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ON THE FIRST AND SECOND ZAGREB INDICES OF QUASI UNICYCLIC GRAPHS

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ABSTRACT. Let G be a simple graph. The graph G is called a quasi unicyclic graph if there exists a vertex $x \in V(G)$ such that $G - x$ is a connected graph with a unique cycle. Moreover, the first and the second Zagreb indices of G denoted by $M_1(G)$ and $M_2(G)$, are the sum of $\deg^2(u)$ overall vertices u in G and the sum of $\deg(u)\deg(v)$ of all edges uv of G , respectively. The first and the second Zagreb indices are defined relative to the degree of vertices. In this paper, sharp upper and lower bounds for the first and the second Zagreb indices of quasi unicyclic graphs are given.

1. Basic Definitions

The first and the second Zagreb indices are among the oldest topological indices defined in 1972 by Gutman and Trinajstić [9]. These numbers have been used to study the molecular complexity, chirality and some other chemical quantities. The *first Zagreb index* is defined as the sum of the squares of the degrees of the vertices, i.e. $M_1(G) = \sum_{u \in V(G)} \deg^2(u)$ and the *second Zagreb index* is the sum of $\deg(u)\deg(v)$ overall edges uv of G . This means that $M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v)$. The first and the second Zagreb indices are defined relative to the degree of vertices, which we summarize them without referring to the degree of vertices.

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Suppose G is a simple graph and $\Delta(G)$ and $\delta(G)$ denote the maximum and minimum degrees of vertices in G . For each $u \in V(G)$, the set of all neighbors of the vertex u is denoted by $N_G(u)$. For a subset W of the vertex set $V(G)$, let $G-W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, for a subset E of the edge set $E(G)$, $G-E$ denotes the subgraph of G obtained by deleting the edges of $E(G)$. If $W=\{v\}$ and $E=\{xy\}$, the subgraphs $G-W$ and $G-E$ will be simply written as $G-v$ and $G-xy$, respectively. For any two non-adjacent vertices x and y of G , we let $G+xy$ be the graph obtained from G by adding an edge xy , and also for any two adjacent vertices u and v of G , we let $G-uv$ be the graph obtained from G by deleting an edge uv .

The cycle C_n for $n \geq 3$, is a path of n edges and n vertices where starting and ending at the same vertex. The wheel graph W_n for $n \geq 4$, is a graph formed by connecting a single universal vertex x to all vertices of a cycle graph C_{n-1} . The complete graph K_n for $n \geq 2$, is a graph in which each pair u and v of vertices are adjacent and finally the star graph S_n is a tree with exactly n vertices such that there is one vertex of degree $n-1$ and other vertices have degree one.

A graph G is called *unicyclic graph*, if it is connected and has a unique cycle. If the graph G has the property that $G-x$ induces a unicyclic graph for a suitable vertex x , then G is called a *quasi unicyclic graph*. It is clear that the cycle C_n of length $n \geq 3$ or even the cycle C_n together with some pendant edges are unicyclic graphs. The complete graph K_4 is not unicyclic, but it is a quasi unicyclic graph, because if we remove a vertex from K_4 then we will get a cycle C_3 and so K_4 is a quasi unicyclic graph. Moreover, a wheel graph W_n is quasi unicyclic, since by removing the center we will get a cycle C_n . Throughout this paper, the set of all unicyclic and quasi unicyclic graphs with n vertices will be denoted by $U(n)$ and $QU(n)$, respectively.

2. History

In this section, we review the important properties of the Zagreb group indices. We refer to Gutman and Das [8] for a survey on important results on the first Zagreb index until 2004. We encourage to the interested readers to consult [2, 12] for more information on distribution of Zagreb group indices on some binary graph operations.

