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Bounds on Vertex Zagreb Indices of Graphs

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Keywords: *degree, zagreb index, topological index.*

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BOUNDSONVERTEXZAGREBINDICESOFGRAPHS

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Bounds on Vertex Zagreb Indices of Graphs

K. Pattabiraman [α] & M. Seenivasan [σ]

Abstract- The vertex version of first and second Zagreb indices were introduced by Tavakoli et al. [2] are defined as $\overline{M}_1^*(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u)+d_G(v)$ and $\overline{M}_2^*(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u)d_G(v)$. In this paper, we obtained the relation between the first and second vertex Zagreb indices of graphs using some well-known results.

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I. Introduction

A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix which represents the whole graph, and these representations are aimed to be uniquely defined for that graph. A topological index is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. There are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. Among these classes degree based topological indices are y and particularly in chemistry. In more precise way, a topological index $Top(G)$ of a graph G, is a number with the property that for every graph H isomorphic to G, $Top(G) = Top(H)$. The topological indices are graph invariants which has been used for examine quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) extensively in which the biological activity or other properties of molecules are correlated with their chemical structures, see [4].

For a (molecular) graph G, The *first Zagreb index* $M_1(G)$ is the equal to the sum of the squares of the degrees of the vertices, and the *second Zagreb index* $M_2(G)$ is the equal to the sum of the products of the degrees of pairs of adjacent vertices, that is, $M_1(G) = \sum_{u\in V(G)} d_G^2(u) = \sum_{uv\in E(G)} (d_G(u) + d_G(v))$, $M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)$, where $d_G(v)$ is a degree of a vertex v in G. There are various study of different versions of Zagreb indices. One of the modified versions of classical Zagreb indices, the vertex version of first and second Zagreb indices were introduced by Tavakoli et al. [2] are defined as $\overline{M}_1^*(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))$ and $\overline{M}_2^*(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u)d_G(v)$.

Another topological index, defined as sum of cubes of degrees of all the vertices was also introduced in the same paper, where the first and second Zagreb indices were introduced [14]. Furtula and Gutman in [13] recently investigated this index and named this index as *forgotten topological index* (or) F-index and showed that the predictive ability of this index is almost similar to that of first Zagreb index and for the entropy and acetic factor, both of them yield correlation coefficients greater than 0.95. The F-index of a graph G is defined as $F = F(G) = \sum_{u\in V(G)} d_G^3(u) = \sum_{uv\in E(G)} (d_G^2(u) + d_G^2(v))$.

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For the survey on theory and application of Zagreb indices, see [11]. Feng et al.[10] have given a sharp bounds for the Zagreb indices of graphs with a given matching number. Khalifeh et al. [3] have obtained the Zagreb indices of the Cartesian product, composition, join, disjunction and symmetric difference of graphs. Ashrafi et al. [9] determined the extremal values of Zagreb coindices over some special class of graphs. Hua and Zhang [12] have given some relations between Zagreb coindices and some other topolodical indices. In [2], the vertex version of Zagreb indices for the generalized hierarchical product of two connected graphs are computed. The vertex Zagreb indices of different types of operations of graphs are computed by De [1]. In this sequence, we have obtained the relation between the first and second vertex Zagreb indices of graphs.

II. Main Results

In this section, we present the relation between the first and second vertex Zagreb indices of graph. The *inverse degree* of a graph G is the sum of reciprocal of the vertex degrees, that is, $ID(G) = \sum_{u\in V(G)} \frac{1}{d_G(u)}$.

Lemma 2.1. *[15]Let $\overrightarrow{x} = (x_1, x_2, \ldots, x_N)$ and $\overrightarrow{y} = (y_1, y_2, \ldots, y_N)$ be sequences of real numbers $\overrightarrow{z} = (z_1, z_2, \ldots, z_N)$ and $\overrightarrow{w} = (w_1, w_2, \ldots, w_N)$ be nonnegative sequences, then*

$$\sum_{i=1}^{N} w_i \sum_{i=1}^{N} z_i x_i^2 + \sum_{i=1}^{N} z_i \sum_{i=1}^{N} w_i y_i^2 \geq 2 \sum_{i=1}^{N} z_i x_i \sum_{i=1}^{N} w_i y_i. \tag{2.1}$$

In particular, if z_i and w_i are positive, then the equality holds in (2.1) if and only if $\overrightarrow{x} = \overrightarrow{y} = \overrightarrow{k}$, where $\overrightarrow{k} = (k, k, \ldots, k)$ is a constant sequence. ■

Theorem 2.2. *Let G be a connected graph with n vertices and m edges. Then*

$$2\overline{M}_1^*(G)\overline{M}_2^*(G) \leq (n-1)ID(G) + \frac{(n-1)\delta\Delta}{\delta+\Delta} + \frac{(n-1)(n-2)\Delta}{4} + 2mM_1(G) - F(G) \tag{2.2}$$

with equality if and only if G is regular.

