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The second Zagreb indices of unicyclic graphs with given degree sequences

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ABSTRACT

Let $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ be two different non-increasing degree sequences. We write $\pi \lhd \pi'$, if and only if $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n$. Let $\Gamma(\pi)$ be the class of connected graphs with degree sequence π. The second Zagreb index of a graph G is denoted by $M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$. In this paper, we characterize an extremal unicyclic graph that achieves the maximum second Zagreb index in the class of unicyclic graphs with given degree sequence, and we also prove that if $\pi \lhd \pi'$, π and π' are unicyclic degree sequences and U^* and U^{**} have the maximum second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively, then $M_2(U^*) < M_2(U^{**})$. Furthermore, we determine the first to ninth largest second Zagreb indices together with the corresponding extremal unicyclic graphs in the class of unicyclic graphs on $n \geq 17$ vertices.

1. Introduction

Throughout this paper, we are concerned with connected undirected simple graph only. Let S_n, C_n and P_n be the star, cycle and path of order n, respectively. The *second Zagreb index* of G is denoted by [2]

$$M_2(G) = \sum_{uv\in E(G)} (d(u)d(v)) . \tag{1.1}$$

For the chemical applications and mathematical properties of the second Zagreb index, we refer the readers to [1,2,5,6] and the references therein.

The sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G if $d_i = d(v_i)$ holds for $1 \leq i \leq n$. Throughout this paper, we use d_i to denote the ith largest degree of G and we suppose that $d(v_i) = d_i$, where $1 \leq i \leq n$. Let $\Gamma(\pi)$ be the class of connected graphs with degree sequence π.

Suppose $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two different non-increasing degree sequences, we write $\pi \lhd \pi'$ if and only if $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n$. Such an ordering is sometimes called *majorization* (see [4]).

A unicyclic graph is a connected graph with n vertices and n edges. In [3], an extremal tree with the maximum second Zagreb index in the class of trees with given degree sequence was characterized. In this note, we identify an extremal unicyclic graph with the maximum second Zagreb index in the class of unicyclic graphs with given degree sequence, and we also prove

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that if $\pi \lhd \pi'$, π and π' are two different unicyclic degree sequences, U^* and U^{**} have the maximum second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively, then $M_2(U^*) < M_2(U^{**})$. Furthermore, we determine the first to ninth largest second Zagreb indices together with the corresponding extremal unicyclic graphs in the class of unicyclic graphs on $n \geq 17$ vertices.

2. The main results

Let $G - uv$ and $G + uv$, respectively, denote the new graph obtained from G by deleting and adding the edge uv.

Lemma 2.1 ([3]). *Let $G = (V, E)$ be a connected graph with $v_1u_1 \in E$, $v_2u_2 \in E$, $v_1v_2 \notin E$ and $u_1u_2 \notin E$. Let $G' = G - u_1v_1 - u_2v_2 + v_1v_2 + u_1u_2$. If $d(v_1) \geq d(u_2)$ and $d(v_2) \geq d(u_1)$, then $M_2(G') \geq M_2(G)$, where $M_2(G') > M_2(G)$ if and only if both two inequalities are strict.*

Lemma 2.2 ([3]). *Suppose $G \in \Gamma(\pi)$, and there exist three vertices u, v, w of a connected graph G such that $uv \in E(G)$, $uw \notin E(G)$, $d(v) < d(w) \leq d(u)$, and $d(u) > d(x)$ for all $x \in N(w)$. Then, there exists another connected graph $G' \in \Gamma(\pi)$ such that $M_2(G) < M_2(G')$.*

Lemma 2.3. *For any degree sequence π with $n \geq 3$, there exists an extremal graph $G \in \Gamma(\pi)$ with the maximum second Zagreb index in $\Gamma(\pi)$ such that $\{v_2, v_3\} \subseteq N(v_1)$.*

