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UNICYCLIC GRAPHS WITH THE FIRST THREE SMALLEST AND LARGEST FIRST GENERAL ZAGREB INDEX

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Abstract

The first general Zagreb index of a graph G is defined as $M_1^\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha$, where $d(u)$ denotes the degree of the vertex u in G and α is an arbitrary real number except 0 and 1. A graph is called *unicyclic* if it is connected and contains a unique cycle. In this paper, we characterize all unicyclic graphs with the smallest, the second and third smallest values of the first general Zagreb index. The same is done for unicyclic graphs with the largest, the second and third largest values of this index.

1 Introduction

The original Zagreb indices, including the first Zagreb index M_1 and the second Zagreb index M_2, were introduced 33 years ago [6]. These indices reflect the extent of branching of the molecular carbon-atom skeleton and can be viewed as molecular structure-descriptors [1, 11]. Recently, the Zagreb indices and their variants have been used to study molecular complexity, chirality, ZE-isomerism and heterosystems etc. The Zagreb indices are also used by various researchers in their QSPR and QSAR studies. Mathematical properties of the Zagreb indices have also been studied [3, 4, 10]. The development and use of the Zagreb indices were summarized in [5, 9].

Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The *first Zagreb index* of G is defined as

$$M_1(G) = \sum_{u \in V(G)} d(u)^2,$$

where $d(u)$ denotes the degree of the vertex u in G. In [8], Li and Zheng introduced the concept of the *first general Zagreb index* of G as

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} d(u)^{\alpha},$$

where α is an arbitrary real number except 0 and 1. Li and Zhao [7] characterized all trees with the first three smallest and largest values of the first general Zagreb index when α is any integers (including negative integers) or any of the fractions $\frac{1}{k}$ for any nonzero integer k.

A graph is called *unicyclic* if it is connected and contains a unique cycle. Our aim in this paper is to consider the problem of determining the extremal values of the first general Zagreb index of unicyclic graphs for general α, and characterizing the corresponding extremal graphs.

Let G be a graph. By $\Delta(G)$ and $\delta(G)$, we denote its maximum degree and minimum degree respectively, and by n_i, we denote the number of vertices of degree i. If G has a_i vertices of degree x_i $(i = 1, 2, \cdots, t)$, where $\Delta(G) = x_1 > x_2 > \cdots > x_t = \delta(G)$ and $\sum_{i=1}^{t} a_i = |V(G)|$, we define $D(G) = [x_1^{a_1}, x_2^{a_2}, \cdots, x_t^{a_t}]$. If $a_i = 1$, we use x_i instead of $x_i^{a_i}$ for convenience. Usually, a path with end-vertices u and v is denoted by $P[u, v]$. If C is a cycle, then a path P is called a C-*path* if

$|V(C) \cap V(P)| = 1$. Furthermore, a C-path P is called *maximal* if it is not a subpath of any other C-path different from P. For notations and terminology not given here, we refer to [2, 12].

The structure of this paper is as follows. In Section 2, we provide a lemma which will be heavily used in the proofs of the main results of this paper. In Section 3, we characterize all unicyclic graphs with the smallest, the second and third smallest values of the first general Zagreb index. Similar results for unicyclic graphs with the largest, the second and third largest values of this index are given in Section 4.

The problem we are concerned with in this paper would be trivial if the graphs under consideration have fewer than 7 vertices. So in the following, we only consider unicyclic graphs with at least 7 vertices.

2 A useful lemma

The following lemma will be frequently used in the proofs of the main results of this paper.

Lemma 1. *Let a and b be positive numbers such that $a \geq b+2$, and α a real number other than 0 and 1. Then*
(i) $a^\alpha + b^\alpha > (a-1)^\alpha + (b+1)^\alpha$ if $\alpha \in (-\infty, 0) \cup (1, +\infty)$;
(ii) $a^\alpha + b^\alpha < (a-1)^\alpha + (b+1)^\alpha$ if $\alpha \in (0, 1)$.

