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Bipartite Graphs with the Maximal Value of the Second Zagreb Index

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Abstract. The second Zagreb index of a graph G is an adjacency-based topological index, which is defined as $\sum_{uv\in E(G)}(d(u)d(v))$, where uv is an edge of G, $d(u)$ is the degree of vertex u in G. In this paper, we consider the second Zagreb index for bipartite graphs. Firstly, we present a new definition of ordered bipartite graphs, and then give a necessary condition for a bipartite graph to attain the maximal value of the second Zagreb index. We also present an algorithm for transforming a bipartite graph to an ordered bipartite graph, which can be done in $O(n_2+n_1^2)$ time for a bipartite graph B with a partition $|X|=n_1$ and $|Y|=n_2$.

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1. Introduction

The topological index can reflect the property of a molecular graph, so there has been rising interest in it since Wiener put forward the Wiener index in [14]. The Zagreb indices are important indices which were introduced by Gutman *et al.* in [5, 6]. For a graph $G=(V,E)$, the first Zagreb index $Z_1(G)$ and the second Zagreb index $Z_2(G)$ are defined as $Z_1(G)=\sum_{u\in V(G)}(d(u)^2)$, $Z_2(G)=\sum_{uv\in E(G)}(d(u)d(v))$. In the early work, the Zagreb indices appeared in the formulation of computing π-electron energy. They are later used separately as topological indices in QSPR/QSAR [12]. Main properties of Zagreb indices can be found in [3, 7, 8]. The problem of finding the graphs with extreme values of the Zagreb indices was studied by many researchers and the extreme values were gotten over some significant classes of graphs, see [13, 4, 11, 16, 10, 15]. Especially, the maximal value of $Z_2(G)$ of trees was obtained by Damir *et al.* [13]; the extreme values of $Z_2(G)$ of graphs with connectivity at most k were obtained in [16, 10]; the bounds of $Z_2(G)$ of unicyclic graphs were obtained by Yan *et al.*[15]. The extreme values of $Z_1(G)$ of bipartite graphs were obtained in [2]. The sharp bounds for $Z_2(G)$ of bipartite graphs with a given diameter were obtained in [9].

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In this paper we consider the second Zagreb index $Z_2(G)$ of bipartite graphs with a given number of vertices and edges. The rest of the paper is organized as follows. In Section 2, we present a new definition of ordered bipartite graphs and discuss the main character of ordered bipartite graphs. We also give a necessary condition for the bipartite graphs attaining the maximal value of $Z_2(G)$ in Section 2.

All graphs considered in this paper are undirected, simple and connected, and the notation not defined here can be found in [1].

2. Results

Let $G=(V,E)$ be a graph. For $v\in G$, let $N_G(v)$ be the set of all neighbors of v in G. We use $B(X,Y:E)$ to denote a connected bipartite graph with a bipartition (X,Y) and $\mathscr{B}(X,Y:E)$ to denote the set of bipartite graphs $B(X,Y:E)$. Let x be a real number. We use $\lfloor x\rfloor$ to represent the largest integer not greater than x and $\lceil x\rceil$ to represent the smallest integer not less than x.

Definition 2.1 (Ordered sets)**.** *Let $\{u,v\}\subset V$. The pair of vertices $\{u,v\}$ is called ordered if $d(u)\geq d(v)$ implies $N_G(v)\subseteq N_G(u)$. A subset $S\subset V$ is called an ordered set of vertices if any pair of vertices of S is ordered.*

Definition 2.2 (Ordered bipartite graphs)**.** *$B(X,Y:E)$ is called an ordered bipartite graph if X and Y are all ordered sets of vertices. Otherwise, the graph $B(X,Y:E)$ is called an unordered bipartite graph.*

Definition 2.3 (Ordered translations)**.** *Let $\{u,v\}\subset V(G)$ such that $uv\notin E(G)$, $d(u)\geq d(v)$, $N_G(u)\bigcap N_G(v)\neq\emptyset$, $N_G(v)\nsubseteq N_G(u)$. Then the ordered translation $F(G:u,v)$ is defined as*

$$F(G:u,v)=G-\{vv_k|v_k\in S\}+\{uv_k|v_k\in S\}$$

where $S=N_G(v)\setminus N_G(u)$.

