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The second Zagreb indices of graphs with given degree sequences[☆]

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ABSTRACT

The second Zagreb index of a simple undirected graph G is defined as $M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$, where $d(x)$ is the degree of vertex x in G. In this paper, we investigate properties of the extremal graphs with the maximum second Zagreb indices with given graphic sequences, in particular graphic bicyclic sequences. Moreover, we obtain the relations of the second Zagreb indices among the extremal graphs with different degree sequences.

1. Introduction

Throughout this paper, $G = (V, E)$ is a simple undirected graph with vertex set V and edge set E. The distance between two vertices u and v which is denoted by $d(u, v)$ is the length of the shortest path that connects u and v. For a vertex $v \in V$, $N(v)$ denotes the neighbor set of v and $d(v) = |N(v)|$ denotes the degree of v. A vertex whose degree is one is called *leaf*. Moreover, $(d(v_1), \ldots, d(v_n))$ is called *degree sequence* of G. A nonnegative non-increased integer sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called the *graphic sequence* if there exists a simple graph G such that its degree sequence is exactly π. For convenience, we use $d^{(k)}$ to denote the k same degrees d in π. For example, $\pi = (4, 4, 2, 2, 1, 1)$ is denoted by $(4^{(2)}, 2^{(2)}, 1^{(2)})$. Let π be a given graphic sequence. Let

$$\Gamma(\pi) = \{G \mid G \text{ is a connected graph with degree sequences } \pi\}.$$

Without loss of generality, assume $d(v_i) = d_i$, for $1 \le i \le n$, $v_i \in V(G)$, $G \in \Gamma(\pi)$.

The *second Zagreb index* [1] of a simple graph G is defined by:

$$M_2(G) = \sum_{uv\in E} d(u)d(v). \tag{1}$$

For a given graphic sequence π, let

$$M_2(\pi) = \max\{M_2(G) : G \in \Gamma(\pi)\}.$$

A simple connected graph G is called an *optimal graph* in $\Gamma(\pi)$ if $G \in \Gamma(\pi)$ and $M_2(G) = M_2(\pi)$.

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The second Zagreb index, whose origin may be dated back to [6,5], plays an important role in total π-electron energy on molecular structure in chemical graph theory. There are two excellent surveys [4,14] on the Zagreb index, which summarize main properties and characterization of the topological index. Das et al. [2] investigated the connections between the Zagreb index and the Wiener index. Estes and Wei [3] presented the sharp upper and lower bounds for the Zagreb indices of k-tree. For more information, the readers are referred to [1,4,5,7–10], [14,15] and the references therein.

Recently, Liu and Liu [11] characterized all optimal trees in the set of trees with a given degree sequence. Further, they [12] investigate some optimal graphs in the set of unicycle graphs with a given graphic sequence. In this paper, we study properties of the optimal graphs in the set of all connected graphs with a given graphic sequence π that satisfies some conditions, which generalize the main results in [11] and [12]. In addition, we present some optimal graphs in the set of all bicyclic graphs with a given graphic sequence and some relations of the maximum values of the second Zagreb indices with different bicyclic graphic sequences.

The rest of this paper is organized as follows. In Section 2, some notations and the main results of this paper are presented. In Sections 3–5, the proofs of the main results are presented, respectively.

2. Preliminary and main results

In order to present the main results of this paper, we introduce some more notations. Assume G is a rooted graph with root v_1. Let $h(v)$ be the distance between v and v_1 and $V_i(G)$ be the set of vertices with distance i from vertex v_1.

Definition 2.1 (*[17]*). Let $G = (V, E)$ be a graph of root v_1. A well-ordering $\prec$ of the vertices is called breadth-first search ordering with non-increasing degrees (BFS-ordering for short) if the following holds for all vertices $u, v \in V$:

(1) $u \prec v$ implies $h(u) \leq h(v)$;

(2) $u \prec v$ implies $d(u) \geq d(v)$;

(3) if there are two edges $uu_1 \in E(G)$ and $ww_1 \in E(G)$ such that $u \prec w$, $h(u) = h(u_1) + 1$ and $h(w) = h(w_1) + 1$, then $u_1 \prec w_1$.

