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New Bounds on Zagreb indices and the Zagreb Co-indices

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ABSTRACT: In this short note, we studied the *first*, *second Zagreb indices* and the *Zagreb Co-indices.* Also, established the connections of bounds to the above sighted indices.

Key Words: Simple graph, Zagreb index, Zagreb coindex, Maximal Degree.

Contents

1. Introduction and Terminologies

Graph theory has provided chemists with a variety of useful tools, such as topological indices [11]. Let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $e = |E = E(G)|$ edges. For the vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of the shortest path between u and v in G. In theoretical Chemistry, molecular structure descriptors, the topological indices are used for modeling physico - chemical, toxicologic, biological and other properties of chemical compounds. Arguably, the best known of these indices is the *Wiener index* W [12], defined as the sum of the distances between all pairs of vertices of the graph G.

$$W(G) = \sum d(u, v).$$

The various extensions and generalization of the *Wiener index* are recently put forward. The degree of the vertex v is denoted by $d(v)$. Specially, $\triangle = \triangle(G)$ is the maximum degree of G.

A graph invariant is a function on a graph that does not depend on the labeling of its vertices. Such quantities are also called topological indices. Two of these graph invariants are known under various names, the most commonly used ones are the first and second Zagreb indices. The *Zagreb index* was first introduced in [5] and the survey of the properties of the *first Zagreb index* is given. The first zagreb index is

$$M_1(G) = \sum [d(u)]^2$$

where $u \in V(G)$. The *second Zagreb index* is

$$M_2(G) = \sum [d(u).d(v)]$$

2000 *Mathematics Subject Classification:* 05C07, 92E10 where $uv \in E(G)$. Recently, there was a vast research on comparing the *Zagreb indices* [3,4,7] and the relation involving the other graph invariants. The zagreb co-indices is defined in [9,10]. The first zagreb co-index is

$$\overline{M_1(G)} = \sum [d(u) + d(v)]$$

where uv is not an edge in $E(G)$. The second zagreb co-index

$$\overline{M_2(G)} = \sum [d(u).d(v)]$$

where uv is not an edge in $E(G)$. In our paper, we established some bounds for the Zagreb co-indices in terms of the cardinality n of the vertex set, the cardinality e of the edge set and the maximum degree $\triangle$ of G. The readers interested in more information on Zagreb indices can be referred to [2,6,8] and to the references therein.

The paper is organized as follows: After the Introduction and terminologies in the second section, we will concentrate our efforts on initiate a systematic study on the *Zagreb co-indices* and obtained some bounds for these indices. For other undefined notations and terminology from graph theory, the readers are referred to J.A. Bondy and et al [1].

2. Bounds on Zagreb indices and co-indices

In this section, we derived the bounds for the relations connecting the Zagreb co-indices in terms of the maximal degree and the cardinality of the vertex set and edge set.

Theorem 2.1. *For a simple graph G, with n vertices and e edges having the maximal degree $\triangle$,*

$$\overline{M_1(G)} \leq 2e(n-1) - M_1(G) + \triangle e(n-1) - 2\triangle e.$$

and

$$\overline{M_2(G)} \leq 2\triangle e(n-1) - \triangle M_1(G)$$

Proof: For each edge $uv \in E(G)$, for a vertex $u \in V(G)$, the $n-1-d(u)$ vertices are non adjacent with the vertex u. Let $\triangle$ be the maximal degree of G. For uw not belongs to $E(G)$,

$$d(u) + d(w) \leq [d(u) + \triangle][n-1-d(u)]$$

$$d(u) + d(w) \leq (n-1)d(u) - d(u)^2 + \triangle(n-1) - \triangle d(u)$$

$$\sum [d(u) + d(w)] \leq (n-1)\sum [d(u)] - \sum d(u)^2 + \sum \triangle(n-1) - \triangle \sum d(u)$$

$$\sum [d(u) + d(w)] \leq (n-1)2e - M_1(G) + \triangle e(n-1) - 2\triangle e$$

$$\overline{M_1(G)} \leq 2e(n-1) - M_1(G) + \triangle e(n-1) - 2\triangle e.$$

$$\overline{M_1(G)} \leq e[2(n-1) + \triangle(n-1) - 2\triangle] - M_1(G)$$

For uw not belongs to $E(G)$,

$$d(u).d(w) \leq d(u)[n-1-d(u)]\triangle.$$
$$d(u).d(w) \leq \triangle(n-1)d(u) - \triangle d(u)^2$$
$$\sum d(u).d(w) \leq \triangle(n-1)\sum d(u) - \triangle \sum d(u)^2$$
$$\leq \triangle(n-1)2e - \triangle \sum d(u)^2$$
$$\leq \triangle(n-1)2e - \triangle M_1(G)$$
$$\overline{M_2(G)} \leq 2\triangle e(n-1) - \triangle M_1(G)$$

□

Theorem 2.2. *For a simple connected graph G,*

$$M_2(G) \leq 2\triangle e$$

.

Proof: For an edge $uv \in E(G)$,

$$d(u).d(v) \leq d(u)\triangle.$$

Hence

$$\sum d(u).d(v) \leq \triangle \sum d(u)$$
$$M_2(G) \leq 2\triangle e.$$

□

Theorem 2.3. *For the connected simple graph G,*

$$M_2(G) + \overline{M_2(G)} \leq \frac{n(n-1)}{2}\triangle^2.$$

Proof: For $uv \in E(G)$ and uv not belongs to $E(G)$,

$$\sum d(u).d(v) = \sum_{uv \in E(G)} d(u).d(v) + \sum_{uv \text{ not belongs to } E(G)} d(u).d(v)$$

$$M_2(G) + \overline{M_2(G)} = \sum d(u).d(v)$$

Since every vertex is adjacent or non adjacent with the remaining $n-1$ vertices with each having the maximum degree $\triangle$,

$$\sum d(u).d(v) \leq \frac{1}{2}\triangle^2 n(n-1).$$

Hence,

$$M_2(G) + \overline{M_2(G)} \leq \frac{1}{2}\triangle^2 n(n-1)$$

□

Theorem 2.4. *For the connected simple graph G,*

$$\overline{M_1(G)} + M_2(G) \leq n(n-1)\triangle.$$

Proof: For $uv \in E(G)$ and not belongs to $E(G)$,

$$\sum[d(u)+d(v)] = \sum_{uv \in E(G)} [d(u)+d(v)] + \sum_{uv \text{ not belongs to } E(G)} [d(u)+d(v)]$$

$$\sum[d(u)+d(v)] = \sum_{uv \in E(G)} [d(u)+d(v)] + \overline{M_1(G)}$$

But $d(u) + d(v) \leq d(u).d(v)$ Since every vertex is adjacent or non adjacent with the remaining $n-1$ vertices with each having the maximum degree $\triangle$,

$$\sum[d(u)+d(v)] \leq n(n-1).$$

Hence

$$\overline{M_1(G)} \leq \sum[d(u)+d(v)] - M_2(G).$$

Hence,

$$\overline{M_1(G)} + M_2(G) \leq \triangle n(n-1).$$

□

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