In the following, we discuss the main character of ordered translations and ordered bipartite graphs. We also give an algorithm for transforming a bipartite graph to an ordered bipartite graph. A necessary condition for the bipartite graphs attaining the maximal value of $Z_2(G)$ is given. In the end of this section, the bipartite graphs $B(X,Y:E)$ with $|X|=n_1$,$|Y|=n_2$ and $\Delta=\{v\in X|d(v)=n_2\}=p_x$ or $\Delta=\{v\in Y|d(v)=n_1\}=p_y$ are considered.

Theorem 2.1. *Let $\{u,v\}\subset V(G)$ such that $uv\notin E(G)$, $d(u)\geq d(v)$, $N_G(u)\bigcap N_G(v)\neq\emptyset$, $N_G(v)\nsubseteq N_G(u)$. Then $G'=F(G:u,v)$ is connected, where $F(G:u,v)$ is an ordered translation.*

Proof. Since $N_G(v)\nsubseteq N_G(u)$, $N_G(v)\setminus N_G(u)\neq\emptyset$. Let $v_k\in N_G(v)\setminus N_G(u)$. vv_k is replaced by uv_k after the ordered translation $F(G:u,v)$. Therefore the ordered translation $F(G:u,v)$ only effects the path passing the edge vv_k.

Since $N_G(u)\bigcap N_G(v)\neq\emptyset$, $N_{G'}(u)\bigcap N_{G'}(v)\neq\emptyset$. We take a vertex $w\in N_{G'}(u)\bigcap N_{G'}(v)$. Namely there is a path uwv between u and v in G'. On the other hand, it is obvious that $uv_k\in G'$ and $vv_k\notin G'$. Therefore in G', the path passing vv_k can be obtained by linking uv_k and the path between u and v. ∎

Theorem 2.2. *Let $\{u,v\}\subset V(G)$ such that $uv\notin E(G)$, $d(u)\geq d(v)$, $N_G(u)\bigcap N_G(v)\neq\emptyset$, $N_G(v)\nsubseteq N_G(u)$. Then $Z_2(G')>Z_2(G)$, where $G'=F(G:u,v)$.*

Proof. Let $N_G(v) \setminus N_G(u) = S$ and $|S| = \lambda$. It is clear that $\lambda > 0$. By Definition 2.3,

$$F(G:u,v) = G - \{vv_k | v_k \in S\} + \{uv_k | v_k \in S\}.$$

Then

$$\begin{aligned}
Z_2(G') = & \sum_{\substack{xy \in E(G),\\ x,y \neq u,v}} d(x)d(y) + [d(u)+\lambda]\Big(\sum_{v_k \in N_G(u)} d(v_k) + \sum_{v_k \in S} d(v_k)\Big) \\
& + [d(v)-\lambda] \sum_{\substack{v_k \in N_G(v),\\ v_k \notin S}} d(v_k) \\
= & Z_2(G) + \lambda\Big(\sum_{v_k \in N_G(u)} d(v_k) + \sum_{v_k \in S} d(v_k)\Big) + d(u)\sum_{v_k \in S} d(v_k) \\
& - \lambda \sum_{\substack{v_k \in N_G(v),\\ v_k \notin S}} d(v_k) - d(v)\sum_{v_k \in S} d(v_k) \\
= & Z_2(G) + \lambda\Big(\sum_{v_k \in N_G(u)} d(v_k) + \sum_{v_k \in S} d(v_k)\Big) \\
& + (d(u)-d(v))\sum_{v_k \in S} d(v_k) - \lambda \sum_{\substack{v_k \in N_G(v),\\ v_k \notin S}} d(v_k) \\
= & Z_2(G) + \lambda\Big(\sum_{v_k \in N_{G'}(u)} d(v_k) - \sum_{v_k \in N_{G'}(v)} d(v_k)\Big) + (d(u)-d(v))\sum_{v_k \in S} d(v_k).
\end{aligned}$$

Since $N_{G'}(u) \supset N_{G'}(v)$, $\lambda(\sum_{v_k \in N_{G'}(u)} d(v_k) - \sum_{v_k \in N_{G'}(v)} d(v_k)) > 0$. Therefore $Z_2(G') > Z_2(G)$. ∎

Theorem 2.3. *If one set of $\{X,Y\}$ of a bipartite graph $B(X,Y:E)$ is ordered , then $B(X,Y:E)$ is an ordered bipartite graph.*

Proof. We prove this by contradiction. Without loss of generality, suppose X is ordered.