Proof. If $v_1v_2 \notin E(G)$, then there is some vertex v such that $v_1v \in E(G)$ and $d(v_1) \geq d(v_2) > d(v)$ and $d(v_1) > d(x)$ holds for all $x \in N(v_2)$, which contradicts Lemma 2.2. Thus, $v_1v_2 \in E(G)$. Now, we assume that $v_1v_3 \notin E(G)$. Then, $d(v_3) > d(v)$ holds for every $v \in N(v_1) \setminus \{v_2\}$. By Lemma 2.2, we may assume that there exists some vertex $u \in N(v_3)$ such that $d(u) = d_1$. If $u = v_2$, the result already holds. If $u \neq v_2$, then $d(u) = d_1 = d_2 = d_3$. Let P be a shortest path from v_1 to v_3.

If $v_2 \notin V(P)$, choose $x \in N(v_1) \cap V(P)$, since $v_1 \in N(x) \setminus N(v_3)$, there must exist some vertex $y \in N(v_3) \setminus V(P)$ such that $y \notin N(x)$. Let $G_1 = G + v_1v_3 + xy - v_1x - v_3y$. By Lemma 2.1, $G_1 \in \Gamma(\pi)$ and $M_2(G_1) \geq M_2(G)$, the result holds. If $v_2 \in V(P)$, we may suppose that $v_2v_3 \notin E(G)$ (otherwise, the result already holds). Choose $x \in N(v_2) \cap V(P)$ such that $x \neq v_1$. It can be proved similarly with the case $v_2 \notin V(P)$. ■

Lemma 2.4. *If π is a unicyclic degree sequence with $d_n = 1$, then there exists an extremal graph $G \in \Gamma(\pi)$ with the maximum second Zagreb index in $\Gamma(\pi)$ such that the unique cycle of G is a triangle with $V(C_3) = \{v_1, v_2, v_3\}$.*

Proof. Suppose C_t is the unique cycle of G. Now, it suffices to prove the following claims.

Claim 1. There is an extremal graph $G \in \Gamma(\pi)$ such that $v_1 \in V(C_t)$ and $\{v_2, v_3\} \subseteq N(v_1)$.

Assume that Claim 1 does not hold for any extremal graph $G \in \Gamma(\pi)$. By Lemma 2.3, we may suppose that G is an extremal graph of $\Gamma(\pi)$ such that $\{v_2, v_3\} \subseteq N(v_1)$. Then, $v_1 \notin C_t$. Suppose that $P = u \cdots v_1 \cdots xy$ is the unique path connecting u and y such that v_1 is on the path P, where $u \in C_t$ and $d(y) = 1$. Let $w \in N(u) \cap V(C_t)$.

If $d(w) \leq d(x)$, let $G_1 = G + ux + wy - wu - xy$. By Lemma 2.1, $M_2(G_1) \geq M_2(G)$. Note that $G_1 \in \Gamma(\pi)$, v_1 is in the unique cycle of G_1 and $\{v_2, v_3\} \subseteq N(v_1)$, a contradiction. If $d(u) \leq d(x)$, let $G_2 = G + uy + wx - wu - xy$. By Lemma 2.1, $M_2(G_2) \geq M_2(G)$. Note that $G_2 \in \Gamma(\pi)$, v_1 is in the unique cycle of G_2 and $\{v_2, v_3\} \subseteq N(v_1)$, a contradiction. Thus, $\min\{d(u), d(w)\} > d(x)$.

Now, choose $z \in (N(x) \cap V(P)) \setminus \{y\}$. Similarly, $\min\{d(u), d(w)\} > d(z)$. Repeating the above process, we will yield that $\min\{d(u), d(w)\} > d(v_1)$, a contradiction. Thus, Claim 1 holds.

Claim 2. There is an extremal graph $G \in \Gamma(\pi)$ such that $v_1v_2 \in E(C_t)$ and $v_3 \in N(v_1)$.