For a graphic sequence $\pi = (d_1, d_2, \ldots, d_n)$ with $\sum_{i=1}^{n} d_i = 2(n+c)$, $d_1 \geq d_2 \geq c+2$, c is an integer and $c \geq -1$. We may construct a graph $G_M^*(\pi)$ by following steps.

Select v_1 as the root vertex and begin with v_1 of the zeroth layer. Select the vertices $v_2, v_3, v_4, \ldots, v_{d_1+1}$ as the first layer such that $N(v_1) = \{v_2, v_3, v_4, \ldots, v_{d_1+1}\}$; then append $d_2 - 1$ vertices to v_2, $d_3 - 2$ vertices to $v_3, \ldots,$ $d_{c+3} - 2$ vertices to v_{c+3} such that $N(v_2) = \{v_1, v_3, \ldots, v_{c+3}, v_{d_1+2}, v_{d_1+3}, \ldots, v_{d_1+d_2-c-1}\}$, $N(v_3) = \{v_1, v_2, v_{d_1+d_2-c}, \ldots,$ $v_{d_1+d_2+d_3-c-3}\}, \ldots, N(v_{c+3}) = \{v_1, v_2, v_{(\sum_{i=1}^{c+2} d_i)-3c}, \ldots, v_{(\sum_{i=1}^{c+3} d_i)-3c-3}\}$. After that, append $d_{c+4} - 1$ vertices to v_{c+4} such that $N(v_{c+4}) = \{v_1, v_{(\sum_{i=1}^{c+3} d_i)-3c-2}, \ldots, v_{(\sum_{i=1}^{c+4} d_i)-3c-4}\}; \cdots$. Note that $v_1v_2v_3, \ldots, v_1v_2v_{c+3}$ form $c+1$ triangles in $G_M^*(\pi)$. Obviously, $G_M^*(\pi)$ is a BFS-ordering graph. In particular, if $c = -1$, there are no triangles; if $c = 1$, the graph $G_M^*(\pi)$ is denoted by $B_M^*(\pi)$.

The first main result in this paper can be stated as follows.

Theorem 2.2. *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a graphic sequence. If it satisfies the following conditions:*

(i) $\sum_{i=1}^{n} d_i = 2(n+c)$, *c is an integer and* $c \geq -1$;

(ii) $d_1 \geq d_2 \geq c+2$;

(iii) $d_3 \geq d_4 = d_5 = \cdots = d_{c+3}$, *for* $c \geq 0$;

(iv) $d_n = 1$;

then $G_M^*(\pi)$ is an optimal graph in $\Gamma(\pi)$. In other words, for any graph $G \in \Gamma(\pi)$, $M_2(G) \leq M_2(G_M^*(\pi))$.

Remark 2.3. If π is a tree degree sequence, then there exists only one tree with degree π having a BFS order (for example, see [16]). Hence it follows from Theorem 2.2 that the main results in [11] and [12] hold for $c = -1$ and $c = 0$, respectively.

Corollary 2.4 (*[11]*). *Let π be a tree degree sequence. The BFS-tree in $\Gamma(\pi)$ reaches the maximum second Zagreb index.*

Corollary 2.5 (*[12]*). *Let $\pi = (d_1, \ldots, d_n)$ be a unicycle graphic sequence with $d_n = 1$. Then there exists an optimal graph $G \in \Gamma(\pi)$ which has a BFS-ordering $\{v_1, \ldots, v_n\}$ with a triangle $v_1v_2v_3$.*

Moreover, condition(iii) in Theorem 2.2 cannot be deleted. For example, let $\pi = (4, 4, 3, 3, 2, 1, 1)$ which does not satisfy condition(iii) . In Fig. 1, G is produced by the method in Theorem 2.2 and G' is not isomorphic to G. It is easy to see that $M_2(G') = M_2(G) + 1$.

In order to present the results of bicyclic graphs with given graphic sequences, we introduce some more notations.

A *bicyclic graph* is a connected graph with $n \geq 4$ vertices and $n+1$ edges. Let $\pi = (d_1, \ldots, d_n)$ be a graphic sequence. If π is a degree sequence of some bicyclic graphs, π is called a *bicyclic graphic sequence*. For a given bicyclic graphic sequence π, let

$$\mathcal{B}_\pi = \{\, G \mid G \text{ is a bicyclic graph with degree sequences } \pi \}.$$