We assume that Y is not ordered. There is at least a pair of vertices $\{u,v\} \subset Y$ such that $d(u) \geq d(v)$ and $N_B(v) \nsubseteq N_B(u)$. Therefore, we have that $N_B(u) \setminus N_B(v) \neq \emptyset$ and $N_B(v) \setminus N_B(u) \neq \emptyset$. Let $x \in N_B(u) \setminus N_B(v)$ and $y \in N_B(v) \setminus N_B(u)$. It is clear that $ux \in E(B)$, $uy \notin E(B)$, $vy \in E(B)$, $vx \notin E(B)$. This implies that $u \in N_B(x)$, $u \notin N_B(y)$, $v \in N_B(y)$, $v \notin N_B(x)$, so $N_B(x) \nsubseteq N_B(y)$ and $N_B(y) \nsubseteq N_B(x)$. Therefore $\{x,y\}$ must be not ordered. It contradicts X being ordered. ∎

Theorem 2.4. *If $B(X,Y:E)$ is an ordered bipartite graph with $|X| = n_1$ and $|Y| = n_2$, then there is at least a pair of vertices $u \in X$ and $v \in Y$ such that $d(u) = n_2$ and $d(v) = n_1$.*

Proof. Let $u \in X$ with $d(u) = \max\{d(u_i) | u_i \in X\}$. Since $B(X,Y:E)$ is an ordered bipartite graph, $N_B(x) \subseteq N_B(u)$ for any $x \in X$. This implies that $\bigcup_{x \in X} N_B(x) \subseteq N_B(u)$. On the other hand, $N_B(u) \subseteq \bigcup_{x \in X} N_B(x)$, by $u \in X$. Therefore $\bigcup_{x \in X} N_B(x) = N_B(u)$. Since $B(X,Y:E)$ is a simple connected graph, $\bigcup_{x \in X} N_B(x) = Y$. We have that $d(u) = n_2$. By a similar way, we can find a vertex $v \in Y$ such that $d(v) = n_1$. ∎

The following is an algorithm for transforming one set of vertices of a bipartite graph to an ordered set of vertices. Let $B(X,Y:E)$ be a bipartite graph with $|X| = n_1$ and $|Y| = n_2$. Let $S = \{u | u \in X, d(u) = n_2\}$ and $v \in Y$ such that $d(v) = \max\{d(v_i) | v_i \in Y\}$. Let $H =$

$\{y|y \in Y, d(y) \le d(v), N_B(y) \bigcap N_B(v) \ne \emptyset, N_B(y) \setminus N_B(v) \ne \emptyset\}$. If $d(v) < n_1$, then $H \ne \emptyset$, since $B(X,Y:E)$ is connected.

Algorithm 1.

Input: $B(X,Y:E)$ with $|X| = n_1$ and $|Y| = n_2$.

Output: $B'(X,Y:E)$ with $|X| = n_1$ and $|Y| = n_2$ such that X being ordered.

Step 1: If $d(v) < n_1$, then take $y \in H$ and do the ordered translation $F(B:v,y)$. Go to step 2. Otherwise, go to Step 3.

Step 2: Let $H = H - \{y\}$, go to Step 1.

Step 3: Let $S_1 = X \setminus S$. If $S_1 \ne \emptyset$, then take a vertex u such that $u \in S_1$ and $d(u) = \max\{d(u_i)|u_i \in S_1\}$. Let $S_2 = S_1 - \{u\}$ and go to Step 4. Otherwise, stop.

Step 4: If $S_2 \ne \emptyset$, go to Step 5. Otherwise, go to Step 6.

Step 5: Take a vertex $v \in S_2$. If v satisfies $N_G(v) \nsubseteq N_G(u)$, then we do ordered translation $F(B,u,v)$. Let $S_2 = S_2 \setminus \{v\}$ and go to Step 4.

