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# ORDERING UNICYCLIC GRAPHS WITH RESPECT TO ZAGREB INDICES

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**Abstract**

For a graph, 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. This paper investigates the Zagreb indices of unicyclic graphs by introducing some transformations, and characterize the unicyclic graphs with the first five largest Zagreb indices and the unicyclic graphs with the first two smallest Zagreb indices, respectively.

## 1 Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For any $v \in V$, $N(v)$ denotes the neighbors of $v$, and $N_G[v] = \{v\} \cup \{u|uv \in E(G)\}$, $d_G(v) = |N(v)|$ is the degree of $v$. A leaf is a vertex of degree one and a stem is a vertex adjacent to at least one leaf, pendant edges are edges incident to a leaf and stem. The distance $d(x, y)$ from a vertex $x$ to another vertex $y$ is the minimum number of edges in an $x - y$ path. The distance $d_G(x, S)$ from a vertex $x$ to the set $S$ is $\min_{y \in S} d(x, y)$. Let $P_n$, $C_n$ and $K_{1,n-1}$ be the path, cycle and the star on $n$ vertices.

Let $\mathcal{U}_n$ denote the set of the unicyclic graphs with $n$ vertices.

Let $\mathcal{U}_n^k$ denote the set of the unicyclic graphs with $n$ vertices and cycle length $k$.

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Let $G_{k,1}^{(n)}$ denote the unicyclic graph constructed by attaching $n-k$ leaves to one vertex on a cycle of length $k$, see figure 1(a).

Let $G_{k,2}^{(n)}$ be the unicyclic graph constructed by attaching $n-k-1$ leaves to one vertex $u$ of the cycle, and a $K_2$ attached to adjacent vertex of $u$, see figure 1(b).

Let $S_{p,q,r}(p, q, r \geq 0$ and $p+q+r = n-3)$ denote the unicyclic graph constructed by attaching $K_{1,p}$, $K_{1,q}$, $K_{1,r}$ to the vertices of $C_3$, respectively, see figure 1(c).

Other graph notations and terminologies undefined will conform to [1].

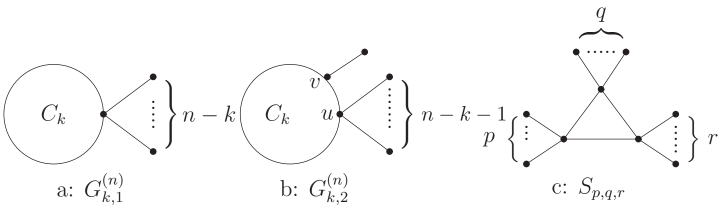



Figure 1.

The first Zagreb index $M_1$ and the second Zagreb index $M_2$ of $G$ are defined as

$$M_1(G) = \sum_{x \in V(G)} (d_G(x))^2$$

$$M_2(G) = \sum_{xy \in E(G)} d_G(x) d_G(y)$$

where $d_G(x)$ is the degree of vertex $x$ in $G$.

The Zagreb indices $M_1$ and $M_2$ were introduced in [2] and elaborated in [3]. The main properties of $M_1$ and $M_2$ were summarized in [4,5]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [5,6].

Recently, finding the extremal values or bounds for the topological indices of graphs, as well as related problems of characterizing the extremal graphs, attracted the attention of many researchers and many results are obtained (see [3-18]). [4] showed that the trees with the smallest and largest $M_1$ are the path and the star, respectively. [7] also showed that the trees with the smallest and largest $M_2$ are the path and the star, respectively. [8] characterized the graphs with the smallest and largest $M_2$ among all unicyclic graphs. [9] gave the the unicyclic graphs with the first three smallest and largest $M_1$. [10] gave the bicyclic graph with the largest $M_1$. [15] presented a unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs.

In this paper, we present investigate the Zagreb indices of unicyclic graphs by introducing some transformations, and characterize the unicyclic graphs with the first five largest Zagreb indices and the unicyclic graphs with the first two smallest Zagreb indices.

## 2 Two transformations which increase the Zagreb indices

Let $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of $G$ obtained by deleting the edges of $E'$. $W \subseteq V(G)$, $G - W$ denotes the subgraph of $G$ obtained by deleting the vertices of $W$ and the edges incident with them.

We give two transformations which will increase the Zagreb indices as follows:

**Transformation** $\alpha$: Let $uv$ be an edge $G$, $d_G(u) \geq 2$, $N_G(v) = \{u, w_1, w_2, \cdots, w_s\}$, and $w_1, w_2, \cdots, w_s$ are leaves. $G' = G - \{vw_1, vw_2, \cdots, vw_s\} + \{uw_1, uw_2, \cdots, uw_s\}$, as shown in Figure 2.

