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On The Zagreb Index Of Quasi-Tree Graphs*

Sheng Ning Qiao†

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Abstract

A topological index is a map from the set of chemical compounds represented by molecular graphs to the set of real numbers. Let G be a simple graph. *The first Zagreb index* $M_1(G)$ of G is the sum of $(d(u))^2$ for all vertices u of G, and *the second Zagreb index* $M_2(G)$ of G is the sum of $d(u)d(v)$ for all edges uv of G, where $d(u)$ denotes the degree of the vertex u in G. A graph G is called *quasi-tree graph*, if there exists a vertex $u \in V(G)$ such that $G - u$ is a tree. In this paper, we give sharp lower and upper bounds on the Zagreb indices of quasi-tree graphs on n vertices, and corresponding extremal graphs are characterized.

1 Introduction

We use Bondy and Murty [2] for terminology and notation not defined here and consider finite simple connected graphs only.

A topological index is a map from the set of chemical compounds represented by molecular graphs to the set of real numbers. Many topological indices are closely correlated with some physico-chemical characteristics of the underlying compounds.

Let G be a simple graph. *The first Zagreb index* $M_1(G)$ and *the second Zagreb index* $M_2(G)$ of G are defined in [7] respectively as

$$M_1(G) = \sum_{u \in V(G)} (d(u))^2, \qquad M_2(G) = \sum_{uv \in E(G)} d(u)d(v),$$

where $d(u)$ denotes the degree of the vertex u in G.

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 [1, 5, 8, 14]. The development and use of the Zagreb indices were summarized in [6, 11]. Mathematical properties of the first Zagreb index for general graphs can be found in [3, 4, 12, 13]. Zhou [16] presented sharp upper bounds for the Zagreb indices M_1 and M_2 of a graph, especially for triangle-free graphs, in terms of the number of vertices and the number of edges. Yan et al. [15] gave sharp upper and lower bounds on the second Zagreb index of unicyclic graphs with n vertices and k pendant vertices.

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†Department of Applied Mathematics, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, P. R. China

A graph G is called *quasi-tree graph*, if there exists a vertex $x \in V(G)$ such that $G-x$ is a tree. In this paper, we give sharp lower and upper bounds on the Zagreb indices of quasi-tree graphs on n vertices, and corresponding extremal graphs are characterized.

Let y be a vertex of G. By $G-y$ we denote $G[V(G) \setminus \{y\}]$. Let z be a vertex of G with $yz \notin E(G)$. By $G+yz$ we denote $G[E(G) \cup \{yz\}]$. Let G be a quasi-tree graph on n vertices and x a vertex of G such that $G-x$ is a tree. If $d_G(x)=1$, then G is a tree. Li et al. [10] and Lang et al. [9] proved the following results.

THEOREM 1 [10]. Let T be a tree on n vertices. Then
(i) $M_1(G) \geq 4n-6$ equality holds if and only if T is a path on n vertices;
(ii) $M_1(G) \leq n(n-1)$ equality holds if and only if T is a star on n vertices.

THEOREM 2 [9]. Let T be a tree on n vertices. Then
(i) $M_2(G) \geq 4(n-2)$ equality holds if and only if T is a path on n vertices;
(ii) $M_2(G) \leq (n-1)^2$ equality holds if and only if T is a star on n vertices.

So, we may assume that $d_G(x) \geq 2$ for all quasi-tree graphs on n vertices. Let $\mathbb{QT}(n)$ be the set of all quasi-tree graphs G on n vertices and $d_G(x) \geq 2$. By $K_{1,1,n-2}$ we denote the complete tripartite graph. Our main results are as follows.

THEOREM 3. Let $n \geq 3$ be a positive integer and G be a graph with $G \in \mathbb{QT}(n)$. Then we have
(i) $M_1(G) \geq 4n$ equality holds if and only if $G = C_n$;
(ii) $M_1(G) \leq 2n^2-6$ equality holds if and only if $G = K_{1,1,n-2}$.

THEOREM 4. Let $n \geq 3$ be a positive integer and G be a graph with $G \in \mathbb{QT}(n)$. Then we have
(i) $M_2(G) \geq 4n$ equality holds if and only if $G = C_n$;
(ii) $M_2(G) \leq 5n^2-14n+9$ equality holds if and only if $G = K_{1,1,n-2}$.

