Extremal Zagreb indices of unicyclic graphs

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Abstract

The Zagreb indices are topological indices of graphs, which defined as, $M_1(G) = \sum_{v \in V(G)} (d(v))^2$, $M_2(G) = \sum_{uv \in E(G)} (d(u)d(v))$. In this paper, we determine the upper and lower bounds for the Zagreb indices of unicyclic graphs in terms of their order and girth. In each case, we characterize the extremal graphs.

1 Introduction

We denote by G a graph of order $n = |V(G)|$ and size $m = |E(G)|$. For any $v \in V$, $N(v)$ denotes the neighbors of v, and $d(v) = |N(v)|$ 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. The stems and their corresponding leaves consist of the pendent edges of the graph. The girth of a graph G is the length of the shortest cycle in G. 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. The Zagreb indices of G were introduced more than 30 years ago [1], they were given by different names in the literatures, such as the Zagreb group indices, the Zagreb group parameters, and most often the Zagreb indices. In the early work of the Zagreb Mathematical Chemistry Group on the topological basis of the π-electron energy, two terms appeared in the topological formula for the total π-energy of conjugated molecules [1,12], where the first used as branching indices and later as topological indices in QSPR / QSAR studies [3]. The original Zagreb indices, which defined as

$$M_1(G) = \sum_{v \in V(G)} (d(v))^2, \tag{1}$$

$$M_2(G) = \sum_{uv \in E(G)} (d(u)d(v)) \tag{2}$$

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Recently, the Zagreb indices and their variants have been used to study molecular complexity,chirality, ZE-isomerism and heterosystems in [4]. The Zagreb indices are referred to in most books reporting topological indices and their uses in QSPR and QSAR. The research background of Zagreb indices together their generalization appears in chemistry or mathematical chemistry and can be found in the literatures [5-18].

A graph is called unicyclic if it is connected and contains exactly one cycle, a graph is unicyclic if and only if it is connected and has size equal to its order. In this paper, we investigate the unicyclic graph with the largest, the second largest and the smallest Zagreb indices, and the corresponding extremal unicyclic graphs achieve the bounds also been characterized.

2 Preliminaries

For convenience of our discussion, we first need to introduce two transformations.

Transformation A: Let u_iv be an edge G, $N_G(v)$ is the neighborhood of v and $N_G(v) - \{u_i\} = \{v_1, v_2, \cdots, v_s\}$, $G_0 = G - N_G[v] + u_i$. $G' = G - \{vv_1, vv_2, \cdots, vv_s\} + \{u_iv_1, u_iv_2, \cdots, u_iv_s\}$, as shown in Figure 1.

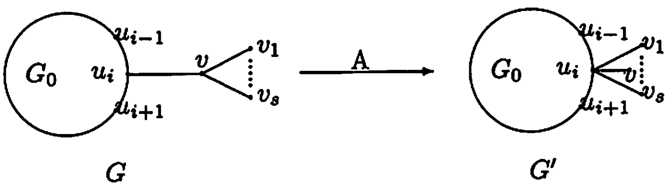

Figure 1. Transformation A

Lemma 2.1. Let G' is obtained from G by transformation A, then $M_i(G') > M_i(G) (i = 1, 2)$.

Proof. From Figure 1, we let $d(u_{i-1}) = p$, $d(u_i) = q$, $d(u_{i+1}) = r$ $(q \geq 3)$ in G, and $d(u_{i-1}) = p$, $d(u_i) = q + s$, $d(u_{i+1}) = r$, in G'. By the definition of the Zagreb indices, we have

$$\begin{aligned} \Delta_1 &= M_1(G) - M_1(G') \\ &= q^2 + (s+1)^2 - (s+q)^2 - 1 \\ &= 2s(1-q) \\ \Delta_2 &= M_2(G) - M_2(G') \\ &= (q+s)(s+1) + q(p+r) - (s+1)(q+s) - (p+r)(q+s) \\ &= -s(p+r) \end{aligned}$$

Therefore $\Delta_1 < 0$, $\Delta_2 < 0$.

So the proof is completed.

Remark: Repeating transformation A, any unicyclic graph can be changed into an unicyclic graph such that all the edges not on the cycle are pendent edges, and the Zagreb indices increase.

Transformation B: 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. $G' = G - \{uu_1, uu_2, \cdots, uu_s\} + \{vu_1, vu_2, \cdots, vu_s\}$, $G'' = G - \{vv_1, vv_2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$. u_{i-1}, u_{i+1} be the adjacent vertices of u in G_0, and v_{i-1}, v_{i+1} be the adjacent vertices of v in G_0, as shown in Figure 2.

