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# Old and New Zagreb Indices of Graphs

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**Abstract**

In this paper, some bounds for the first and second Zagreb indices of graphs are presented. A new graph invariant, named third Zagreb index, is introduced. Some mathematical properties of this new graph invariant are also presented.

## 1. Introduction

Graph theory has provided chemist with a variety of useful tools, such as topological indices. Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds.

A topological index is a graph invariant applicable in chemistry. The Wiener index is the first topological index introduced by chemist Harold Wiener.[1-3] There are some topological indices based on degrees such as the first and second Zagreb indices of molecular graphs. The first Zagreb index $M_1 = M_1(G)$ and the second Zagreb index $M_2 = M_2(G)$ of a graph G are defined as:

$$\mathrm{M}_1(G) = \sum_{e=uv\in E(G)} [\mathrm{d(u)} + \mathrm{d(v)}] , \qquad \mathrm{M}_2(G) = \sum_{e=uv\in E(G)} \mathrm{d(u)\,d(v)}$$

where d(u) denotes the degree of a vertex u in G. [4-10]

Suppose G is a simple graph. We denote minimum and maximum degree of vertices of G by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. The path $P_n$ is the shortest walk between two vertices. We denote Star, wheel, cycle and complete graph by $S_n$, $W_n$, $C_n$ and $K_n$, respectively.

The union of $G \cup H$ of graphs G and H is a graph such that $V(G \cup H) = V(G) \cup V(H)$, and $E(G \cup H) = E(G) \cup E(H)$. The Cartesian product $G \times H$ of graphs G and H is a graph such that $V(G \times H) = V(G) \times V(H)$, and any two vertices (a,b) and (u,v) are adjacent in $G \times H$ if and only if either a = u and b is adjacent with v, or b = v and a is adjacent with u. [11-14]

We now define a new graph invariant, names the third Zagreb index. This new graph invariant is denoted by $M_3 = M_3(G)$ and defined as follows:

$$M_3(G) = \sum_{e=uv \in E(G)} |d(u) - d(v)|.$$

Throughout this paper consider only simple graphs are considered. Our notation is standard and taken from as the following.

## 2. Some Bounds on the First and second Zagreb Indices

In this section, we present some new bounds for the first and second Zagreb indices of graphs and compare them with each other.

**Lemma 1.** Let G be a graph. Then $M_1(G) \leq 2M_2(G)$ with equality if and only if G is an empty graph or a complete graphs with two vertices.

**Lemma 2.** Let G be a graph with $\delta(G) \geq 2$. Then $M_1(G) \leq M_2(G)$ with equality if and only if G is isomorphic to $C_n$.

**Proof.** Suppose a and b are greater than one then $a + b \leq ab$ with equality if and only if $a = b = 2$. Thus $M_1(G) \leq M_2(G)$. □

**Lemma 3.** Suppose G is an n-vertex graph, $n \geq 3$, without isolated vertices. Then $M_1 \geq 3m$ and $M_2 \geq 2m$ with equality if and only if G is isomorphic to $P_3$.

**Proof.** Suppose $n \geq 3$ then $d(u) + d(v) \geq 3$ and $d(u)d(v) \geq 2$. By definition, $M_1 \geq 3m$ and $M_2 \geq 2m$. □

**Theorem 1.** $M_1(G) \le \Delta(G)/2 + \sqrt{\Delta^2/4 + 2M_2(G) + 4m(m-1)\Delta(G)^2}$ with equality if and only if G is $\Delta(G)$-regular.

**Proof.** By definition of the first Zagreb index, we have:

$$\begin{aligned} M_1^2 &= \sum_{e=uv\in E(G)} [d(u)^2 + d(v)^2 + 2d(u)d(v)] \\ &+ 2\sum_{e=uv,e'=xy\in E(G)} [d(u)+d(v)][d(x)+d(y)] \\ &\le \Delta(G)M_1(G) + 2M_2(G) + 4m(m-1)\Delta(G)^2. \end{aligned}$$

Thus by a simple calculation $(M_1-\Delta(G)/2)^2 \le 2M_2(G) + 4m(m-1)\Delta(G)^2 + \Delta(G)^2/4$ Therefore

$$M_1(G) \le \Delta(G)/2 + \sqrt{\Delta^2/4 + 2M_2(G) + 4m(m-1)\Delta(G)^2}.$$

Since d(u) and d(v) are less than or equal to $\Delta(G)$, one can see that $M_1(G) = \Delta(G)/2 + \sqrt{\Delta^2/4 + 2M_2(G) + 4m(m-1)\Delta(G)^2}$ if and only if G is $\Delta(G)$-regular. □

**Theorem 2.** $M_1(G) \ge \delta(G)/2 + \sqrt{\delta(G)^2/4 + 2M_2(G) + 4m(m-1)\delta(G)^2}$ with equality if and only if G is $\delta(G)$-regular.

**Theorem 3.** $M_1(G) \le \dfrac{2m^2}{n} + \left(\dfrac{\Delta(G)}{\delta(G)} + \dfrac{\delta(G)}{\Delta(G)}\right)\dfrac{m^2}{n}$.