Step 6: Let $S = S \bigcup \{u\}$ and go to Step 3.

Obviously, Algorithm 1 can be done in $O(n_2 + n_1^2)$ time. On the other hand, according to Theorem 2.3, when a bipartite graph need to be transformed to an ordered bipartite graph, it is sufficient to transform one set of $\{X,Y\}$ to be ordered. Hence, we have the following result.

Theorem 2.5. *Any simple connected bipartite graph $B(X,Y:E)$ can be translated into an ordered bipartite graph by a finite number of ordered translations.*

Theorem 2.6. *Let m and n be two integers with $n-1 \le m \le \lfloor n/2 \rfloor \lceil n/2 \rceil$. If $B(X,Y:E)$ attains the maximum value of the second Zagreb index among $\mathscr{B}(X,Y:E)$ with n vertices and m edges, then $B(X,Y:E)$ must be an ordered bipartite graph.*

Proof. We prove this by contradiction. Suppose B_1 is a bipartite graph with n vertices and m edges such that $Z_2(B_1) = \max\{Z_2(B)|B \in \mathscr{B}(X,Y:E)\}$, but B_1 isn't an ordered bipartite graph. It follows from Theorem 2.5 that B_1 can be translated into an ordered bipartite graph B'. By Theorem 2.2, $Z_2(B') > Z_2(B_1)$. This contradicts that B_1 attains the maximal value of the second Zagreb index. ∎

In fact, Theorem 2.6 gives a necessary condition, that is not sufficient for a bipartite graph attaining the maximal value of $Z_2(G)$, since the ordered bipartite graphs with $|X| = n_1$, $|Y| = n_2$ and m edges are not unique. In the following, we discuss the bipartite graphs $B(X,Y:E)$ with $|X| = n_1$,$|Y| = n_2$ and $\Delta = \{v \in X|d(v) = n_2\} = p_x$ or $\Delta = \{v \in Y|d(v) = n_1\} = p_y$.

Theorem 2.7. *Let m,n and p be three integers with $m = (n-1)+(p-1)(n_2-1)+k$, where $p \ge 1, k \le n_2 - 1$. If $B(X,Y:E)$ with $|X| = n_1$, $|Y| = n_2$ satisfies $\Delta = |\{v \in X|d(v) = n_2\}| = p$, then*

$$Z_2(B) \le pn_1n_2 + p^2n_2^2 + n_1^2 + (k-p)n_1 + p(k-p)n_2 + (p+1)k(k+1)$$

Proof. We prove this by induction. Suppose B is a bipartite graph with n vertices and m edges such that $m = (n-1)+(p-1)(n_2-1)+k$.

(1) when $k = 0$,

$$Z_2(B) = pn_1n_2 + p^2n_2^2 + n_1^2 - n_1p - p^2n_2.$$

Therefore, when $k = 0$,

$$Z_2(B) \le pn_1n_2 + p^2n_2^2 + n_1^2 + (k-p)n_1 + p(k-p)n_2 + (p+1)k(k+1)$$

(2) Suppose when $k = r, r \le n_2 - 2$,

$$Z_2(B) \le pn_1n_2 + p^2n_2^2 + n_1^2 + (r-p)n_1 + p(r-p)n_2 + (p+1)r(r+1).$$

In the following, we prove

$$Z_2(B) \le pn_1n_2 + p^2n_2^2 + n_1^2 + (k-p)n_1 + p(k-p)n_2 + (p+1)k(k+1),$$

when $k = r+1$.

We prove this by contradiction. Suppose $B_1(X,Y:E)$ is a bipartite graph with n vertices and m edges such that $m = (n-1)+(p-1)(n_2-1)+(r+1)$ and $\Delta = |\{v \in X | d(v) = n_2\}| = p$, which attains the maximum value of the second Zagreb index, but $Z_2(B_1) > pn_1n_2 + p^2n_2^2 + n_1^2 + (r+1-p)n_1 + p[(r+1)-p]n_2 + (p+1)(r+1)(r+2)$. Let $\eta \in Y$ such that $d(\eta) = min\{d(v)|v \in Y, d(v) \ne p)\} = \delta$, and $\xi\eta \in E$ such that $d(\xi) = min\{d(u)|u \in N_{B_1}(\eta)\}$. Since B_1 attains the maximum value of the second Zagreb index, according to Theorem 2.6, B_1 is an ordered bipartite graph.