Proof. Let us calculate

$$a^\alpha + b^\alpha - [(a-1)^\alpha + (b+1)^\alpha] = [a^\alpha - (a-1)^\alpha] - [(b+1)^\alpha - b^\alpha]. \tag{1}$$

Using Lagrange's mean value theorem, we conclude that there is a number $\xi_1 \in (b, b+1)$ such that $(b+1)^\alpha - b^\alpha = \alpha \xi_1^{\alpha-1}$, and there is a number $\xi_2 \in (a-1, a)$ such that $a^\alpha - (a-1)^\alpha = \alpha \xi_2^{\alpha-1}$. Hence expression (1) transforms into $\alpha(\xi_2^{\alpha-1} - \xi_1^{\alpha-1})$. Note that $0 < \xi_1 < \xi_2$. Again, from Lagrange's mean value theorem, there is a number $\xi \in (\xi_1, \xi_2)$ such that $\alpha(\xi_2^{\alpha-1} - \xi_1^{\alpha-1}) = \alpha(\alpha-1)\xi^{\alpha-2}(\xi_2 - \xi_1)$. Clearly, $\xi^{\alpha-2}$ and $(\xi_2 - \xi_1)$ are positive. At the same time, $\alpha(\alpha-1)$ is positive if $\alpha \in (-\infty, 0) \cup (1, +\infty)$ and negative if $\alpha \in (0, 1)$. The result follows. $\square$

3 Unicyclic graphs with the first three smallest values of the first general Zagreb index

Theorem 1. *Let G be a unicyclic graph with $n \geq 7$ vertices and α a real number with $\alpha \in (-\infty, 0) \cup (1, +\infty)$. Then*
(i) $M_1^\alpha(G)$ attains the smallest value if and only if $D(G) = [2^n]$;
(ii) $M_1^\alpha(G)$ attains the second smallest value if and only if $D(G) = [3, 2^{n-2}, 1]$;
(iii) $M_1^\alpha(G)$ attains the third smallest value if and only if $D(G) = [3^2, 2^{n-4}, 1^2]$.

Proof. (i) By contradiction. Suppose $M_1^\alpha(G)$ attains the smallest value and $D(G) \neq [2^n]$. Let $C = u_1u_2 \cdots u_ku_1$ be the unique cycle in G. Then $k < n$ and there is at least one vertex u_i with $d(u_i) \geq 3$. Without loss of generality, we assume $d(u_1) \geq 3$. Choose a maximal C-path $P[u_1, v_1]$ in G. Clearly $d(v_1) = 1$. Let $G' = G - u_1u_2 + u_2v_1$. Then by Lemma 1 (i), we have

$$M_1^\alpha(G) - M_1^\alpha(G') = [d(u_1)^\alpha + d(v_1)^\alpha] - [(d(u_1) - 1)^\alpha + (d(v_1) + 1)^\alpha] > 0,$$

i.e., $M_1^\alpha(G) > M_1^\alpha(G')$, a contradiction.

(ii) Suppose $M_1^\alpha(G)$ attains the second smallest value. Let G_1^s and G_2^s be unicyclic graphs with $D(G_1^s) = [2^n]$ and $D(G_2^s) = [3, 2^{n-2}, 1]$.

Claim 1. $\Delta(G) = 3$.

Proof. Let $C = u_1u_2 \cdots u_ku_1$ be the unique cycle in G. From (i), we can choose a maximal C-path, say $P[u_1, v_1]$. Set $G' = G - u_1u_2 + u_2v_1$. By Lemma 1 (i), we have $M_1^\alpha(G) > M_1^\alpha(G')$. Moreover, if $\Delta(G) \geq 4$, then $\Delta(G') \geq 3$. From (i), $M_1^\alpha(G') > M_1^\alpha(G_1^s)$. So we have $M_1^\alpha(G) > M_1^\alpha(G') > M_1^\alpha(G_1^s)$, a contradiction. $\square$

Claim 2. $n_1 = n_3 = 1$.

Proof. It follows from Claim 1 that $n_1 + n_2 + n_3 = n$. On the other hand, by the handshaking lemma, $n_1 + 2n_2 + 3n_3 = 2n$. So we have $n_1 = n_3$. Then $D(G) = [3^{n_3}, 2^{n-2n_3}, 1^{n_3}]$.