**Lemma 2.1**[15]. Let $G'$ be obtained from $G$ by transformation $\alpha$, then

$$M_1(G') > M_1(G) \text{ and } M_2(G') > M_2(G).$$

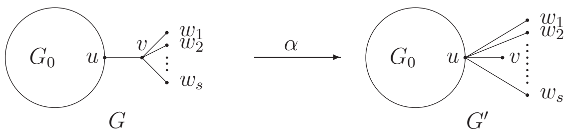



Figure 2. Transformation $\alpha$.

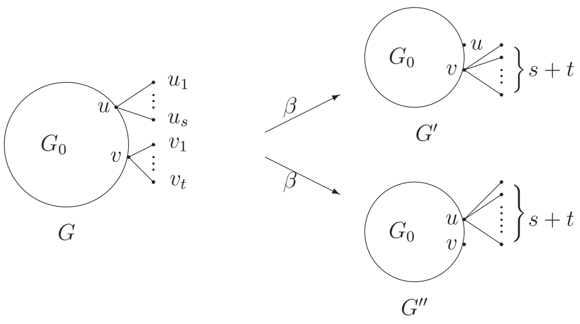



Figure 3. Transformation $\beta$.

**Remark 1**. Repeating Transformation $\alpha$, any unicyclic graph can be changed into an unicyclic graph such that all the edges not on the cycle are pendant edges.

**Transformation** $\beta$: Let $u$ and $v$ be two vertices in $G$. $u_1, u_2, \cdots, u_s$ are the leaves adjacent to $u$, $v_1, v_2, \cdots, v_t$ are the leaves adjacent to $v$. $G' = G - \{uu_1, uu_2, \cdots, uu_s\} +$

$\{vu_1, vu_2, \cdots, vu_s\}$, $G'' = G - \{vv_1, vv_2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$, as showed in Figure 3.

**Lemma 2.2**[**15**]. Let $G'$ and $G''$ be obtained from $G$ by transformation $\beta$, then either $M_i(G') > M_i(G)$ or $M_i(G'') > M_i(G)$, $i = 1, 2$.

**Remark 2**. Repeating Transformation $\beta$, any unicyclic graph can be changed into an unicyclic graph such that all the pendant edges are attached to the same vertex.

# 3 Some transformations which decrease the Zagreb indices

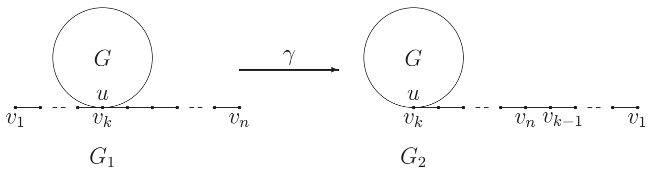



Figure 4. Transformation $\gamma$.

**Transformation** $\gamma$. Let $G \neq P_1$ be a connected graph and choose $u \in V(G)$. $G_1$ denotes the graph that results from identifying $u$ with the vertex $v_k$ of a simple path $v_1v_2 \cdots v_n$, $1 < k < n$; $G_2$ is obtained from $G_1$ by deleting $v_{k-1}v_k$ and adding $v_{k-1}v_n$ (see Figure 4).

**Lemma 3.1**[**15**]. Let $G_1$ and $G_2$ be the graphs in Figure 4. Then $M_i(G_1) > M_i(G_2)$, $i = 1, 2$.

**Remark 3**. Repeating Transformation $\gamma$, any tree $T$ attached to a graph $G$ can be changed into a path as showed in Figure 5. And the Zagreb indices decrease.

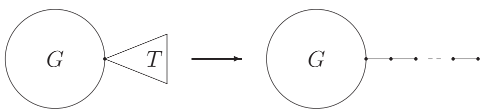



Figure 5.

**Transformation** $\delta$. Let $u$ and $v$ be two vertices in a graph $G$. $G_1$ denotes the graph that results from identifying $u$ with the vertex $u_0$ of a path $u_0u_1u_2 \cdots u_s$ and identifying $v$ with the vertex $v_0$ of a path $v_0v_1v_2 \cdots v_t$; $G_2$ is obtained from $G_1$ by deleting $uu_1$ and adding $v_tu_1$ (see Figure 6).