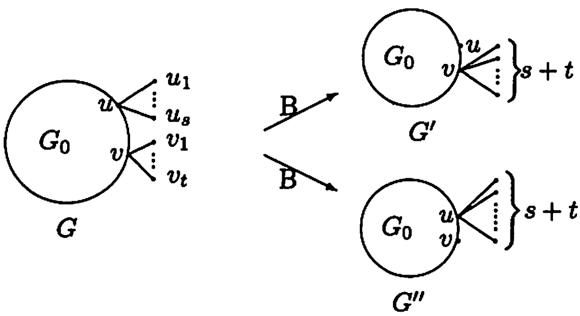

Figure 2. Transformation B.

Lemma 2.2. Let the graphs G' and G'' are obtained by transformation B on G as shown in Figure 2, then $M_i(G') > M_i(G)$, or $M_i(G'') > M_i(G)(i = 1, 2)$.

Proof. From Figure 2, we let:

$d(u_{i-1}) = a$, $d(u) = b + s$, $d(u_{i+1}) = c$, $d(v_{i-1}) = d$, $d(v) = e + t$, $d(v_{i+1}) = f$ in G;

$d(u_{i-1}) = a$, $d(u) = b$, $d(u_{i+1}) = c$, $d(v_{i-1}) = d$, $d(v) = e + s + t$, $d(v_{i+1}) = f$ in G';

$d(u_{i-1}) = a$, $d(u) = b + s + t$, $d(u_{i+1}) = c$, $d(v_{i-1}) = d$, $d(v) = e$, $d(v_{i+1}) = f$ in G''.

(1) By the definition of the Zagreb indices, we have

$$\begin{aligned} \Delta_1 &= M_1(G') - M_1(G) \\ &= (e+s+t)^2 + b^2 - (b+s)^2 - (e+t)^2 \\ &= 2s(e+t-b) \\ \Delta_2 &= M_1(G'') - M_1(G) \\ &= (b+s+t)^2 + e^2 - (b+s)^2 - (e+t)^2 \\ &= 2t(b+s-e) \end{aligned}$$

If $\Delta_1 \le 0$, such that $b \ge e + t$, then $\Delta_2 \ge 2t(s + t) > 0$.

(2) Let $d(u, v) = k$, there are three cases about $M_2(G)$

Subcase I: $k \ge 3$

$$\begin{aligned}
\Delta_3 &= M_2(G') - M_2(G) \\
&= ab + bc + d(e+s+t) + f(e+s+t) + (s+t)(e+s+t) \\
&\quad -[a(b+s) + c(b+s) + s(b+s) + d(e+t) + f(e+t) + t(e+t)] \\
&= s[(d+e+f) - (a+b+c)] + 2st \\
\Delta_4 &= M_2(G'') - M_2(G) \\
&= a(b+s+t) + c(b+s+t) + (s+t)(b+s+t) + de + ef \\
&\quad -[a(b+s) + c(b+s) + s(b+s) + d(e+t) + f(e+t) + t(e+t)] \\
&= t[(a+b+c) - (d+e+f)] + 2st
\end{aligned}$$

If $\Delta_3 \leq 0$, then $d+e+f \leq a+b+c-2t$, thus $\Delta_4 \geq 2t^2 + 2st > 0$.

Subcase II: $k = 2$,that's $u_{i+1} = v_{i-1} = w$, let $d(w) = g$

$$\begin{aligned}
\Delta_3 &= M_2(G') - M_2(G) \\
&= ab + bg + eg + g(e+s+t) + (s+t)(e+s+t) + f(e+s+t) \\
&\quad -[a(b+s) + g(b+s) + s(b+s) + g(e+t) + t(e+t) + f(e+t)] \\
&= s[(e+f) - (a+b)] + 2st \\
\Delta_4 &= M_2(G'') - M_2(G) \\
&= a(b+s+t) + g(b+s+t) + (s+t)(b+s+t) + ge + ef \\
&\quad -[a(b+s) + g(b+s) + s(b+s) + g(e+t) + t(e+t) + f(e+t)] \\
&= t[(a+b) - (e+f)] + 2st
\end{aligned}$$

If $\Delta_3 \leq 0$, then $e+f \leq a+b+c-2t$, thus $\Delta_4 \geq 2t^2 + 2st > 0$.

Subcase III: $k = 1$, that's u, v are adjacent

$$\begin{aligned}
\Delta_3 &= M_2(G') - M_2(G) \\
&= ab + b(e+s+t) + (s+t)(e+s+t) + f(e+s+t) \\
&\quad -[a(b+s) + s(b+s) + (b+s)(e+t) + t(e+t) + f(e+t)] \\
&= s[t+f-a] \\
\Delta_4 &= M_2(G'') - M_2(G) \\
&= a(b+s+t) + e(b+s+t) + (s+t)(b+s+t) + ef \\
&\quad -[a(b+s) + s(b+s) + (b+s)(e+t) + t(e+t) + f(e+t)] \\
&= t[a+s-f]
\end{aligned}$$

If $\Delta_3 \leq 0$, then $a \leq t+f$, thus $\Delta_4 \geq t^2 + st > 0$.