If $n_3 \geq 2$, then

$$\begin{aligned} M_1^\alpha(G) - M_1^\alpha(G_2^s) &= [n_3 3^\alpha + (n - 2n_3)2^\alpha + n_3] - [3^\alpha + (n-2)2^\alpha + 1] \\ &= (n_3 - 1)(3^\alpha + 1 - 2 \cdot 2^\alpha) > 0, \end{aligned}$$

i.e., $M_1^\alpha(G) > M_1^\alpha(G_2^s)$. At the same time, it is easy to check that $M_1^\alpha(G_2^s) > M_1^\alpha(G_1^s)$. So $M_1^\alpha(G) > M_1^\alpha(G_2^s) > M_1^\alpha(G_1^s)$, a contradiction. $\square$

By Claims 1 and 2, and the result in (i), we can easily see that $M_1^\alpha(G)$ attains the second smallest value if and only if $D(G) = [3, 2^{n-2}, 1]$.

(iii) Suppose $M_1^\alpha(G)$ attains the third smallest value. Let G_3^s be a unicyclic graph with $D(G_3^s) = [3^2, 2^{n-4}, 1^2]$.

Claim 3. $\Delta(G) = 3$.

Proof. By contradiction. Suppose $\Delta(G) = \Delta \geq 4$ and let $C = u_1u_2\cdots u_ku_1$ be the cycle in G and $\gamma = n - n_1 - n_2$. We distinguish two cases.

Case 1. $\gamma = 1$.

Clearly, the vertex with the maximum degree must lie on C, and $n_1 = \Delta - 2$, $n_2 = n - \Delta + 1$. Then $D(G) = [\Delta, 2^{n-\Delta+1}, 1^{\Delta-2}]$. By Lemma 1 (i), we have

$$\begin{aligned}
&M_1^\alpha(G) - M_1^\alpha(G_3^s) \\
=&[\Delta^\alpha + (n-\Delta+1)2^\alpha + \Delta - 2] - [2\cdot 3^\alpha + (n-4)2^\alpha + 2] \\
=&(\Delta^\alpha - 3^\alpha) - (3^\alpha - 2^\alpha) - (\Delta - 4)(2^\alpha - 1) \\
=&[(\Delta^\alpha - 3^\alpha) - (\Delta - 3)(2^\alpha - 1)] - [(3^\alpha - 2^\alpha) - (2^\alpha - 1)] \\
=&(\Delta - 3)(\Delta^{\alpha-1} + 3\Delta^{\alpha-2} + \cdots + 3^{\alpha-1} - 2^\alpha + 1) - [(3^\alpha - 2^\alpha) - (2^\alpha - 1)] \\
\geq&(4-3)(4^{\alpha-1} + 3\cdot 4^{\alpha-2} + \cdots + 3^{\alpha-1} - 2^\alpha + 1) - [(3^\alpha - 2^\alpha) - (2^\alpha - 1)] \\
=&[(4^\alpha - 3^\alpha) - (2^\alpha - 1)] - [(3^\alpha - 2^\alpha) - (2^\alpha - 1)] \\
=&(4^\alpha - 3^\alpha) - (3^\alpha - 2^\alpha) > 0,
\end{aligned}$$

i.e., $M_1^\alpha(G) > M_1^\alpha(G_3^s)$. On the other hand, it is easy to check that $M_1^\alpha(G_3^s) > M_1^\alpha(G_2^s)$. Then we have $M_1^\alpha(G) > M_1^\alpha(G_3^s) > M_1^\alpha(G_2^s)$, a contradiction.

Case 2. $\gamma \geq 2$.

Case 2.1. All vertices with degree at least 3 lie on C.

Without loss of generality, assume that $d(u_1) \geq 3$ and $d(u_i) = \Delta(G) \geq 4$ $(i \neq 1)$. Choose a maximal C-path $P[u_1, v_1]$, and set $G' = G - u_1u_2 + u_2v_1$. Then by Lemma 1

(i), we have $M_1^\alpha(G) > M_1^\alpha(G')$. Moreover, $\Delta(G') = d(u_i) \geq 4$. From (ii), $M_1^\alpha(G') > M_1^\alpha(G_2^s)$. So we have $M_1^\alpha(G) > M_1^\alpha(G') > M_1^\alpha(G_2^s)$, a contradiction.