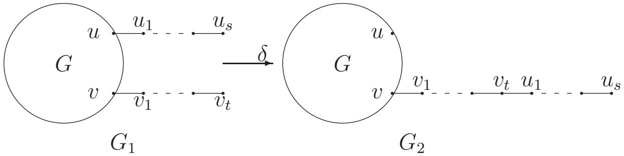



Figure 6. Transformation $\delta$.

**Lemma 3.2[15]**. Let $G_1$ and $G_2$ be the graphs in Figure 6. $d_G(u) \geq d_G(v) > 1$, $s \geq 1$ and $t \geq 0$.

$(i)$ If $t > 0$, then $M_1(G_1) > M_1(G_2)$ and $M_2(G_1) > M_2(G_2)$;

$(ii)$ If $t = 0$ and $d_G(u) > d_G(v)$, then $M_1(G_1) > M_1(G_2)$;

$(iii)$ If $t = 0$ and $\sum\limits_{x \in N_G(u)-\{v\}} d_G(x) > \sum\limits_{y \in N_G(v)-\{u\}} d_G(y)$, then $M_2(G_1) > M_2(G_2)$.

**Remark 4**. After repeating transformation $\delta$, then any tree attached on the unicyclic graph can be changed into such an unicyclic graph that a path attached to a cycle, and the Zagreb indices decrease.

# 4 Unicyclic graphs with larger Zagreb indices

In this section we shall get the upper bounds of the unicyclic graphs with respect to their Zagreb indices.

**Lemma 4.1[15,16].** Let $G \in \mathcal{U}_n^k$, then $M_i(G) \leq M_i(G_{k,1}^{(n)})(i = 1, 2)$, with equality if and only if $G \cong G_{k,1}^{(n)}$.

**Lemma 4.2[16].** Let $G \in \mathcal{U}_n$, then

$(i)$ $M_i(G) \leq M_i(G_{3,1}^{(n)})$, with equality if and only if $G \cong G_{3,1}^{(n)}(i = 1, 2)$;

$(ii)$ If $G \ncong G_{3,1}^{(n)}$, then $M_i(G) \leq M_i(G_{3,2}^{(n)})$, with equality if and only if $G \cong G_{3,2}^{(n)}(i = 1, 2)$.

Note that for given integers $k \geq 3$ and $n \geq k$. We can calculate out the Zagreb indices of $G_{k,1}^{(n)}$ in the following, $M_1(G_{k,1}^{(n)}) = (n-k)^2+5n-k$, $M_2(G_{k,1}^{(n)}) = (n-k)^2+6n-2k$.

**Theorem 4.1.** Let $G \in \mathcal{U}_n^k(k \geq 3)$, we have $M_i(G_{k,1}^{(n)}) > M_i(G_{k,2}^{(n)})(i = 1, 2)$.

**Proof.** From the definition of $G_{k,2}^{(n)}$ and the Zagreb indices, we have
$M_1(G_{k,2}^{(n)}) = (n-k)^2 + 3n + k + 2$, $M_2(G_{k,2}^{(n)}) = (n-k)^2 + 5n - k + 1$.
Then

$$\begin{aligned} \Delta_1 &= M_1(G_{k,1}^{(n)}) - M_1(G_{k,2}^{(n)}) \\ &= n - k - 1 > 0 \end{aligned}$$

$$\begin{aligned}\Delta_2 &= M_2(G_{k,1}^{(n)}) - M_2(G_{k,2}^{(n)})\\ &= n-k-1>0\end{aligned}$$

**Theorem 4.2.** Let $G \in \mathcal{U}_n^k$ be an arbitrary unicyclic graph, then $M_i(G_{k,2}^{(n)}) > M_i(G_{k+1,2}^{(n)})(i = 1, 2)$.

**Proof.** From above proof, we have

$$\begin{aligned}\Delta_1 &= M_1(G_{k,2}^{(n)}) - M_1(G_{k+1,2}^{(n)})\\ &= 2(n-k-1)>0\\ \Delta_2 &= M_2(G_{k,2}^{(n)}) - M_2(G_{k+1,2}^{(n)})\\ &= 2(n-k)>0\end{aligned}$$

**Theorem 4.3.** Let $p \geq q \geq r \geq 0$, $p+q+r = n-3$, we have

$(i)$ $M_i(S_{p,q,r}) < M_1(S_{p+1,q-1,r})$, for $i = 1, 2$;

$(ii)$ $M_i(S_{p,q,r}) < M_1(S_{p,q+1,r-1})$, for $i = 1, 2$.