All these cases showed that(i) $M_1(G') > M_1(G)$, or $M_1(G'') > M_1(G)$; (ii) $M_2(G') > M_2(G)$, or $M_2(G'') > M_2(G)$.

The proof of Lemma 2.2 is completed.

Remark: Repeating transformation B, any unicyclic graph can be changed into an unicyclic graph such that all the pendent edges are attached to the same vertex of the cycle, and the Zagreb indices increase.

3 Extremal Zagreb indices of unicyclic graphs

Theorem 3.1. Let G be an arbitrary unicyclic graph of girth $k(k \geq 3)$, then

$$M_i(G) \leq M_i(H_{n,k})(i = 1, 2).$$

The equalities hold if and only if $G \cong H_{n,k}$, where $H_{n,k}$ denote the unicyclic graph constructed by attaching $n-k$ leaves to one vertex on a cycle of length k as shown in Figure 3(a).

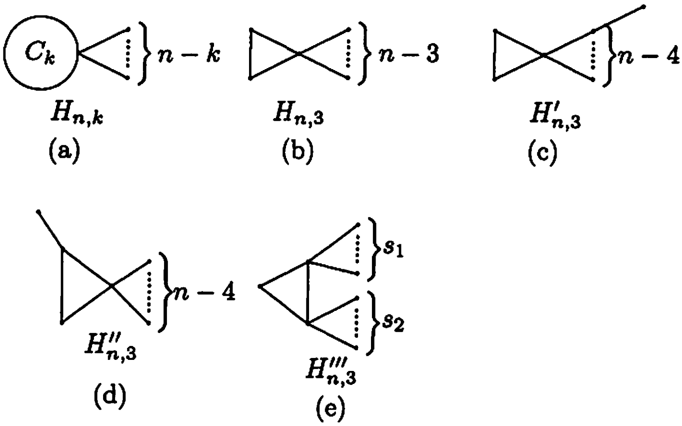

Figure.3

Proof. For G be an arbitrary unicyclic graph of the cycle length k, after many times transformation A on G, the graph G can be changed into G', in which the edges not on the cycle C_k are attached to the vertex of the cycle, and (i) $M_1(G) < M_1(G')$; (ii) $M_2(G) < M_2(G')$. Then repeating the transformations B on graph G', we can get a graph G'' such that all the pendant edges attached to the same vertex v. $G'' \cong H_{n,k}$, and we have (i) $M_1(G') < M_1(H_{n,k})$; (ii) $M_2(G') < M_2(H_{n,k})$. At last, we will get (i) $M_1(G) \leq M_1(H_{n,k})$; (ii) $M_2(G) \leq M_2(H_{n,k})$.

The proof is completed.

Theorem 3.2. Let $H_{n,k}(k-1 \geq 3)$ be the graph described above, then $M_i(H_{n,k}) < M_i(H_{n,k-1})(i = 1, 2)$.

Proof. From above proof and the definition of Zagreb indices, we have

$$\begin{aligned}
\Delta_1 &= M_1(H_{n,k}) - M_1(H_{n,k-1}) \\
&= (n-k) + (n-k+2)^2 + 2^2 - (n-k+1) - (n-k+3)^2 \\
&= -2(n-k) - 2 < 0 \\
\Delta_2 &= M_2(H_{n,k}) - M_2(H_{n,k-1}) \\
&= (n-k)(n-k+2) + 4(n-k+2) + 4 - (n-k+1)(n-k+3) \\
&\quad -4(n-k+3) \\
&= -2(n-k) - 3 < 0
\end{aligned}$$

Therefore, $M_1(H_{n,k}) < M_1(H_{n,k-1})$, $M_2(H_{n,k}) < M_2(H_{n,k-1})$

So the proof is completed.

Note that by the definition of the Zagreb indices, we can calculate the Zagreb indices of $H_{n,3}$ as following

$$M_1(H_{n,3}) = n^2 - n + 6, \ \ M_2(H_{n,3}) = n^2 + 3$$

Theorem 3.3. Let G be an arbitrary unicyclic graph with n vertices, then

(i) $M_1(G) \leq n^2 - n + 6$; (ii) $M_2(G) \leq n^2 + 3$,

the equalities hold if and only if $G \cong H_{n,3}$. (see Figure 3(b));

(iii) $M_1(G) \geq 4n$; (iv) $M_2(G) \geq 4n$,

the equalities hold if and only if $G \cong C_n$.