Suppose G is a simple graph with exactly n vertices and m edges. The first important property of Zagreb group indices is related to an inequality named “Zagreb indices inequality (ZII property)”. Hansen and Vukičević [10] proved that all graphs with this condition that $\Delta(G) \leq 4$ satisfy ZII property. These authors observed that the union of a complete graph of order 3 and the star graph S_6 is a counterexample for this inequality when the graph is disconnected. Also, for connected graphs they constructed a counterexample of order 48. Vukičević and Graovac [16] proved that the ZII property holds for trees and Caporossi et al. [3] verified the ZII property for unicyclic graphs. We refer to [1] for a simple proof of ZII property when the graph is a tree or a unicyclic graph. Das [6] investigated this

property under some unary graph operations and Horoldagva and Das [11] continued this approach by investigating some binary graph operations.

Das and Gutman [4] provided some identities for Zagreb indices by which the authors obtained some bounds for the second Zagreb index and in [5], the author established some bound for the first Zagreb index. Deng [7] presented a unified approach to the largest and smallest Zagreb indices for trees, unicyclic and bicyclic graphs by introducing some transformations. He also characterized the graphs with the largest and smallest Zagreb indices. Li et al. [13] determined sharp bounds for the first and second Zagreb indices of n -vertex cacti with k pendant vertices. As a consequence, they also obtained the n -vertex cacti with a perfect matching having maximal Zagreb indices. Li and Zhao [14] investigated the Zagreb indices of bicyclic graphs with a given matching number and provided some sharp upper bounds for the first and second Zagreb indices of these graphs in terms of the order and given size of matchings. Xu [17] characterized the connected n -vertex graphs with clique number k with respect to Zagreb indices and determined the values of the corresponding indices. Yarahmadi et al. [18] computed the Zagreb indices of polyomino chains. Zhao and Li [19] determined sharp bounds for both of Zagreb indices in the class of all n -vertex bicyclic graphs with k pendant vertices. Zhou [20] provided upper bounds for the Zagreb indices of triangle-free graphs in terms of the number of vertices and the number of edges and determined the graphs for which the bounds are attained. Zhou and Stevanović [21] continued the mentioned work by providing upper bounds for the Zagreb indices of quadrangle-free graphs. Zhou [22] found upper bounds for the Zagreb indices and the spectral radius of series-parallel graphs in terms of the number of vertices and the number of edges. He also determined the graphs for which the bounds are attained.

Qiao [15] gave sharp lower and upper bounds for the Zagreb group indices of n -vertex quasi-tree graphs and the corresponding extremal graphs were characterized. The second Zagreb indices of graphs with given degree sequences was discussed in [23]. In this paper, we continue this work for quasi unicyclic graphs.

3. Quasi Unicyclic Graphs

The aim of this section is to present sharp upper and lower bounds for the first and the second Zagreb indices of quasi unicyclic graphs. We start by the following simple lemma which plays an important role in the proof of our main theorems.

Lemma 3.1. *Let G be an n -vertex graph, $xy \in E(G)$ and $uv \notin E(G)$. Then,*

- (i) $M_1(G) \leq M_1(G + uv)$,
- (ii) $M_1(G - xy) \leq M_1(G)$,
- (iii) $M_2(G) \leq M_2(G + uv)$,
- (iv) $M_2(G - xy) \leq M_2(G)$.

Proof. Since the proof of the Part (ii) is similar to the proof of the Part (i) and the proof of (iv) is similar to the proof of (iii), it is enough to prove (i) and (iii).

- (i). $uv \notin E(G)$. By connecting the vertices u and v , we can see that $M_1(G + uv) - M_1(G) = (\deg u + 1)^2 + (\deg v + 1)^2 - \deg^2 u - \deg^2 v = 2(1 + \deg u \deg v) > 0$. Hence, $M_1(G) \leq M_1(G + uv)$.
- (iii). $uv \notin E(G)$, $N_G(v) = \{x_1, \dots, x_s\}$ and $N_G(u) = \{y_1, \dots, y_r\}$. Therefore, $M_2(G + uv) - M_2(G) = (\deg u + 1)(\deg v + 1) + \sum_{i=1}^r (\deg u + 1)(\deg y_i) + \sum_{i=1}^s (\deg v + 1)(\deg x_i) - \sum_{i=1}^r (\deg u)(\deg y_i) - \sum_{i=1}^s (\deg v)(\deg x_i) = (\deg u + 1)(\deg v + 1) + \sum_{i=1}^r \deg y_i + \sum_{i=1}^s \deg x_i > 0$. As a consequence, $M_2(G) \leq M_2(G + uv)$.