Proof. Note that each i in Lemma 2.1 corresponds a vertex pair $\{u_i, u_j\}$ such that $N = \frac{n(n-1)}{2}$. setting $z_i = w_i = \frac{1}{x_i y_i}$ and each x_i is replaced by $\frac{1}{d_G(u_i)d_G(u_j)}$ and each y_i is replaced by $\frac{1}{d_G(u_i)+d_G(u_j)}$, then we obtain

$$\sum_{\{u_i,u_j\}\subseteq V(G)} d_G(u_i)d_G(u_j)\big(d_G(u_i)+d_G(u_j)\big) \sum_{\{u_i,u_j\}\subseteq V(G)} \left(\frac{d_G(u_i)+d_G(u_j)}{d_G(u_i)d_G(u_j)} + \frac{d_G(u_i)d_G(u_j)}{d_G(u_i)+d_G(u_j)}\right)$$
$$\geq 2 \sum_{\{u_i,u_j\}\subseteq V(G)} \big(d_G(u_i)+d_G(u_j)\big) \sum_{\{u_i,u_j\}\subseteq V(G)} d_G(u_i)d_G(u_j). \tag{2.3}$$

One can observe that $\frac{2}{\Delta} \leq \frac{1}{d_G(u_i)} + \frac{1}{d_G(u_j)} \leq \frac{2}{\delta}$, it immediately follows that $\frac{d_G(u_i)d_G(u_j)}{d_G(u_i)+d_G(u_j)} \leq \frac{\Delta}{2}$. Also $\frac{1}{\delta} + \frac{1}{\Delta} \leq \frac{1}{d_G(u_i)} + \frac{1}{\delta}$, we have $\frac{d_G(u_i)\delta}{d_G(u_i)+\delta} \leq \frac{\delta\Delta}{\delta+\Delta}$. Let v_k be the minimum degree vertex in G. Then

$$\sum_{\{u_i,u_j\}\subseteq V(G)} \left(\frac{d_G(u_i)+d_G(u_j)}{d_G(u_i)d_G(u_j)} + \frac{d_G(u_i)d_G(u_j)}{d_G(u_i)+d_G(u_j)}\right) = \sum_{\{u_i,u_j\}\subseteq V(G)} \frac{d_G(u_i)+d_G(u_j)}{d_G(u_i)d_G(u_j)} + \sum_{\{u_i,u_j\}\subseteq V(G)} \frac{d_G(u_i)d_G(u_j)}{d_G(u_i)+d_G(u_j)}$$
$$= \sum_{\{u_i,u_j\}\subseteq V(G)} \left(\frac{1}{d_G(u_i)} + \frac{1}{d_G(u_j)}\right) + \sum_{\{u_i,u_k\}\subseteq V(G)} \frac{d_G(u_i)\delta}{d_G(u_i)+\delta}$$

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10. L. Feng, A. Ilic, Zagreb, Harary and hyper- Wiener indices of graphs with a given matching number, Appl. Math. Lett. 23 (2010) 943948.

$$+\sum_{\substack{\{u_i,u_j\}\subseteq V(G)\\ u_j\neq u_k}}\frac{d_G(u_i)d_G(u_j)}{d_G(u_i)+d_G(u_j)}$$

$$\leq \sum_{u_i\in V(G)}^{n}\frac{n-1}{d_G(u_i)}+\frac{(n-1)\delta\Delta}{\delta+\Delta}+\Big(\frac{n(n-1)}{2}-(n-1)\Big)\frac{\Delta}{2}$$

$$= (n-1)ID(G)+\frac{(n-1)\delta\Delta}{\delta+\Delta}+\frac{(n-1)(n-2)\Delta}{4}, \quad (2.4)$$

where $ID(G)$ is the inverse degree index of G.

Since $\sum_{u_i\in V(G)} d_G(u_i)=2m,$ then we have

$$\sum_{\{u_i,u_j\}\subseteq V(G)} d_G(u_i)d_G(u_j)\big(d_G(u_i)+d_G(u_j)\big) \leq \sum_{u_i\in V(G)} d_G(u_i)^2\big(2m-d_G(u_i)\big).$$

From the definitions of first Zagreb index and F-index of G, we obtain

$$\sum_{\{u_i,u_j\}\subseteq V(G)} d_G(u_i)d_G(u_j)\big(d_G(u_i)+d_G(u_j)\big) \leq 2mM_1(G)-F(G). \quad (2.5)$$

Using (2.4) and (2.5) in (2.3), we obtain the required result in (2.2).