**Proof.** Firstly, we get the Zagreb indices of $S_{p,q,r}$ as follows.

$M_1(S_{p,q,r}) = (p+2)^2 + (q+2)^2 + (r+2)^2 + n - 3$;

$M_2(S_{p,q,r}) = p^2 + q^2 + r^2 + pq + pr + qr + 6p + 6q + 6r + 12$.

Consequently, we have

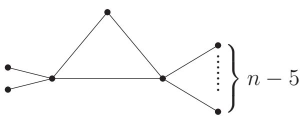
$$\begin{aligned}\Delta_1 &= M_1(S_{p+1,q-1,r}) - M_1(S_{p,q,r})\\ &= 2(p-q+1)>0\\ \Delta_2 &= M_2(S_{p+1,q-1,r}) - M_2(S_{p,q,r})\\ &= p-q+1>0\end{aligned}$$

and

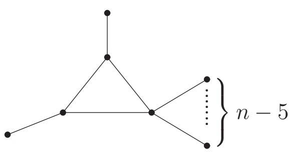
$$\begin{aligned}\Delta_1' &= M_1(S_{p,q+1,r-1}) - M_1(S_{p,q,r})\\ &= 2(q-r+1)>0\\ \Delta_2' &= M_2(S_{p,q+1,r-1}) - M_2(S_{p,q,r})\\ &= q-r+1>0\end{aligned}$$

So the proof of theorem is completed.

Let $G_{3,3}^{(n)}$ be the graph obtained from attaching $K_{1,n-5}$ and $K_{1,2}$ to the adjacent vertices of $C_3$, respectively. See figure 7(a). $G_{3,4}^{(n)}$ be the graph obtained from attaching $K_{1,n-5}$ to one vertex of $C_3$, and $K_{1,2}$ to another two vertices of $C_3$, respectively. See figure 7(b).




(a) $G_{3,3}^{(n)}$




(b) $G_{3,4}^{(n)}$

Figure 7.

From Figure 7, we can work out:

$M_1(G_{3,3}^{(n)}) = n^2 - 5n + 26,\ M_2(G_{3,3}^{(n)}) = n^2 - 2n + 13;$
$M_1(G_{3,4}^{(n)}) = n^2 - 5n + 24,\ M_2(G_{3,4}^{(n)}) = n^2 - 2n + 12;$
By Lemma 4.1, Lemma 4.2, Theorem 4.3 and above calculation, we have

**Theorem 4.4.** When $n \geq 6$, we have $M_i(G_{3,3}^{(n)}) > M_i(G_{3,4}^{(n)}) > \cdots (i = 1, 2)$.

Let $S_\Delta$ denote the set of graphs belong to $S_{p,q,r}$. Then by Lemma 4.1, Lemma 4.2 and Theorem 4.3, Theorem 4.4 we have

**Theorem 4.5.** When $n \geq 6$, the order in $S_\Delta$ with respect to the Zagreb indices is (for $i = 1, 2$)

$$M_i(G_{3,1}^{(n)}) > M_i(G_{3,2}^{(n)}) > M_i(G_{3,3}^{(n)}) > M_i(G_{3,4}^{(n)}) > \cdots$$

Let $\mathcal{U'}_n^3$ be the set of graphs, which there are at least one vertex is at distant $\geq 2$ from $C_3$. Obviously, $\mathcal{U'}_n^3 = \mathcal{U}_n^3 - S_\Delta$. By Lemma 2.1 and Lemma 2.2, we know, graphs with the largest Zagreb indices in $\mathcal{U'}_n^3$ must be made from attaching $K_{1,l} (l \geq 1)$ to one of the pendent vertices of $S_{i,j,k} (i, j \geq 0, k \geq 1)$, denote the graph as $R_{i,j,k,l}$, is showed in Figure 8.

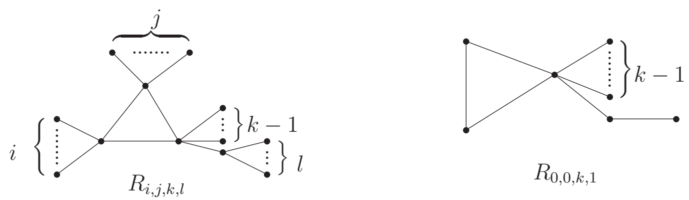



Figure 8.