**Proof.** Suppose $a_i = d(v_i)$ and $b_i = 1$, $1 \le i \le n$. Then by the Polya-Szego inequality[15], we have

$$\sum_{i=1}^{n} d(v_i)^2 \sum_{i=1}^{n} 1^2 \le \frac{1}{4}\left(\sqrt{\frac{\Delta(G)}{\delta(G)}} + \sqrt{\frac{\delta(G)}{\Delta(G)}}\right)^2 \left(\sum_{i=1}^{n} d(v_i)\right)^2.$$

Thus $nM_1 \le \dfrac{1}{4}\left(\sqrt{\dfrac{\Delta(G)}{\delta(G)}} + \sqrt{\dfrac{\delta(G)}{\Delta(G)}}\right)^2 (2m)^2$ and this concludes that $M_1(G) \le \dfrac{2m^2}{n} + \left(\dfrac{\Delta(G)}{\delta(G)} + \dfrac{\delta(G)}{\Delta(G)}\right)\dfrac{m^2}{n}$. □

**Theorem 3.** $M_1(G) \le \dfrac{4m^2}{n} + \dfrac{n}{4}(\Delta(G) - \delta(G))^2$.

**Proof.** Suppose $a_i = d(v_i)$ and $b_i = 1$, $1 \le i \le n$. Then by Oseki's inequality[16],

$$\sum_{i=1}^{n} d(v_i)^2 \sum_{i=1}^{n} 1^2 - \left(\sum_{i=1}^{n} d(v_i)\right)^2 \le \frac{n^2}{4}(\Delta(G)-\delta(G))^2.$$

We now apply a simple calculation to complete the theorem. □

**3. The third Zagreb index**

Suppose a and b are greater than or equal to 1. Then $a + b \ge |a - b| + 2$. Therefore, $M_1(G) \ge \sum_{e=uv\in E(G)} |d(u)-d(v)| + 2m$. We name this summation, the third Zagreb index, $M_3(G)$. In fact, $M_3(G) = \sum_{e=uv\in E(G)} |d(u) - d(v)|$. In this section, we prove some properties of the third Zagreb index.

**Example.** $M_3(S_{n+1}) = n(n-1)$, $M_3(W_{n+1}) = n(n-3)$, $M_3(C_n) = 0$, $M_3(K_n) = 0$ and $M_3(P_n) = 2$.

**Lemma 4.** $M_3(G) = 0$ if and only if G is a union of regular graphs.
**Lemma 4.** $M_3(G \cup H) = M_3(G) + M_3(H)$.

**Theorem 4.** Suppose that G is a graph without isolated vertices. Then $M_3(G) \le m(n-2)$ with equality if and only if G is isomorphic to the star graph $S_n$.

**Proof.** Since $|d(u) - d(v)| \le n - 2$, by definition of $M_3(G) \le m(n-2)$ with equality if and only if $d(u) = n - 1$ and $d(v) = 1$ if and only if G is isomorphic to the star graph $S_n$. □

**Theorem 5.** $M_3(G) \le \sqrt{m}\sqrt{(n-1)M_1(G) - 2M_2(G)}$ with equality if and only if G is isomorphic to $K_n$.

**Proof.** By definition of $M_3$ and Cauchy-Schwarz inequality,

$$\begin{aligned} M_3(G) &= \sum_{e=uv\in E(G)} |d(u) - d(v)| \\ &= \sum_{e=uv\in E(G)} 1\,|d(u) - d(v)| \\ &\le \sqrt{\sum_{e=uv\in E(G)} 1^2}\sqrt{\sum_{e=uv\in E(G)} (d(u)-d(v))^2} \\ &\le \sqrt{m}\sqrt{(n-1)M_1(G) - 2M_2(G)}, \end{aligned}$$

with equality if and only if $d(u) = d(v) = n - 1$ if and only if G is isomorphic to the complete graph $K_n$. □

**Theorem 6.** $M_3(G) \leq \sqrt{\Delta(G)M_1 - 2M_2 + m(m-1)\Delta(G)^2}$ with equality if and only if G is empty graph.

**Proof.** By definition,

$$M_3^2(G) = \sum_{e=uv\in E(G)} [d(u)^2 + d(v)^2 - 2d(u)d(v)]$$
$$+ 2\sum_{e=uv,\, e'=xy\in E(G)} |d(u) - d(v)||d(x) - d(y)|$$
$$\leq \Delta(G)\, M_1(G) - 2M_2(G) + m(m-1)\Delta(G)^2.$$

Thus $M_3 \leq \sqrt{\Delta(G)M_1 - 2M_2 + m(m-1)\Delta(G)^2}$ with equality if and only if $\Delta(G) = 0$ if and only if G is empty graph. □

**Theorem 7.** $M_3 \geq \sqrt{\delta(G)M_1(G) - 2M_2(G)}$ with equality if and only if G is regular graph.

**Theorem 8.** Suppose G and H are graphs then $M_3(G\times H) = |H|\, M_3(G) + |G|\, M_3(H)$.

**Proof.** If e = (a , x)(a , y) is an edge in E(G×H) then d((a, x)) = d(a) + d(x). Thus |d((a, x)) − d((a, y)) | = |d(x) – d(y)|. Now by definition,

$$M_3(G\times H) =$$
$$\sum_{e=(a,x)(a,y)} |d((a,x)) - d((a,y))| + \sum_{e=(x,b)(y,b)} |d((x,b)) - d((y,b))|$$
$$= \sum_{e=(a,x)(a,y)} |d(x) - d(y)| + \sum_{e=(x,b)(y,b)} |d(x) - d(y)|$$
$$= |H|\, M_3(G) + |G|\, M_3(H).$$

This completes our argument. □

**Corollary.** If $G_i$, $1 \leq i \leq k$ are graphs then

$$\frac{M_3(\prod_{i=1}^{k} G_i)}{\prod_{i=1}^{k} |V(G_i)|} = \sum_{i=1}^{k} \frac{M_3(G_i)}{|V(G_i)|}.$$

In particular, $M_3(G^k) = k|G|^{k-1}M_3(G)$.

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