Case 2.2. Not all vertices with degree at least 3 lie on C.

Let v be a vertex in $V(G) \setminus V(C)$ with $d(v) \geq 3$. Choose a maximal C-path, say $P[u_1, v_1]$ with $v \in V(P[u_1, v_1])$. Set $G_1 = G - u_1u_2 + u_2v_1$. Then by Lemma 1 (i), $M_1^\alpha(G) > M_1^\alpha(G_1)$. Clearly, the number of vertices with degrees at least 3 on the unique cycle in G_1 is not less than that of vertices with degree at least 3 on the unique cycle in G, and the degree of u_1 decreases by 1 in this process. If not all vertices with degree at least 3 lie on the unique cycle of graph G_1, repeating the above processes, we can get a sequence of unicyclic graphs $G_2, G_3, \ldots, G_l$, such that for each graph G_i with $2 \leq i \leq l-1$, not all vertices with degrees at least 3 lie on its unique cycle, but all vertices with degree at least 3 of G_l lie on its unique cycle. By Lemma 1 (i), we have $M_1^\alpha(G) > M_1^\alpha(G_1) > \cdots > M_1^\alpha(G_l)$.

If $l = 1$, then G_1 has two vertices of degree 3 or a vertex of degree 4. In both cases, we have $M_1^\alpha(G) > M_1^\alpha(G_1) > M_1^\alpha(G_2^s) > M_1^\alpha(G_1^s)$, a contradiction; If $l = 2$, then G_2 has a vertex of degree 3. Hence, $M_1^\alpha(G) > M_1^\alpha(G_1) > M_1^\alpha(G_2) > M_1^\alpha(G_1^s)$, a contradiction; If $l = 3$, then $M_1^\alpha(G) > M_1^\alpha(G_1) > M_1^\alpha(G_2) > M_1^\alpha(G_3)$, a contradiction. □

Claim 4. $n_1 = n_3 = 2$.

Proof. From Claim 3, it is easy to see that $n_1 = n_3$ and $n_2 = n - 2n_3$. Then $D(G) = [3^{n_3}, 2^{n-2n_3}, 1^{n_3}]$.

If $n_3 \geq 3$, then

$$\begin{aligned} M_1^\alpha(G) - M_1^\alpha(G_3^s) &= [n_3 3^\alpha + (n - 2n_3)2^\alpha + n_3] - [2 \cdot 3^\alpha + (n-4)2^\alpha + 2] \\ &= (n_3 - 2)(3^\alpha + 1 - 2 \cdot 2^\alpha) > 0, \end{aligned}$$

i.e., $M_1^\alpha(G) > M_1^\alpha(G_3^s)$. On the other hand, it is easy to check that $M_1^\alpha(G_3^s) > M_1^\alpha(G_2^s)$. Then we have $M_1^\alpha(G) > M_1^\alpha(G_3^s) > M_1^\alpha(G_2^s)$, a contradiction. □

By Claims 3 and 4, and the results in (i) and (ii), we can easily see that $M_1^\alpha(G)$ attains the third smallest value if and only if $D(G) = [3^2, 2^{n-4}, 1^2]$. □

Theorem 2. *Let G be a unicyclic graph with $n \geq 7$ vertices, α a real number with $\alpha \in (0,1)$, and $g(n) = (n-2)^\alpha - (n-3)^\alpha - (2^\alpha - 1)^2$. Then*
(i) $M_1^\alpha(G)$ attains the smallest value if and only if $D(G) = [n-1, 2^2, 1^{n-3}]$;
(ii) $M_1^\alpha(G)$ attains the second smallest value if and only if $D(G) = [n-2, 3, 2, 1^{n-3}]$;
(iii) If $g(n) < 0$, then $M_1^\alpha(G)$ attains the third smallest value if and only if $D(G) = [n-2, 2^3, 1^{n-4}]$. If $g(n) > 0$ and the unique root of the equation $g(n) = 0$ is $n_0(\alpha)$, then $M_1^\alpha(G)$ attains the third smallest value if and only if $D(G) = [n-3, 4, 2, 1^{n-3}]$ when $7 \leq n < n_0(\alpha)$, $D(G) = [n-2, 2^3, 1^{n-4}]$ when $n > n_0(\alpha)$, and $D(G) = [n-3, 4, 2, 1^{n-3}]$ or $[n-2, 2^3, 1^{n-4}]$ when $n = n_0(\alpha)$ in the case $n_0(\alpha)$ is an integer.