Similar to the proof of Theorem 4.3, we have

**Theorem 4.6.** Let $i \geq j \geq 1$, $i+j+k+l = n-3$, we have $M_i(R_{i+1,j-1,k,l}) > M_i(R_{i,j,k,l})$ (for $i = 1, 2$). In particular, $M_i(R_{i+j,0,k,l}) > M_i(R_{i,j,k,l})$ (for $i = 1, 2$).

**Proof.** At first, we can calculate out the Zagreb indices of $R_{i,j,k,l}$.
$M_1(R_{i,j,k,l}) = (i+2)^2 + (j+2)^2 + (k+2)^2 + (l+1)^2 + n - 4;$
$M_2(R_{i,j,k,l}) = i(i+2) + (j+2)(i+j+2) + (k+2)(n-l) + (l+1)(k+l+2).$
Therefore,
$M_1(R_{i+1,j-1,k,l}) = (i+2+1)^2 + (j+2-1)^2 + (k+2)^2 + (l+1)^2 + n - 4;$
$M_2(R_{i+1,j-1,k,l}) = (i+1)(i+3) + (j+1)(i+j+2) + (k+2)(n-l) + (l+1)(k+l+2).$
Consequently, we have

$$\begin{aligned}\Delta_1 &= M_1(R_{i+1,j-1,k,l}) - M_1(R_{i,j,k,l})\\ &= 2(i-j+1) > 0\\ \Delta_2 &= M_2(R_{i+1,j-1,k,l}) - M_2(R_{i,j,k,l})\\ &= i-j+1 > 0\end{aligned}$$

The proof of $M_i(R_{i+j,0,k,l}) > M_i(R_{i,j,k,l})$ is similar.

So the proof of theorem is completed.

**Theorem 4.7.** Let $i \geq 1$, we have $M_i(R_{i,0,k,l}) < M_i(R_{0,0,i+k,l})(i = 1, 2)$.

For brevity, we shall denote $R_{0,0,k,1}$ simply as $R_{k,1}$, or denote it by $G'^{(n)}_{3,1}$.

**Theorem 4.8.** Let $n \geq 9$, we have $M_i(G^{(n)}_{3,3}) < M_i(R_{k,1}) < M_i(G^{(n)}_{3,2})(i = 1, 2)$.

**Proof.** By simple calculation, we have

$M_1(G^{(n)}_{3,2}) = n^2 - 3n + 14$, $M_2(G^{(n)}_{3,2}) = n^2 - n + 7$;

$M_1(R_{k,1}) = n^2 - 3n + 12$, $M_2(R_{k,1}) = n^2 - n + 4$.

Therefore, $M_i(G^{(n)}_{3,3}) < M_i(R_{k,1}) < M_i(G^{(n)}_{3,2})$ hold.

**Theorem 4.9.** Let $n \geq 6$, $l \geq 2$, $k + l + 3 = n$, we have we have $M_i(G^{(n)}_{3,4}) > M_i(R_{k,l})(i = 1, 2)$.

**Proof.** From the definition of $R_{k,l}$ and $k + l + 3 = n$, we have $M_1(R_{k,l}) = 2 \times l^2 + (4 - 2n)l + n^2 - n + 6$, $M_2(R_{k,l}) = l^2 - nl + (n - 3)^2 + 6(n - 1)$. Let $f(l) = 2 \times l^2 + (4 - 2n)l + n^2 - n + 6$, $g(l) = l^2 - nl + (n - 3)^2 + 6(n - 1)$, $(l \in [2, n - 4])$, then $\max\{f(l)\} = \{f(2), f(n - 4)\} = n^2 - 5n + 22$ (since $f(2) = f(n - 4)$), and $\max\{g(l)\} = \{g(2), g(n - 4)\} = \{n^2 - 2n + 7, n^2 - 4n + 19\} = n^2 - 2n + 7$.

Therefore, $M_i(G^{(n)}_{3,4}) > M_i(R_{k,l})(i = 1, 2)$ hold.

So the proof of theorem is completed.

**Theorem 4.10.** Let $n \geq 9$, the Zagreb indices order in $\mathcal{U}^3_n$ is$(i = 1, 2)$

$$M_i(G^{(n)}_{3,1}) > M_i(G^{(n)}_{3,2}) > M_i(G'^{(n)}_{3,1}) > M_i(G^{(n)}_{3,3}) > M_i(G^{(n)}_{3,4}) > M_i(R_{k,l}) > \cdots$$

Let $G^{(n)}_{4,3}$ be the graph obtained from a $C_4$ by attaching $n - 5$ leaves to one of its vertices and another one leaf to the vertex which 2-distant to the $n - 3$-degree vertex of $C_4$. By the definition, we can work out the Zagreb indices of $G^{(n)}_{4,3}$ easily, $M_1(G^{(n)}_{4,3}) = n^2 - 5n + 22 = M_1(G^{(n)}_{4,2})$, $M_2(G^{(n)}_{4,3}) = n^2 - 4n + 18$.

