Bounds on General Zagreb Indices

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Abstract: *The first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices, and the second Zagreb index $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices of the underlying molecular graph G. In this paper we give some new bounds for the first and second general Zagreb indices $M_1^{\alpha}(G)$ and $M_2^{\alpha}(G)$.*

Keywords: *General Zagreb Indices, Matching, Barycentric Subdivision.*

1. Introduction

All graphs under discussion are finite, undirected and simple. Let G=(V,E) be a simple graph with n vertices and m edges. Denote by uv the edge of G, connecting the vertices u and v. For $u \in V(G)$, N(u) denotes the set of its (first) neighbors in G. The degree of a vertex u is denoted by $d(u) = |N(u)|$. As usual $\Delta = \Delta(G)$ and $\delta = \delta(G)$ are the maximum and minimum degree of G, respectively. $P_n, K_{1,n-1}, C_n$ denotes the paths, star and cycle of n vertices.

In 1972, I.Gutman and N.Trinajsti'c [1,2] explored the study of total π - electron energy on the molecular structure and introduced two vertex degree-based graph varients. These are defined as

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

In Chemical literature M_1 and M_2 are named as first and second Zagreb indices [3]. The Zagreb indices are used by various researchers in their QSPR and QSAR studies. These indices are also viewed as a molecular structure-descriptors [4,5]. Various results on its chemical applications, mathematical properties and developments are identified and the use of Zagreb indices were reviewed and the references are cited there in [6,7].

In 2004, A.Miličević and S.Nikolić [8] constructed the first and second variable Zagreb indices and are defined by

$${}^{\alpha}M_1 = {}^{\alpha}M_1(G) = \sum_{v \in V(G)} d(v)^{2\alpha}; \quad {}^{\alpha}M_2 = {}^{\alpha}M_2(G) = \sum_{uv \in E(G)} \left[d(u)d(v)\right]^{\alpha}.$$

In 2005, X.Li and J.Zheng [9] introduced the first general Zagreb index, immediately which turns the first variable Zagreb index as a special case of it and subsequently the present authors with Gutman [10] introduced the second general Zagreb index which is same as the second variable Zagreb index and these are defined as

$$M_1^{\alpha} = M_1^{\alpha}(G) = \sum_{v \in V(G)} d(v)^{\alpha}; \quad M_2^{\alpha} = M_2^{\alpha}(G) = \sum_{uv \in E(G)} \left[d(u)d(v)\right]^{\alpha}$$

where $\alpha \in \mathbf{R}$. Various properties and relations of the first general Zagreb index are discussed in [11-14].

To the little knowledge of the authors, till date there were no results emerged regarding the Zagreb indices varying over the matching edges of the given graph. This stimulated us to establish some mathematical properties and identities for the general Zagreb indices running over the k-matching of G.

The first and second general Zagreb indices with k-matching in G are defined as

$$M_1^{\alpha}(M) = \sum_{v \in V(M)} d(v)^{\alpha}; \qquad M_2^{\alpha}(M) = \sum_{uv \in E(M)} [d(u)d(v)]^{\alpha},$$

Where $\alpha \in \mathbf{R}$. Obviously $M_1^0(M) = 2k, M_2^0(M) = k$.

2. MAIN RESULTS

Using the definition of $M_1^{\alpha}(G)$ and $M_2^{\alpha}(G)$, we reproduce that

(2.1) $$M_1^{\alpha}(G) = \sum_{u \in V(G)} \sum_{uv \in E(G)} d(v)^{\alpha-1}; \quad M_2^{\alpha}(G) = \frac{1}{2} \sum_{u \in V(G)} d(u)^{\alpha} \sum_{uv \in E(G)} d(v)^{\alpha}.$$

Theorem 2.1. For $\alpha \in [0, \infty)$ and G be a simple graph. Then

(2.2) $$M_1^{\alpha+1}(G) \geq \left(\frac{2m}{n}\right) M_1^{\alpha}(G)$$

with equality holds if and only if $\alpha = 0$ or regular.
Proof: By Chebyshev's sum inequality, we have

$$n\left(\sum_{v \in V(G)} d(v)d(v)^{\alpha}\right) \geq \left(\sum_{v \in V(G)} d(v)\right)\left(\sum_{v \in V(G)} d(v)^{\alpha}\right),$$

which completes our claim. Evidently equality holds for $\alpha = 0$ or G is regular.
In 2009, A. Ilić and D.Stevanović [15] obtained the following results:

Theorem 2.2. It holds that $M_1^2(G) \geq \frac{4m^2}{n}$. The equality is attained if and only if graph is regular.

Remark 2.3. In 1998, D.de Caen [16] have obtained the same result independently.

Theorem 2.4. For $2\alpha \geq 1$ and G be a simple graph. Then

(2.3) $$M_1^{2\alpha}(G) \geq n\left(\frac{2m}{n}\right)^{2\alpha}$$

with equality holds if and only if G is regular.

Remark 2.5. It is recognized that, equality of (2.3) holds for $\alpha = 0$. In addition, for any simple graph G, the inequality (2.3) is always true in the interval $\alpha \in \mathbf{R} \setminus \left(0, \frac{1}{2}\right)$.

Now, we give new upper bound for the first variable Zagreb index. By replacing α by $2\alpha - 1$ in Theorem (2.1), we have the following formula.

Corollary 2.6. For $\alpha \in \left[\frac{1}{2}, \infty\right)$ and G be a simple graph. Then

(2.4) $$M_1^{2\alpha}(G) \geq \left(\frac{2m}{n}\right) M_1^{2\alpha-1}(G),$$

with equality holds if and only if $\alpha = \frac{1}{2}$ or G is regular.

Remark 2.7. Inequalities (2.3) and (2.4) are incomparable except at $\alpha = \frac{1}{2}, 1$. For $\alpha \in \left(\frac{1}{2}, 1\right)$, (2.3) is finer than (2.4) For $\alpha > 1$, (2.4) is finer than (2.3).

Theorem 2.8. Let G be a simple graph with n>2 vertices. Then

(2.5) $$M_2^{\alpha}(G) \geq M_1^{\alpha+1}(G) - m$$

with equality holds if and only if G is a P_3.

Proof: It is clear that for $d(u)^{\alpha}, d(v)^{\alpha} \geq 1$ and for any edge $uv \in E(G)$,

$$d(u)^{\alpha} d(v)^{\alpha} \geq d(u)^{\alpha} + d(v)^{\alpha} - 1$$

$$\sum_{uv \in E(G)} d(u)^{\alpha} d(v)^{\alpha} \geq \sum_{uv \in E(G)} \left[d(u)^{\alpha} + d(v)^{\alpha} - 1 \right] = \sum_{v \in V(G)} d(v)^{\alpha+1} - m,$$

Which completes our claim.

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