In the following, we distinguish two cases.

Case 1: $\delta - p = 1$

Since $\delta - p = 1$, only ξ is adjacent to η except the vertices in Δ. This implies that

$$d(\xi) \le r+2, \qquad \sum_{u_i \in N_{B_1}(\eta), u_i \ne \xi} d(u_i) = pn_2,$$

and

$$\sum_{v_i \in N_{B_1}(\xi), v_i \ne \eta} d(v_i) \le n_1 + (d(\xi)-2)p + [(r+1)-(\delta-p)].$$

Therefore,we can obtain

$$\begin{aligned} Z_2(B_1 - \xi\eta) &= Z_2(B_1) - [d(\xi)d(\eta) + \sum_{u_i \in N_{B_1}(\eta), u_i \ne \xi} d(u_i) + \sum_{v_i \in N_{B_1}(\xi), v_i \ne \eta} d(v_i) \\ &\ge Z_2(B_1) - [\delta(r+2) + pn_2 + n_1 + rp + r] \\ &> pn_1n_2 + p^2n_2^2 + n_1^2 + (r-p)n_1 + p(r-p)n_2 + (p+1)r(r+1) \end{aligned}$$

This contradicts that when $k = r$,

$$Z_2(B) \le pn_1n_2 + p^2n_2^2 + n_1^2 + (r-p)n_1 + p(r-p)n_2 + (p+1)r(r+1).$$

Case 2: $\delta - p \ge 2$

Since $d(\xi) = min\{d(u)|u \in N_{B_1}(\eta)\}$, and B_1 is an ordered bipartite graph,

$$d(\xi) \le \left\lfloor \frac{r+1}{\delta-p} \right\rfloor + 1, \qquad \sum_{v_i \in N_{B_1}(\xi), v_i \ne \eta} d(v_i) \le n_1 + (d(\xi)-2)p + [(r+1)-(\delta-p)].$$

Then

$$\begin{aligned} Z_2(B_1 - \xi\eta) &= Z_2(B_1) - [d(\xi)d(\eta) + \sum_{u_i \in N_{B_1}(\eta), u_i \ne \xi} d(u_i) + \sum_{v_i \in N_{B_1}(\xi), v_i \ne \eta} d(v_i) \\ &\ge Z_2(B_1) - \left[pn_2 + n_1 + 2r + 1 + (\delta+p)\left\lfloor \frac{r+1}{\delta-p} \right\rfloor\right] \\ &\ge Z_2(B_1) - \left[pn_2 + n_1 + 3(r+1) - 1 + 2p\frac{r+1}{\delta-p}\right] \qquad (2.1) \end{aligned}$$

Since $\delta - p \geq 2$, from equation (2.1), we have that

$$\begin{aligned} Z_2(B_1 - \xi\eta) &\geq Z_2(B_1) - [pn_2 + n_1 + 3(r+1) - 1 + p(r+1)] \\ &> pn_1n_2 + p^2n_2^2 + n_1^2 + (r+1-p)n_1 + p[(r+1)-p]n_2 + (p+1)(r+1)(r+2) \\ &\quad - [pn_2 + n_1 + 3(r+1) - 1 + p(r+1)] \\ &> pn_1n_2 + p^2n_2^2 + n_1^2 + (r-p)n_1 + p(r-p)n_2 + (p+1)r(r+1) \end{aligned}$$

This contradicts that when $k = r$,

$$Z_2(B) \leq pn_1n_2 + p^2n_2^2 + n_1^2 + (r-p)n_1 + p(r-p)n_2 + (p+1)r(r+1).$$

From the above discussion, we can get that

$$Z_2(B) \leq pn_1n_2 + p^2n_2^2 + n_1^2 + (k-p)n_1 + p(k-p)n_2 + (p+1)k(k+1),$$

when $k = r+1$. ∎

Although only one set of bipartite graphs is considered in Theorem 2.7, the same result is correct for the other set of bipartite graphs according to the proof of the Theorem 2.7.

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