Similar to Theorem 4.10, we have

**Theorem 4.11.** Let $n \geq 6$, the Zagreb indices order in $\mathcal{U}^4_n$ is

$(i)$ $M_1(G^{(n)}_{4,1}) > M_1(G^{(n)}_{4,2}) = M_1(G^{(n)}_{4,3}) > M_1(G'^{(n)}_{4,1}) > \cdots$

(*ii*) $M_2(G_{4,1}^{(n)}) > M_2(G_{4,2}^{(n)}) > M_1(G_{4,1}^{\prime(n)}) > M_2(G_{4,3}^{(n)}) > \cdots$
where $G_{4,1}^{\prime(n)}$ is obtained from by attaching $K_2$ to one of the pendent edges of $G_{4,1}^{(n-1)}$.

**Theorem 4.12.** Let $n \geq 6$, we have
(*i*) $M_1(G_{4,1}^{(n)}) = M_1(G_{3,1}^{\prime(n)})$;
(*ii*) $M_1(G_{3,4}^{(n)}) > M_1(G_{4,2}^{(n)})$;
(*iii*) $M_2(G_{3,4}^{(n)}) > M_2(G_{4,1}^{(n)})$.
**Proof.**By simple calculation, we have $M_1(G_{4,1}^{(n)}) = n^2-3n+12$, $M_2(G_{4,1}^{(n)}) = n^2-2n+8$, $M_2(G_{4,2}^{(n)}) = n^2-3n+13$.
Then the results is obvious.

Combining all the results, we shall get the upper bounds of unicyclic graphs with respect to Zagreb indices.
**Theorem 4.13.** Let $n \geq 6$, we have
(*i*) $M_1(G_{3,1}^{(n)}) > M_1(G_{3,2}^{(n)}) > M_1(G_{3,1}^{\prime(n)}) = M_1(G_{4,1}^{(n)}) > M_1(G_{3,3}^{(n)}) > M_1(G_{3,4}^{(n)}) > \cdots$
(*ii*) $M_2(G_{3,1}^{(n)}) > M_2(G_{3,2}^{(n)}) > M_2(G_{3,1}^{\prime(n)}) > M_2(G_{3,3}^{(n)}) > M_2(G_{3,4}^{(n)}) > \cdots$

# 5 The lower bounds of the unicyclic graphs with respect to Zagreb indices

Given integers $n$ and $k$ with $3 \leq k \leq n-1$, the *lollipop* $L_{n,k}$ is the unicyclic graph of order $n$ obtained from the two vertex disjoint graphs $C_k$ and $P_{n-k}$ by adding an edge joining a vertex of $C_k$ to an endvertex of $P_{n-k}$.

**Theorem 5.1**([8,9]). The cycle $C_n$ is the unique graph with the smallest Zagreb indices $M_1$ and $M_2$ among all unicyclic graphs with $n$ vertices.

**Theorem 5.2**. Let $G \in \mathcal{U}_n^k$, $3 \leq k \leq n-1$ be an arbitrary unicyclic graph, then $M_i(G) \geq M_i(L_{n,k})(i=1,2)$, with equality if and only if $G \cong L_{n,k}$.
**Proof.** By transformation $\gamma$, $\delta$ and Lemma 3.1, Lemma 3.2, the conclusion is obvious.

**Theorem 5.3**. Let $G \in \mathcal{U}_n - C_n$ be an arbitrary unicyclic graph, then $M_i(G) > M_i(L_{n,k})(i=1,2)$, $k \in \{3, \cdots, n-1\}$.
**Proof.** By the definition of $L_{n,k}$, we have $M_1(L_{n,k}) = 4n+2$, $M_2(L_{n,k}) = 4n+4$. Consequently, the values of $M_1$ and $M_2$ are the function of $n$, not related to $k$, and we know $M_i(L_{n,k}) = M_i(L_{n,l})$, which $k \in \{3, \cdots, n-1\}$ and $k \neq l$. That's to say, if $G \ncong C_n$, then $M_i(G) > M_i(L_{n,k})$ for $k \in \{3, \cdots, n-1\}$.

So the proof of theorem is completed.

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