This proves the lemma. \square

In the following lemma, we give a class of graphs which are not quasi unicyclic.

Lemma 3.2. *Let G be an n -vertex graph such that $n \geq 5$. If the number of vertices of degree $n - 1$ is greater than 2, then G is not a quasi unicyclic graph.*

Proof. Since $|V(G)| = n \geq 5$, there are 5 distinct vertices x_1, x_2, x_3, x_4 and x_5 such that $\deg x_1 = \deg x_2 = \deg x_3 = n - 1$. It is clear that x_1, x_2, x_3 are adjacent to each other and so the subgraph of G induced by the above five vertices is not quasi unicyclic, because the graph constructed from G by removing any of these five vertices has at least two cycles. Hence G can not be a quasi unicyclic graph. \square

The following corollary is a direct consequence of Lemma 2.3.

Corollary 3.3. *If $G \in QU(n)$, then G has at most two vertices of degree $n - 1$.*

Lemma 3.4. *Let $G \in QU(n)$, $n \geq 4$ and $m = |E(G)|$. Then $n \leq m \leq 2n - 2$ and $1 \leq \delta(G) \leq 3$.*

Proof. Suppose $G \in QU(n)$ and $n \geq 4$. Since G is connected and has a cycle, $m \geq n$. By our assumption, G has a suitable vertex x such that $G - x \in U(n)$. Thus, $|E(G - x)| = |V(G - x)| = n - 1$. Since $\deg(x) \leq n - 1$, $m = |E(G)| \leq |E(G - x)| + n - 1 = 2n - 2$. Furthermore, if $G \in QU(n)$ has a pendant vertex, then $\delta(G) = 1$. Suppose G has no pendant vertex. Then $\delta(G) \geq 2$ and for a suitable vertex x , we have $G - x \in U(n - 1)$ which implies that $G - x$ has a vertex y of degree 2. If y is adjacent to x , then the minimum degree of G can be at most 3. Hence $1 \leq \delta(G) \leq 3$, as desired. \square

Apply Lemmas 3.2 and 3.4 to find lower and upper bounds for the Zagreb indices of an arbitrary quasi unicycle graph. We first define a class $\Omega(n)$ of n -vertex quasi unicyclic graphs that plays an important role in our results. Let $\Omega(n)$ be the set of all quasi unicyclic graphs with exactly n vertices that contains two vertices of degree $n - 1$, two vertices of degree 3 and the rest of vertices have degree 2, see Figure 1.

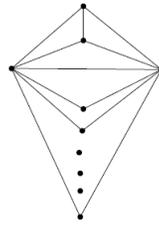


FIGURE 1. The Graph Structure of a Member of $\Omega(n)$.

Theorem 3.5. *Let $G \in QU(n)$ and $n \geq 4$. Then $M_1(G) \leq 2n^2 + 4$. The equality holds if and only if $G \in \Omega(n)$.*

Proof. Suppose $G \in QU(n)$, $n \geq 4$, and x is a vertex of G such that $G - x \in U(n - 1)$. We have the following two cases:

Case 1. G has no pendant vertex. By Lemma 3.4, $\delta(G) = 2$ or 3 . Suppose $\delta(G) = 2$. We proceed by induction on n . If $n = 4$, then it is clear that $M_1(G) \leq 36 = 2n^2 + 4$, see Figure 2. We now assume that $n \geq 5$ and the result holds for $n - 1$. If $\deg(x) < n - 1$, then we construct a graph G' from G by adding some new edges to G to obtain $\deg_{G'}(x) = n - 1$. By Lemma 3.1, $M_1(G) \leq M_1(G')$. Let u be a vertex adjacent to x and v such that $\deg(u) = 2$, $\deg(x) = n - 1$ and $2 \leq \deg(v) \leq n - 1$. If we remove the vertex u , then by inductive assumption $M_1(G' - u) \leq 2(n - 1)^2 + 4$. Therefore,

$$\begin{aligned} M_1(G') - M_1(G' - u) &= 4 + [(n - 1)^2 - (n - 2)^2] + [(\deg(v))^2 - (\deg(v) - 1)^2] \\ &= 2 + 2[(n - 1) + \deg(v)]. \end{aligned}$$