Assume that Claim 2 does not hold for any extremal graph $G \in \Gamma(\pi)$. By Claim 1, there exists an extremal graph $G \in \Gamma(\pi)$ such that $v_1 \in V(C_t)$ and $\{v_2, v_3\} \subseteq N(v_1)$. Then, $v_2 \notin V(C_t)$. Choose $\{u, v\} \subseteq V(C_t) \setminus \{v_1\}$ such that $uv \in E(C_t)$. Suppose that $P = v_1v_2xy \cdots z$ is the unique path connecting v_1 and z such that v_2 is on the path P, where $d(z) = 1$.

Suppose that $\max\{d(u), d(v)\} = d(u)$. If $d(u) \geq d(x)$, let $G_1 = G + uv_2 + vx - uv - v_2x$. By Lemma 2.1, $M_2(G_1) \geq M_2(G)$. But Claim 2 holds for G_1, a contradiction. Thus, $\max\{d(u), d(v)\} = d(u) < d(x)$. Similarly, $\max\{d(u), d(v)\} < d(y)$. Repeating the above process, we will yield that $\max\{d(u), d(v)\} < d(z) = 1$, a contradiction. Thus, Claim 2 holds.

Claim 3. There is an extremal graph $G \in \Gamma(\pi)$ such that $\{v_1v_2, v_1v_3\} \subseteq E(C_t)$.

By Claim 2, there is an extremal graph $G \in \Gamma(\pi)$ such that $v_1v_2 \in E(C_t)$ and $v_3 \in N(v_1)$. If $v_3 \notin V(C_t)$, then $v_2v_3 \notin E(G)$. Choose $u \in (V(C_t) \cap N(v_2)) \setminus \{v_1\}$ and $v \in N(v_3) \setminus \{v_1\}$. Let $G_1 = G + v_2v_3 + uv - vv_3 - uv_2$. By Lemma 2.1, $M_2(G_1) \geq M_2(G)$ and $G_1 \in \Gamma(\pi)$. It is easily checked that Claim 3 holds for G_1.

Claim 4. There is an extremal graph $G \in \Gamma(\pi)$ such that $\{v_1, v_2, v_3\} = V(C_t)$.

If $d_2 = 2$, it is easily checked that the result holds. So, we may suppose that $d_2 \geq 3$. By Claim 3, there exists an extremal graph $G \in \Gamma(\pi)$ such that $\{v_1v_2, v_1v_3\} \subseteq E(C_t)$. If $\{v_1, v_2, v_3\} \neq V(C_t)$, then $v_2v_3 \notin E(G)$. Choose $u \in N(v_2) \setminus V(C_t)$, and choose $v \in (N(v_3) \cap V(C_t)) \setminus \{v_1\}$. Let $G_1 = G + v_2v_3 + uv - vv_3 - uv_2$. By Lemma 2.1, $M_2(G_1) \geq M_2(G)$. Since $G_1 \in \Gamma(\pi)$ and $\{v_1, v_2, v_3\} = V(C_t)$, Claim 4 holds. ■

To give our main result, we have to introduce the following notation.

Suppose $\pi = (d_1, d_2, \ldots, d_n)$, where $d_n = 1$. Let $U_M(\pi)$ be the unique unicyclic graph such that the unique cycle of $U_M(\pi)$ is a triangle with $V(C_3) = \{v_1, v_2, v_3\}$, and the remaining vertices appear in *BFS*-ordering with respect to C_3 starting from v_4 that is adjacent to v_1. It means that, $U_M(\pi)$ can be constructed by the breadth-first-search method as follows: select the vertices $\{v_1, v_2, v_3\}$ as the root vertices and begin with $\{v_1, v_2, v_3\}$ of the zeroth layer. Select the vertices $v_4, v_5, \ldots, v_{d_1+d_2+d_3-3}$ as the first layer such that $N(v_1) = \{v_2, v_3, v_4, v_5, \ldots, v_{d_1+1}\}$, $N(v_2) = \{v_1, v_3, v_{d_1+2}, v_{d_1+3}, \ldots, v_{d_1+d_2-1}\}$,