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New Upper Bounds for the First Zagreb Index

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Abstract

The first Zagreb index $M_1(G)$ of a graph G is defined as the sum of squares of the degrees of the vertices. This paper presents some new upper bounds for the first Zagreb index.

1 Introduction

Let $G = (V, E)$ be a graph. The number of vertices of G we denote by n and the number of edges we denote by m, thus $|V(G)| = n$ and $|E(G)| = m$. The degree of a vertex v, denoted by $d_G(v)$.Specially, $\Delta = \Delta(G)$ and $\delta = \delta(G)$ are called the maximum and minimum degree of vertices of G respectively. G is said to be r-regular if $\delta(G) = \Delta(G) = r$ for some positive integer r.

The Zagreb indices were first introduced by Gutman [8], they are important molecular descriptors and have been closely correlated with many chemical properties [17].

The first Zagreb index is defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2$$

Recently, there was a vast research on comparing Zagreb indices [2,10,11,14], establishing various upper bounds [3,4,12,13,18,20] and relation involving graph invariants [6,15,19, 21], a survey on the first Zagreb index see [9].

In this paper, we obtain some new sharp upper bounds for $M_1(G)$.

2 Main Results

In this section, a new of upper bounds for the first Zagreb index of a graph G are presented. At this point, let us remind the lower bound for the first Zagreb index is $\frac{4m^2}{n}$, i.e., $M_1(G) \geq \frac{4m^2}{n}$ [11].

We begin with the following straightforward, previously known, auxiliary result.

Theorem 1. [1] *Suppose a_i and b_i, $1 \leq i \leq n$ are positive real numbers, then*

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \alpha(n)(A-a)(B-b) \tag{1}$$

where a, b, A and B are real constants, that for each i, $1 \leq i \leq n$, $a \leq a_i \leq A$ and $b \leq b_i \leq B$. Further, $\alpha(n) = n\lceil\frac{n}{2}\rceil\left(1 - \frac{1}{n}\lceil\frac{n}{2}\rceil\right)$.

We can see the appearance of Theorem 1, in [16].

Theorem 2. *Let G be a nontrivial graph of order n and size m. Then*

$$M_1(G) \leq \frac{\alpha(n)(\Delta-\delta)^2 + 4m^2}{n},$$

where $\alpha(n) = n\lceil\frac{n}{2}\rceil(1 - \frac{1}{n}\lceil\frac{n}{2}\rceil)$, where $\lceil x\rceil$ largest integer greater than or equal to x. Further, equality holds if and only if G is regular graph.

Proof. Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be real numbers for which there exist real constants a, b, A and B, so that for each i, $i = 1, 2, \cdots, n, a \leq a_i \leq A$ and $b \leq b_i \leq B$. Then by Theorem 1, the following inequality is valid

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \alpha(n)(A-a)(B-b) \tag{2}$$

$\alpha(n) = n\lceil\frac{n}{2}\rceil(1-\frac{1}{n}\lceil\frac{n}{2}\rceil)$, where $\lceil x\rceil$ largest integer greater than or equal to x. Equality holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.
We choose $a_i = d_G(v_i) = b_i$, $A = \Delta = B$ and $a = \delta = b$, inequality (2), becomes

$$\begin{aligned} n\sum_{i=1}^{n} d_G(v_i)^2 - \left(\sum_{i=1}^{n} d_G(v_i)\right)^2 &\leq \alpha(n)(\Delta-\delta)(\Delta-\delta) \\ nM_1(G) &\leq \alpha(n)(\Delta-\delta)^2 + 4m^2 \\ M_1(G) &\leq \frac{\alpha(n)(\Delta-\delta)^2 + 4m^2}{n} . \end{aligned}$$

Since equality in (2) holds if and only if $a_1 = a_2 = \cdots, = a_n$ and $b_1 = b_2 = \cdots, = b_n$. Therefore equality of the theorem holds if and only if G is regular graph. ■

Corollary 3. *Since,* $\alpha(n) \leq \frac{n^2}{4}$. *Therefore,* $M_1(G) \leq \dfrac{n^2(\Delta-\delta)^2 + 16m^2}{4n}$.

Theorem 4. *Let G be a nontrivial graph of order n and size m. Then*

$$M_1(G) \leq (\delta + \Delta)2m - n\delta\Delta .$$

Equality holds if and only if G is regular graph.

Proof. Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be real numbers for which there exist real constants r and R so that for each i, $i = 1, 2, \cdots, n$ holds $ra_i \leq b_i \leq Ra_i$. Then the following inequality is valid (see [5]).

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \leq (r+R)\sum_{i=1}^{n} a_i b_i . \tag{3}$$

Equality of (3) holds if and only if, for at least one i, $1 \leq i \leq n$ holds $ra_i = b_i = Ra_i$. We choose $b_i = d_G(v_i)$, $a_i = 1$, $r = \delta$ and $R = \Delta$ in inequality (2), then

$$\begin{aligned} \sum_{i=1}^{n} d_G(v_i)^2 + \delta\Delta\sum_{i=1}^{n} 1 &\leq (\delta+\Delta)\sum_{i=1}^{n} d_G(v_i) \\ M_1(G) + \delta\Delta n &\leq (\delta+\Delta)2m \\ M_1(G) &\leq (\delta+\Delta)2m - n\delta\Delta . \end{aligned}$$

if for some i holds that $ra_i = b_i = Ra_i$, then for some i also holds $b_i = r = R$. Therefore equality holds if and only if $\delta = \Delta$, i.e., for regular graphs. ■

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