On the other hand, we have

$$\begin{aligned} M_1(G) &\leq M_1(G') = M_1(G' - u) + 2 + 2[(n - 1) + \deg(v)] \\ &\leq 2(n - 1)^2 + 4 + 2 + 2[(n - 1) + \deg(v)] \\ &\leq 2(n - 1)^2 + 6 + 2(2n - 2) = 2n^2 + 4. \end{aligned}$$

If $\delta(G) = 3$, then G is the wheel graph W_n and so $M_1(G) = M_1(W_n) = n^2 + 2n - 3 < 2n^2 + 4$ as required.

Case 2. G has a pendant vertex x . In this case, we can see that x is not adjacent to other pendant vertices of G . Again we obtain a new graph G' by connecting all pendant vertices to x and Lemma 3.4, $M_1(G) \leq M_1(G')$. So, the proof is completed by using the previous case.

For the second part, we first note that if $G \in \Omega$, then $M_1(G) = \sum_{u \in V(G)} \deg^2 u = 2n^2 + 4$. Conversely, if $M_1(G) = \sum_{u \in V(G)} \deg^2 u = 2n^2 + 4$, then we can see that the vertex v has degree $n - 1$. This shows that we have two vertices x and v of degree $n - 1$. Moreover, we have only two

distinct vertices $y, u \notin \{x, v\}$ such that x and v are adjacent to y and u and $\deg y = \deg u = 3$. If for instance y is adjacent to a vertex different from x and v then we will have a new cycle which is a contradiction. Thus $\deg y = \deg u = 3$. For the rest of vertices as $z \notin \{x, y, u, v\}$, we should have $\deg z = 2$. Otherwise, a new cycle will be appeared. Hence $G \in \Omega(n)$. \square

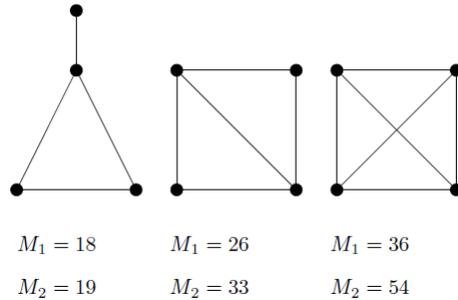


FIGURE 2. The Zagreb Indices of Members on $QU(4)$.

Let us now state another class of quasi unicyclic graphs. Define $\Gamma(n)$ to be a quasi unicyclic graph that contains a cycle of length $n - 1$ and a pendant vertex that is attached to C_{n-1} , see Figure 3. The following theorem gives a necessary and sufficient condition for a graph G to be isomorphic to $\Gamma(n)$.

Theorem 3.6. *Let $G \in QU(n)$ and $n \geq 4$. Then $M_1(G) \geq 4n + 2$ with equality if and only if $G \cong \Gamma(n)$.*

Proof. Suppose $G \in QU(n)$, where $n \geq 4$. Hence, there exists a vertex $x \in V(G)$ such that $G - x \in U(n)$. Two cases can be happened as follows:

Case 1. G has no pendant vertex. We can proceed by induction on n . Let $n = 4$, then we have three kinds of quasi unicyclic graphs depicted in Figure 2. For the graph depicted on the left hand side of Figure 2, we have $M_1 = 18 = 4(4) + 2$ and the equality holds. For other two graphs, we can see that $M_1 > 18$, as desired. Suppose that $n \geq 5$ and the result holds for $n - 1$.

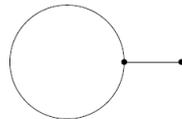


FIGURE 3. The Graph $\Gamma(n)$.