Proof. (i) Suppose $M_1^\alpha(G)$ attains the smallest value. Let $C = u_1u_2 \cdots u_ku_1$ be the unique cycle in G.

Claim 1. There is at least one vertex $u_i \in V(C)$ with $d(u_i) = \Delta(G)$.

Proof. Assume there is no vertex on C with the maximum degree in G. Choose a maximal C-path, say $P[u_1, v_1]$, such that $v \in V(P[u_1, v_1])$ and $d(v) = \Delta(G)$. Set $G' = G - u_1u_2 + u_2v$. Then by Lemma 1 (ii), we have

$$M_1^\alpha(G) - M_1^\alpha(G') = [d(u_1)^\alpha + d(v)^\alpha] - [(d(u_1) - 1)^\alpha + (d(v) + 1)^\alpha] > 0,$$

i.e., $M_1^\alpha(G) > M_1^\alpha(G')$, a contradiction. □

Claim 2. $|V(C)| = 3$.

Proof. Suppose $d(u_1) = \Delta(G)$. If $|V(C)| \geq 4$, set $G' = G - u_3u_4 + u_1u_3$. Then by Lemma 1 (ii), we have $M_1^\alpha(G) > M_1^\alpha(G')$, a contradiction. □

Claim 3. $\Delta(G) = n - 1$.

Proof. Suppose $d(u_1) = \Delta(G)$. Obviously, $\Delta(G) > 2$. If $\Delta(G) \leq n-2$, then by Claims 1 and 2, there is at least one vertex $v \in V(G)$ with $d(v) = 1$ and $u_1v \notin E(G)$. Denote the neighbor of v by w and set $G' = G - vw + u_1v$. Then by Lemma 1 (ii), we have $M_1^\alpha(G) > M_1^\alpha(G')$, a contradiction. □

By Claims 2 and 3, we can easily see that $M_1^\alpha(G)$ attains the smallest value if and only if $D(G) = [n-1, 2^2, 1^{n-3}]$.

(ii) Suppose $M_1^{\alpha}(G)$ attains the second smallest value. Let G_1^s and G_2^s be unicyclic graphs with $D(G_1^s) = [n-1, 2^2, 1^{n-3}]$ and $D(G_2^s) = [n-2, 3, 2, 1^{n-3}]$. It is easy to check that $M_1^{\alpha}(G_2^s) > M_1^{\alpha}(G_1^s)$. Let $C = u_1 u_2 \cdots u_k u_1$ be the unique cycle in G.

Claim 4. There is at least one vertex $u_i \in V(C)$ with $d(u_i) = \Delta(G)$.

Proof. Assume there is no vertex on C with the maximum degree in G. Then, choose a maximal C-path, say $P[u_1, v_1]$, such that $v \in V(P[u_1, v_1])$ and $d(v) = \Delta(G)$. Set $G' = G - u_1 u_2 + u_2 v$. By Lemma 1 (ii), we have $M_1^{\alpha}(G) > M_1^{\alpha}(G')$. Let C' be the cycle in G'. Then $|V(C')| > |V(C)| \geq 3$, i.e., $|V(C')| \geq 4$. From (i), $M_1^{\alpha}(G') > M_1^{\alpha}(G_1^s)$. So $M_1^{\alpha}(G) > M_1^{\alpha}(G') > M_1^{\alpha}(G_1^s)$, a contradiction. □

Claim 5. $|V(C)| = 3$.

Proof. Assume $|V(C)| \geq 4$. We distinguish two cases.

Case 1. $|V(C)| = 4$.

Let $C = u_1 u_2 u_3 u_4 u_1$ and $d(u_1) = \Delta(G)$. Then $d(u_1) \leq n-2$.