Since the methods of the proofs of Theorem 3 and Theorem 4 are similar, we only prove Theorem 4 in the next section.

2 The Proof of Theorem 4

PROOF of (i). We prove (i) by induction on n. If $n=3$, then (i) holds obviously. In the following we may assume $n \geq 4$. We consider two cases as follows.

Case 1. There exists a vertex u in G such that $d_G(u)=1$.

Let v be a vertex in G with $uv \in E(G)$. Suppose that $N_G(v) = \{u, u_1, u_2, \ldots, u_p\}$. Clearly $p \geq 1$. Let $G' = G-u$. It is not difficult to see that $G' \in \mathbb{QT}(n-1)$. If $p \geq 2$, then by the induction hypothesis, we can get that

$$M_2(G) \geq M_2(G') + 5 \geq 4n-4+5 > 4n.$$

If $p=1$, then we have $d_G(u_1) \geq 2$ and $G' \neq C_{n-1}$. So, by the induction hypothesis, we have

$$M_2(G) \geq M_2(G') + 4 > 4n-4+4 = 4n.$$

Case 2. The minimum degree of G is at least two.

Since G is a quasi-tree graph, there exists a vertex with exactly two degrees in G. Without loss of generality, we let u be the vertex in G such that $d_G(u) = 2$ and $N_G(u) = \{v_1, v_2\}$. Suppose $G \neq C_n$. We will show that $M_2(G) > 4n$. Let $G' = G - u$. Since the minimum degree of G is at least two, we have $G' \in \mathbb{QT}(n-1)$. So, by the induction hypothesis, we have

$$M_2(G) \geq M_2(G') + 8 > 4n - 4 + 8 > 4n.$$

The proof of (i) is complete.

PROOF of (ii). We prove (ii) by induction on n. If $n = 3$, then (ii) follows immediately. We may assume $n \geq 4$. Choose $G \in \mathbb{QT}(n)$ such that $M_2(G)$ is as large as possible.

We claim that the minimum degree of G is at least two. If not, then we let y be a vertex with exactly one degree in G. Let x be a vertex in G such that $G - x$ is a tree. It is easy to see that $xy \not\in E(G)$. Since $G + xy \in \mathbb{QT}(n)$ and $M_2(G + xy) > M_2(G)$, by the choice of G in $\mathbb{QT}(n)$ we can obtain a contradiction. So the minimum degree of G is at least two. In fact, it follows from the choice of G in $\mathbb{QT}(n)$ that $d_G(x) = n - 1$.

If there exists a vertex $x' \neq x$ in G such that $G - x'$ is a tree, then by the choice of G in $\mathbb{QT}(n)$ we have $d_G(x') = n - 1$. Since G is a quasi-tree graph, we can get that $G - x - x'$ contains no edges. This implies that $G = K_{1,1,n-2}$. Thus, in the following we assume $G \neq K_{1,1,n-2}$ and we show that $M_2(G) < M_2(K_{1,1,n-2}) = 5n^2 - 14n + 9$, a contradiction.

Since the minimum degree of G is at least two and G is a quasi-tree graph, we can deduce that G contains a vertex v with exactly two degrees. Set $N_G(v) = \{u, w\}$. It is not difficult to see that $G \neq C_n$. Then we have $G - v \in \mathbb{QT}(n-1)$. By $G \neq K_{1,1,n-2}$, it follows that $G - v \neq S_{1,1,n-3}$. By the induction hypothesis, we have

$$\begin{aligned}
M_2(G) &\leq M_2(G - v) + 2(n-1) + 2d_G(w) \\
&\quad + \Big(4n - 6 - n - 1 - d_G(w)\Big) + \Big(n - 2 + d_G(w)\Big) + \Big(n + d_G(w) - 3\Big) \\
&= M_2(G - v) + 7n + 3d_G(w) - 14 \\
&< 5(n-1)^2 - 14(n-1) + 9 + 7n + 3(n-2) - 14 \\
&= 5n^2 - 14n + 8 \\
&< 5n^2 - 14n + 9.
\end{aligned}$$

The proof of (ii) is complete.

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