Proceed by induction, we assume that $2 \leq \deg x = r \leq n - 1$ and $N_G(x) = \{x_1, \dots, x_r\}$. If we remove all edges xx_2, xx_3, \dots, xx_r and obtain the new graph G' , then we can see that

$$M_1(G) > M_1(G - xx_2) > M_1(G - \{xx_2, xx_3\}) > \dots > M_1(G - \{xx_2, \dots, xx_r\}) = M_1(G').$$

If we remove vertex x from G' , then by induction hypothesis, $M_1(G' - x) \geq 4(n - 1) + 2$. Therefore,

$$\begin{aligned} M_1(G') - M_1(G' - x) &= 1 + [\deg^2(x_1) - (\deg(x_1) - 1)^2] \\ &= 2 \deg(x_1) \geq 4. \end{aligned}$$

Hence, $M_1(G') \geq 4(n - 1) + 2 + 2 \deg(x_1) \geq 4n + 2$, as desired.

Case 2. G has pendant vertex u adjacent to v , where $2 \leq \deg(v) \leq n - 1$. By removing the vertex u we achieved a new graph G'' that by induction hypothesis satisfies $M_1(G'') > 4(n - 1) + 2$. So,

$$M_1(G) = M_1(G'') + 1 + [\deg^2 v - (\deg(v) - 1)^2] \geq 4(n - 1) + 2 + 1 + 1 + 2 \deg(v) \geq 4n + 2$$

and the proof is completed.

To prove the second part, we first assume that $G \in \Gamma$. It is clear that $M_1(G) = \sum_{u \in V(G)} \deg^2 u = 4n + 2$. Conversely one can easily see that the minimum value of $M_1(G)$ occurs when $\deg(x) = 1$. Since $M_1(G) = 4n + 2$, x must be adjacent to only one vertex of C_{n-1} , and the result follows. \square

As similar as the method for giving lower and upper bounds of $M_1(G)$, we can state it for $M_2(G)$ as the following theorem.

Theorem 3.7. *Let $G \in QU(n)$ and $n \geq 4$. Then $4n + 3 \leq M_2(G) \leq 5n^2 - 10n + 14$ with equality on the left or right whenever $G \cong \Gamma(n)$ or $G \in \Omega(n)$, respectively.*

Proof. Suppose $G \in QU(n)$, $n \geq 4$, and x is a vertex in G such that $G - x \in U(n)$. We prove the theorem in two parts. For the right hand side of the inequality, we may consider two cases as follows:

Case 1. G has no pendant vertex. By Lemma 3.4, $\delta(G) = 2$ or 3. Suppose $\delta(G) = 2$ and apply induction on n . If $n = 4$, then equality holds, see Figure 2. We assume that $n \geq 5$ and the result holds for $n - 1$. If $\deg(x) < n - 1$, then there are vertices in the graph that are not adjacent to x . We connect these vertices to x and obtain a new graph G' . By Lemma 3.2, $M_2(G) \leq M_2(G')$. Let u be a vertex adjacent to x and v such that $\deg(u) = 2$, $\deg(x) = n - 1$ and $2 \leq \deg(v) = r \leq n - 1$. Suppose x and v have neighbors y_1, \dots, y_{n-1} and y_1, \dots, y_r , respectively. If we remove the vertex u , then by induction assumption, $M_2(G - u) \leq 5(n - 1)^2 - 10(n - 1) + 14$. Therefore,

$$\begin{aligned} M_2(G') - M_2(G' - u) &= 2(n - 1) + 2r + \sum_{i=1}^{n-2} (n - 1) \deg(y_i) + \sum_{i=1}^{r-1} r \deg(y_i) \\ &\quad - \sum_{i=1}^{n-2} (n - 2) \deg(y_i) - \sum_{i=1}^{r-1} (r - 1) \deg(y_i) \end{aligned}$$

and so

$$\begin{aligned}
 M_2(G') &\leq M_2(G' - u) + (4n - 4 - n - 1) + (4n - 4 - n - 1) + 4n - 4 \\
 &\leq 5(n - 1)^2 - 10(n - 1) + 14 + 10n - 14 \\
 &\leq 5n^2 - 10n + 14.
 \end{aligned}$$

If $\delta(G) = 3$, then G is wheel graph and so $M_2(W_n) = 3n^2 + 3n - 6 < 5n^2 - 10n + 14$, as required.