By Lemma 2.1, the equality in (2.2) holds if $\frac{1}{d_G(u_i)d_G(u_j)}=\frac{1}{d_G(u_i)d_G(u_k)}=\frac{1}{d_G(u_i)+d_G(u_j)}+\frac{1}{d_G(u_i)+d_G(u_k)}$ for any three vertices u_i, u_j and u_k in G. This implies G is regular. ■

Proposition 2.3. Let p be the number of pendent vertices in G. Then $F(G)\geq \delta M_1(G)+p(1-\delta)$.

Proof. Since p is the number of pendent vertices in G,

$$F(G)=\sum_{u_i\in V(G)} d_G(u_i)^3 = p+\sum_{\substack{u_i\in V(G)\\ d_G(u_i)\neq 1}} d_G(u_i)^3 \geq p+\delta\sum_{\substack{u_i\in V(G)\\ d_G(u_i)\neq 1}} d_G(u_i)^2$$

$$= p+\delta(M_1(G)-p).$$

■

Using Proposition 2.3 in Theorem 2.2, we obtain the following corollary.

Corollary 2.4. Let G be a connected graph with n vertices and m edges. If p is the number of pendent vertices in G, then

$$2\overline{M}_1^*(G)\overline{M}_2^*(G)\leq (n-1)ID(G)+\frac{(n-1)\delta\Delta}{\delta+\Delta}+\frac{(n-1)(n-2)\Delta}{4}+(2m-\delta)M_1(G)+p(\delta-1)$$

with equality if and only if G is regular. ■

Lemma 2.5.(Radon's inequality) For real numbers $p>0, a_1.a_2,\ldots,a_N\geq 0$ and $b_1,b_2,\ldots,b_N>0$, the following inequality holds:

$$\sum_{i=1}^{N}\frac{a_i^{p+1}}{b_i^{p}}\geq \frac{\Big(\sum_{i=1}^{N}a_i\Big)^{p+1}}{\Big(\sum_{i=1}^{N}b_i\Big)^{p}}.$$

■

Next we obtain the another relation between the first and second vertex Zagreb indices of graphs.

Theorem 2.6. *Let* G *be a connected graph with* n *vertices and* m *edges. Then* $\frac{\left(M_1(G)\right)^2}{M_2(G)} \leq \frac{n(n-1)(\delta+\Delta)^2}{2\delta\Delta}$ *with equality if and only if* G *is regular.*

Proof. For each i in Lemma 2.5 corresponds a vertex (u_i, u_j) with $N = \frac{n(n-1)}{2}$ and $p = 1$, setting each $a_i = d_G(u_i) + d_G(u_i)$ and $b_i = d_G(u_i)d_G(u_i)$, it follows that

$$\sum_{(u_i,u_j)\subseteq V(G)} \frac{\left(d_G(u_i) + d_G(u_i)\right)^2}{d_G(u_i)d_G(u_i)} \geq \frac{\left(\sum_{(u_i,u_j)\subseteq V(G)} d_G(u_i) + d_G(u_i)\right)^2}{\sum_{(u_i,u_j)\subseteq V(G)} d_G(u_i)d_G(u_i)}. \tag{2.6}$$

The equation (2.6) is equivalent to

$$\sum_{(u_i,u_j)\subseteq V(G)} \left(\sqrt{\frac{d_G(u_i)}{d_G(u_j)}} + \sqrt{\frac{d_G(u_j)}{d_G(u_i)}}\right)^2 \geq \frac{\left(\overline{M}_1^*(G)\right)^2}{\overline{M}_2^*(G)}.$$

It has been proved in [15] that

$$\left(\sqrt{\frac{d_G(u_i)}{d_G(u_j)}} + \sqrt{\frac{d_G(u_j)}{d_G(u_i)}}\right)^2 \leq \frac{(\delta+\Delta)^2}{\delta\Delta}.$$

Hence

$$\frac{\left(M_1(G)\right)^2}{M_2(G)} \leq \sum_{(u_i,u_j)\subseteq V(G)} \frac{(\delta+\Delta)^2}{\delta\Delta} = \frac{n(n-1)(\delta+\Delta)^2}{2\delta\Delta}. \tag{2.7}$$

Equality in (2.7) holds if and only if G is regular. ■

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Notes

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