput. Chem. **65** (2011), 85-92.
3. A.T. Balaban, I. Motoc, D. Bonchev and O. Mekenyan, *Topological indices for structure-activity corrections*, Topics Curr. Chem. **114** (1983), 21-55.
4. J.A. Bondy and U.S.R. Murty, *Graph Theory with Applications*, Macmillan Press, New York, 1976.
5. K.C. Das, *Maximizing the sum of the squares of degrees of a graph*, Discrete Math. **257** (2004), 57-66.
6. K.C. Das, N. Akgünes, M. Togan, A. Yurttas, I.N. Cangül and A.S. Cevik, *On the first Zagreb index and multiplicative Zagreb coindices of graphs*, Analele Stiintifice ale Universitatii Ovidius Constanta, in press.
7. K.C. Das, I. Gutman and B. Zhou, *New upper bounds on Zagreb indices*, J. Math. Chem. **46** (2009), 514-521.
8. K.C. Das and I. Gutman, *Some properties of the second Zagreb index*, MATCH Commun. Math. Comput. Chem. **52** (2004), 103-112.
9. H. Deng, *A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs*, MATCH Commun. Math. Comput. Chem. **57** (2007), 597-616.
10. T. Došlić, *Vertex-weighted Wiener polynomials for composite graphs*, Ars Math. Contemp. **1** (2008), 66-80.
11. M. Eliasi, A. Iranmanesh and I. Gutman, *Multiplicative versions of first Zagreb index*, MATCH Commun. Math. Comput. Chem. **68** (2012), 217-230.
12. I. Gutman, *Multiplicative Zagreb indices of trees*, Bulletin of Society of Mathematicians Banja Luka **18** (2011), 17-23.
13. I. Gutman, *Degree-based topological indices*, Croat. Chem. Acta **86** (2013), 351-361.
14. I. Gutman, An exceptional property of first Zagreb index, MATCH Commun. Math. Comput. Chem. **72** (2014) 733–740.
15. I. Gutman and K.C. Das, *The first Zagreb index 30 years after*, MATCH Commun. Math. Comput. Chem. **50** (2004), 83-92.
16. I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
17. I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. III. Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), 535-538.
18. I. Gutman, B. Ruščić, N. Trinajstić and C.F. Wilcox, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. **62** (1975), 3399-3405.

19. B. Lučić, S. Nikolić and N. Trinajstić, *Zagreb indices, in: Chemical information and computational challenges in the 21st century*, edited by M.V. Putz, Nova Sci. Publ. New York, 2012, 261-275.
20. S. Nikolić, G. Kovačević, A. Miličević and N. Trinajstić, *The Zagreb indices 30 years after*, Croat. Chem. Acta **76** (2003), 113-124.
21. R. Todeschini, D. Ballabio and V. Consonni, *Novel molecular descriptors based on functions of new vertex degrees*, In: Novel molecular structure descriptors - Theory and applications I. (I. Gutman, B. Furtula, eds.), pp. 73-100. Kragujevac: Univ. Kragujevac 2010.
22. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
23. R. Todeschini and V. Consonni, *Zagreb indices (M_n), in: Molecular descriptors for chemoinformatics*, Wiley-VCH, Weinheim, **I**(2009), 955-966.
24. R. Todeschini and V. Consonni, *New local vertex invariants and molecular descriptors based on functions of the vertex degrees*, MATCH Commun. Math. Comput. Chem. **64** (2010), 359-372.
25. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL, 1992.
26. K. Xu, *The Zagreb indices of graphs with a given clique number*, Appl. Math. Lett. **24** (2011), 1026-1030.
27. K. Xu and K.C. Das, *Trees, unicyclic, and bicyclic graphs extremal with respect to multiplicative sum Zagreb index*, MATCH Commun. Math. Comput. Chem. **68** (2012), 257-272.
28. K. Xu, K.C. Das and S. Balachandran, *Maximizing the Zagreb indices of (n,m)- graphs*, MATCH Commun. Math. Comput. Chem. **72** (2014), 641-654.
29. K. Xu, K.C. Das and K. Tang, *On the multiplicative Zagreb coindex of graphs*, Opuscula Math. **33** (2013), 197-210.
30. K. Xu and H. Hua, *A unified approach to extremal multiplicative Zagreb indices for trees, unicyclic and bicyclic graphs*, MATCH Commun. Math. Comput. Chem. **68** (2012), 241-256.

Kexiang Xu received M.Sc. from Southeast University and Ph.D at Nanjing Normal University in China. He is an associate professor of Mathematics in Nanjing University of Aeronautics & Astronautics of China. His research interests include graph theory with its applications.

Department of Mathematics, College of Science, Nanjing University of Aeronautics & Astronautics, Nanjing, Jiangsu 210016, PR China.
e-mail: kexxu1221@126.com

Kechao Tang received M.Sc. from Nanjing University of Aeronautics & Astronautics of China.

Department of Mathematics, College of Science, Nanjing University of Aeronautics & Astronautics, Nanjing, Jiangsu 210016, PR China.
e-mail: tangkechao3@163.com

Hongshuang Liu is a M.Sc. student in Nanjing University of Aeronautics & Astronautics of China.

Department of Mathematics, College of Science, Nanjing University of Aeronautics & Astronautics, Nanjing, Jiangsu 210016, PR China.
e-mail: 992868875@qq.com

Jinlan Wang is a M.Sc. student in Nanjing University of Aeronautics & Astronautics of China.

Department of Mathematics, College of Science, Nanjing University of Aeronautics & Astronautics, Nanjing, Jiangsu 210016, PR China.
e-mail: 774189209@qq.com