Case 2. G has a pendant vertex. If G has a pendant vertex x then we can see that x is not adjacent to other pendant vertices and hence we can obtain a new graph G' by connecting all pendant vertices to x . Again by Lemma 3.2, $M_1(G) \leq M_1(G')$ and the proof can be completed by using the Case 1.

To prove the second part, it's clear that if $G \in \Omega(n)$, then $M_2(G) = \sum_{uv \in E(G)} \deg u \deg v = 5n^2 - 10n + 14$. Conversely, if $M_2(G) = \sum_{uv \in E(G)} \deg u \deg v = 5n^2 - 10n + 14$, then we can see that the vertex v should be of degree $n - 1$. Thus, we have two vertices x and v of degree $n - 1$. Moreover, we have only two distinct vertices $y, u \notin \{x, v\}$ such that x and v are adjacent to y and u and $\deg y = \deg u = 3$. If for instance y is adjacent to a vertex different to x and v then we will have a new cycle which is a contradiction. Thus $\deg y = \deg u = 3$ and for the rest of vertices as $z \notin \{x, y, u, v\}$, we should have $\deg z = 2$. Otherwise, a new cycle will be appeared which proves that $G \in \Omega(n)$.

For the left hand side inequality, two cases can be happened as follows:

Case 1'. G has no pendant vertex. Again our proof can be proceed by induction on n . If $n = 4$, then we have three kinds of quasi unicyclic graphs as in Figure 2. For the first graph on the left hand side of Figure 2, we have $M_2 = 19 = 4(4) + 3$ and the equality holds. For other two graphs, we can see that $M_2 > 19$, as desired. We now assume that $n \geq 5$ and the result holds for $n - 1$. To prove the result for n , let $2 \leq \deg x = r \leq n - 1$ and $N_G(x) = \{x_1, \dots, x_r\}$. If we remove the edges xx_2, xx_3, \dots, xx_r then we obtain a new graph G' such that

$$M_2(G) > M_2(G - xx_2) > M_2(G - \{xx_2, xx_3\}) > \dots > M_2(G - \{xx_2, \dots, xx_r\}) = M_2(G').$$

If we remove the vertex x from G' , then by induction hypothesis, we have $M_2(G' - x) \geq 4(n - 1) + 3$. Therefore,

$$\begin{aligned}
 M_2(G') &\geq M_2(G' - x) + r + \sum_{i=1}^{r-1} (r - (r - 1))d(y_i) \\
 &\geq 4n - 4 + 3 + 2 + 2 = 4n + 3
 \end{aligned}$$

that all vertices $y_i, 1 \leq i \leq r$, are adjacent to x_1 .

Case 2'. G has pendant vertex u adjacent to v , where $2 \leq \deg v \leq n-1$. By removing vertex u we achieve a new graph G'' such that $M_2(G'') \geq 4(n-1) + 3$. Therefore,

$$\begin{aligned} M_2(G) &\geq M_2(G'') + r + \sum_{i=1}^{r-1} (r - (r-1)) \deg(y_i) \\ &\geq 4n - 1 + 2 + \sum_{i=1}^{r-1} \deg(y_i) \geq 4n + 3 \end{aligned}$$

that all vertices y_i , $1 \leq i \leq r$, are adjacent to v . Since the degree of at least one vertex y_i is greater than or equal to 2, $r \geq 2$ which completes the proof of this case.

To prove the second part, we note that if $G \cong \Gamma(n)$, then $M_2(G) = \sum_{u \in V(G)} \deg u \deg v = 4n + 3$. Conversely, one can easily see that the minimum value of $M_2(G)$ occurs when $\deg(x) = 1$. Since $M_2(G) = 4n + 3$, x has to be adjacent to only one vertex of C_{n-1} , and the result follows. \square

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