Case 1.1. One of $d(u_2)$, $d(u_3)$ and $d(u_4)$ is greater than 2.

Set $G' = G - u_3 u_4 + u_1 u_3$. From Lemma 1 ($ii$), it is easy to see that $M_1^{\alpha}(G) > M_1^{\alpha}(G')$. Clearly, $D(G') \neq D(G_1^s)$. Then from (i), we have $M_1^{\alpha}(G') > M_1^{\alpha}(G_1^s)$. So $M_1^{\alpha}(G) > M_1^{\alpha}(G') > M_1^{\alpha}(G_1^s)$, a contradiction.

Case 1.2. All of $d(u_2)$, $d(u_3)$ and $d(u_4)$ are 2.

If $d(u_1) = n-2$, then $D(G) = [n-2, 2^3, 1^{n-4}]$. It is easy to check that $M_1^{\alpha}(G) > M_1^{\alpha}(G_2^s) > M_1^{\alpha}(G_1^s)$, a contradiction. If $d(u_1) < n-2$, set $G' = G - u_3 u_4 + u_1 u_3$. It follows from Lemma 1 (ii) that $M_1^{\alpha}(G) > M_1^{\alpha}(G')$. On the other hand, $\Delta(G') \leq n-2$. From (i), we have $M_1^{\alpha}(G') > M_1^{\alpha}(G_1^s)$. So $M_1^{\alpha}(G) > M_1^{\alpha}(G') > M_1^{\alpha}(G_1^s)$, a contradiction.

Case 2. $|V(C)| \geq 5$.

Set $G' = G - u_3 u_4 + u_1 u_3$. It is easy to check that $M_1^{\alpha}(G) > M_1^{\alpha}(G') > M_1^{\alpha}(G_1^s)$, a contradiction.

This completes the proof of Claim 5. □

Claim 6. $\Delta(G) = n - 2$.

Proof. From Claims 4 and 5, and (i), $\Delta(G) \leq n - 2$. If $\Delta(G) < n - 2$, let $d(u_1) = \Delta(G)$. From $|V(C)| = 3$, there is one vertex v with $d(v) = 1$ and $u_1v \notin E(G)$. Denote the neighbor of v by w. Set $G' = G - vw + u_1v$. Then $M_1^\alpha(G) > M_1^\alpha(G')$ and $\Delta(G') \leq n - 2$. From (i), we have $M_1^\alpha(G') > M_1^\alpha(G_1^s)$. So $M_1^\alpha(G) > M_1^\alpha(G') > M_1^\alpha(G_1^s)$, a contradiction. □

Claim 7. $n_2 = 1$.

Proof. From Claims 4, 5 and 6, it is easy to see that $n_2 \leq 3$. If $n_2 = 2$, then G is not a unicyclic graph. If $n_2 = 3$, then $D(G) = [n - 2, 2^3, 1^{n-4}]$. It is easy to check that $M_1^\alpha(G) > M_1^\alpha(G_2^s) > M_1^\alpha(G_1^s)$, a contradiction. □

By Claims 4, 5, 6 and 7, and the result in (i), we can easily see that $M_1^\alpha(G)$ attains the second smallest value if and only if $D(G) = [n - 2, 3, 2, 1^{n-3}]$.

(iii) Suppose $M_1^\alpha(G)$ attains the third smallest value. Let G_2^s be the unicyclic graph with $D(G_2^s) = [n - 2, 3, 2, 1^{n-3}]$, and $C = u_1u_2 \cdots u_ku_1$ be the unique cycle in G. If $|V(C)| \geq 5$, suppose $d(u_1) \geq d(u_5)$ and set $G' = G - u_4u_5 + u_1u_4$. Then, $M_1^\alpha(G) > M_1^\alpha(G')$ and the girth of G' is 4. From (ii), $M_1^\alpha(G') > M_1^\alpha(G_2^s)$. So $M_1^\alpha(G) > M_1^\alpha(G') > M_1^\alpha(G_2^s)$, a contradiction. Thus, we have $|V(C)| \leq 4$.