Proof. By theorem 3.2 (i), (ii)can be easily proved. We will prove (iii), (iv) in the following.

Let G be an arbitrary unicyclic graph and $G \ncong C_n$, then the cycle length of G must less than n, let C denote the cycle. There must be a vertex i, such that $d(i) \geq 3$, and there is a tree T_i located at i, repeating transformation A and B on G, G can be changed into the graph G', where the tree T_i is changed into the path, let P_k denote the path, and by Lemma 2.1 and 2.2, we have $M_1(G') < M_1(G)$,$M_2(G') < M_2(G)$. Let v_k be the endpoint of P_k, then $d(v_k) = 1$. The vertex j be the adjacent vertex of i in the cycle, such that $ij \in E(C)$, define $G'' = G' - \{ij\} + \{jv_k\}$, the graph G'' has order n and is unicyclic. By the definition of the Zagreb indices, we have

$$\begin{aligned} & M_1(G'') - M_1(G') \\ = \ & (d(i) - 1)^2 + 2^2 - (d(i))^2 - 1 \\ = \ & -2d(i) + 4 < 0 \end{aligned}$$

Let x be the adjacent vertex of i in C, y be the adjacent vertex of v_k in P_k, and $d(x) = a$

$$\begin{aligned} & M_2(G'') - M_2(G') \\ = \ & 2d(j) + 4 + a(d(i) - 1) - d(i)d(j) - ad(i) - 2 \\ = \ & (2 - d(i))d(j) + 2 - a < 0 \end{aligned}$$

Therefore $M_1(G'') < M_1(G')$, $M_2(G'') < M_2(G')$, that's to say G'' has smaller Zagreb indices than G'.

Repeating above proof, at last the graph G is changed into C_n.

So the proof is completed.

Theorem 3.4. Let G be an arbitrary unicyclic graph with n vertices. If $G \ncong H_{n,3}$, then

(i) $M_1(G) \leq n^2 - 3n + 14$, the equality holds if and only if $G \cong H''_{n,3}$;

(ii) $M_2(G) \leq n^2 - n + 7$, the equality holds if and only if $G \cong H''_{n,3}$.

Proof. Let $C_k = v_1v_2v_3 \cdots v_kv_1$, if $k \geq 5$, then it follows from the proof of Theorem 3.2 that $M_1(G) \leq M_1(H_{n,4}) = n^2 - 3n + 12$. Hence we may suppose $k \leq 4$

If $k = 4$, then by Theorem 3.3

$$M_1(G) \leq M_1(H_{n,4}) = n^2 - 3n + 12, \ \ M_2(G) \leq M_2(H_{n,4}) = n^2 - 2n + 8$$

and equalities hold if and only if $G \cong H_{n,4}$.

Now suppose $k = 3$. That's $C_k = v_1v_2v_3v_1$, the assumption $G \ncong H_{n,3}$, implies that the pendent edges not all connected to one vertex of C_3. Now, it suffice to consider the following cases.

(1)$d(v_1) = 3$, $d(v_2) = d(v_3) = 2$. In this case, $G \ncong H_{n,3}$, repeating transformation A and B on G, then G can be changed the graph G', where $G' \cong H'_{n,3}$(see Figure 3(c)). By Lemma 2.1 and 2.2, we have $M_1(G) \le M_1(H'_{n,3}) = n^2 - 3n + 12$;$M_2(G) \le M_2(H'_{n,3}) = n^2 - n + 4$ and equalities hold if and only if $G \cong H'_{n,3}$.

(2)$d(v_1), d(v_2) \ge 3, d(v_3) = 2$. In this case,$G \ncong H_{n,3}$, repeating transformation A on G, then G can be changed the graph $H''_{n,3}$(see Figure 3(e)), where $d(v_1) = s_1, d(v_2) = s_2 (s_1, s_2 \ge 1)$, and $s_1 + s_2 = n - 3$, for simple we denote $H'''_{n,3}$ by G'(see figure 3(e)). For $G' \ncong H_{n,3}$, we apply transformation B on G', then G' can be changed into the graph $G'' \cong H''_{n,3}$(see Figure 3(d)). By Lemma 2.2, we have $M_1(G) \le M_1(H''_{n,3}) = n^2 - 3n + 14$; $M_2(G) \le M_2(H''_{n,3}) = n^2 - n + 7$ and equalities hold if and only if $G \cong H''_{n,3}$.

(3)$d(v_1), d(v_2), d(v_3) \ge 3$. This case is similar to case (2).

Compare all the cases, we know $H''_{n,3}$ has the second maximal Zagreb indices among all the graphs G, which $G \ncong H_{n,3}$.

So the proof of theorem is completed.

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