In the following, by $G_3^{s_1}$, $G_3^{s_2}$ and $G_3^{s_3}$ we denote the unicyclic graphs with $D(G_3^{s_1}) = D(G_3^{s_2}) = [n - 2, 2^3, 1^{n-4}]$ and $D(G_3^{s_3}) = [n - 3, 4, 2, 1^{n-3}]$ such that the girth of $G_3^{s_1}$ is 4 and that of $G_3^{s_2}$ and $G_3^{s_3}$ are 3.

Claim 8. If $|V(C)| = 4$, then $G \cong G_3^{s_1}$.

Proof. If there is no vertex with the maximum degree on C in G, then $\Delta(G) \leq n-4$. Choose a maximal C-path, say $P[u_1, v_1]$, such that $v \in V(P[u_1, v_1])$ and $d(v) = \Delta(G)$. Set $G' = G - u_1u_2 + u_2v$. Then, $M_1^\alpha(G) > M_1^\alpha(G')$ and $\Delta(G') \leq n - 3$. From (ii), $M_1^\alpha(G') > M_1^\alpha(G_2^s)$. So $M_1^\alpha(G) > M_1^\alpha(G') > M_1^\alpha(G_2^s)$, a contradiction.

If there is at least one vertex $u_i \in V(C)$ with $d(u_i) = \Delta(G)$, then, without loss of generality, assume $d(u_1) = \Delta(G)$. If $G \ncong G_3^{s_1}$, then $d(u_1) < n - 2$. So there must be at least one vertex $v \in V(G)$ with $d(v) = 1$ and $u_1v \notin E(G)$. Denote the neighbor of v by w and set $G' = G - vw + u_1v$. Then, $M_1^\alpha(G) > M_1^\alpha(G')$ and the girth of

G' is still 4. From (ii), $M_1^\alpha(G') > M_1^\alpha(G_2^s)$. So $M_1^\alpha(G) > M_1^\alpha(G') > M_1^\alpha(G_2^s)$, a contradiction. $\square$

Claim 9. If $|V(C)| = 3$, then $G \cong G_3^{s_2}$ or $G \cong G_3^{s_3}$.

Proof. By contradiction. Suppose that $G \ncong G_3^{s_2}$ and $G \ncong G_3^{s_3}$.

If there is no vertex on C with the maximum degree in G, then, choose a maximal C-path, say $P[u_1, v_1]$, such that $v \in V(P[u_1, v_1])$ and $d(v) = \Delta(G)$. Set $G' = G - u_1u_2 + u_2v$. Then $M_1^\alpha(G) > M_1^\alpha(G')$ and the girth of G' is at least 4. From (ii), $M_1^\alpha(G') > M_1^\alpha(G_2^s)$. So $M_1^\alpha(G) > M_1^\alpha(G') > M_1^\alpha(G_2^s)$, a contradiction.

If there is at least one vertex on C with the maximum degree in G and $\Delta(G) \leq n-4$, then there must be at least one vertex $v \in V(G)$ such that $d(v) = 1$ and $u_1v \notin E(G)$. Denote the neighbor of v by w. Set $G' = G - vw + u_1v$. Then, $M_1^\alpha(G) > M_1^\alpha(G')$ and $\Delta(G') \leq n-3$. From (ii), $M_1^\alpha(G') > M_1^\alpha(G_2^s)$. So $M_1^\alpha(G) > M_1^\alpha(G') > M_1^\alpha(G_2^s)$, a contradiction.

If there is at least one vertex on C with the maximum degree in G and $\Delta(G) = n-3$, then, it is easy to see that $D(G) = [n-3, 3^2, 1^{n-3}]$, $[n-3, 3, 2^2, 1^{n-4}]$, or $[n-3, 2^4, 1^{n-5}]$. In each case, we can prove that $M_1^\alpha(G) > M_1^\alpha(G_3^{s_3}) > M_1(G_2^s)$ and $M_1^\alpha(G) > M_1^\alpha(G_3^{s_2}) > M_1(G_2^s)$, a contradiction. $\square$

For a given $\alpha \in (0,1)$, let $g(n) = M_1^\alpha(G_3^{s_1}) - M_1^\alpha(G_3^{s_3}) = M_1^\alpha(G_3^{s_2}) - M_1^\alpha(G_3^{s_3}) = (n-2)^\alpha - (n-3)^\alpha - (2^\alpha - 1)^2$. Then by Lemma 1 (ii), we have

$$
\begin{aligned}
&g(n+1) - g(n) \\
=&[(n-1)^\alpha - (n-2)^\alpha - (2^\alpha - 1)^2] - [(n-2)^\alpha - (n-3)^\alpha - (2^\alpha - 1)^2] \\
=&[(n-1)^\alpha - (n-2)^\alpha] - [(n-2)^\alpha - (n-3)^\alpha] < 0,
\end{aligned}
$$

when n is an integer not less than 7. So $g(n)$ is a strictly decreasing function.

Thus, if $g(n) < 0$, then $M_1^\alpha(G_3^{s_1}) = M_1^\alpha(G_3^{s_2}) < M_1^\alpha(G_3^{s_3})$. By Claims 8 and 9, $G \cong G_3^{s_1}$ or $G_3^{s_2}$. So we have $D(G) = [n-2, 2^3, 1^{n-4}]$. If $g(n) > 0$, denote the unique root of the equation $g(n) = 0$ by $n_0(\alpha)$. When $7 \leq n < n_0(\alpha)$, $M_1^\alpha(G_3^{s_1}) = M_1^\alpha(G_3^{s_2}) > M_1^\alpha(G_3^{s_3})$. It follows from Claims 8 and 9 that $D(G) = [n-3, 4, 2, 1^{n-3}]$. When $n > n_0(\alpha)$, $M_1^\alpha(G_3^{s_1}) = M_1^\alpha(G_3^{s_2}) < M_1^\alpha(G_3^{s_3})$. It follows from Claims 8 and 9 that $D(G) = [n-2, 2^3, 1^{n-4}]$. If $n_0(\alpha)$ is an integer, then $D(G) = [n-3, 4, 2, 1^{n-3}]$ or $[n-2, 2^3, 1^{n-4}]$ when $n = n_0(\alpha)$.

The result follows from (i) and (ii) immediately. $\square$

4 Unicyclic graphs with the first three largest values of the first general Zagreb index

The following results can be proved with arguments similar to that used in Theorems 1 and 2.

Theorem 3. *Let G be a unicyclic graph with $n \geq 7$ vertices , α a real number with $\alpha \in (-\infty, 0) \cup (1, +\infty)$, and $g(n) = (n-2)^\alpha - (n-3)^\alpha - (2^\alpha - 1)^2$. Then*
(i) $M_1^\alpha(G)$ attains the largest value if and only if $D(G) = [n-1, 2^2, 1^{n-3}]$;
(ii) $M_1^\alpha(G)$ attains the second largest value if and only if $D(G) = [n-2, 3, 2, 1^{n-3}]$;
(iii) If $g(n) > 0$, then $M_1^\alpha(G)$ attains the third largest value if and only if $D(G) = [n-2, 2^3, 1^{n-4}]$. If $g(n) < 0$ and the unique root of the equation $g(n) = 0$ is $n_0(\alpha)$, then $M_1^\alpha(G)$ attains the third largest value if and only if $D(G) = [n-3, 4, 2, 1^{n-3}]$ when $7 \leq n < n_0(\alpha)$, $D(G) = [n-2, 2^3, 1^{n-4}]$ when $n > n_0(\alpha)$, and and $D(G) = [n-3, 4, 2, 1^{n-3}]$ or $[n-2, 2^3, 1^{n-4}]$ when $n = n_0(\alpha)$ in the case $n_0(\alpha)$ is an integer..

Theorem 4. *Let G be a unicyclic graph with $n \geq 7$ vertices and α a real number with $\alpha \in (0, 1)$. Then*
(i) $M_1^\alpha(G)$ attains the largest value if and only if $D(G) = [2^n]$;
(ii) $M_1^\alpha(G)$ attains the second largest value if and only if $D(G) = [3, 2^{n-2}, 1]$;
(iii) $M_1^\alpha(G)$ attains the third largest value if and only if $D(G) = [3^2, 2^{n-4}, 1^2]$.

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