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THE SHARP BOUNDS OF ZAGREB INDICES ON CONNECTED GRAPHS

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Abstract. The analysis of a structure is based on its configuration. The common means available for this purpose is the use of graph products. The rooted product is specially revelent for trees. Chemical application of graph theory predicts different properties like physico-chemical properties, thermodynamics properties, chemical activity, biological activity, etc. Certain graph invariants known as topological indices are used for characterization of these properties. These indices have a promising role in chemical sciences and QSAR/QSPR studies. In this paper the lower and upper bounds of Zagreb indices, multiple Zagreb indices and F-index for rooted product of F-sum on connected graphs are determined.

1. Introduction

The use of structure descriptors is a standard procedure in the study of structure-property relations. To correlate and predict physical, chemical and biological activity (property) from molecular structure is a very important problem in theoretical and computational chemistry [14]. The topological index characterizes the topology of the graph numerically. It is a popular quantifiers of the molecular structures because it is obtained directly from molecular structures and rapidly computed for large number of molecules. Its use was started by the chemist, Wiener in 1947, during study of relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds [15]. Its role in the development of the chemical sciences is worth saying.

In the whole paper, G is a simple, connected and finite graph with vertex set $V(G) = \{u_1, u_2, u_3, \ldots, u_n\}$ and edge set $E(G) = \{e_1, e_2, e_3, \ldots, e_m\}$, where m, n are size and order of G, respectively. An edge with end vertices u_i and u_j is denoted by $u_i u_j$. The number of vertices adjacent to u in G is called *degree* of u in G and is denoted by $deg_G(u)$. δ_G and Δ_G are notations denoting *minimum*, *maximum* degrees of graph G, respectively. P_n and C_n are notations for path and cycle with order n, respectively.

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The first degree-based structure descriptors [10, 11] known as first and second Zagreb indices have been used to study molecular complexity, chirality, ZE-isomorphism and hetero-systems, that are defined as:

$$M_1(G) = \sum_{v \in V(G)} [deg_G(v)]^2 = \sum_{uv \in E(G)} [deg_G(u) + deg_G(v)]$$

$$M_2(G) = \sum_{uv \in E(G)} deg_g(u) deg_G(v)$$

These indices have been used as branching indices [3] and found applications in QSPR and QSAR studies [12, 16].

The augmented Zagreb index is a valuable predictive index in the study of the heat of formation in octanes and heptanes proposed by Furtula et al. in 2010 [5] that is defined as:

$$AZI(G) = \sum_{uv \in E(G)} \left[\frac{deg_G(u) deg_G(v)}{deg_G(u) + deg_G(v) - 2}\right]^3$$

Replacing the exponent 3 with -0.5, we get the ordinary ABC index. Preliminary studies [5] indicate that AZI has an even better correlation potential than ABC index.

The first and second multiple Zagreb indices, introduced by Ghorbani and Azimi in 2012 [7], are defined as:

$$PM_1(G) = \prod_{uv \in V(G)} [deg_G(u) + deg_G(v)] = \prod_{v \in V(G)} [deg_G(v)]^2$$

$$PM_2(G) = \prod_{uv \in V(G)} deg_G(u) deg_G(v)$$

The third Zagreb index, introduced by Shirdel in 2013 [13], is defined as:

$$M_3(G) = \sum_{uv \in E(G)} [deg_G(u) + deg_G(v)]^2$$

Furtula and Gutman showed that the term, $\sum_{v \in V(G)} [deg_G(v)]^3$, have a very promising application potential [6]. They named it the forgotten topological index or shortly the F-index that is defined as:

$$F(G) = \sum_{v \in V(G)} [deg_G(v)]^3 = \sum_{uv \in E(G)} [\{deg_G(u)\}^2 + \{deg_G(v)\}^2]$$

It is notable that,

$$F(G) = M_3(G) - 2M_2(G.$$

The linear combination $M_1 + \lambda F$ yields a highly accurate mathematical model of certain physico-chemical properties of alkanes [6].

Given a graph G of order n and a graph H with root vertex v, the rooted product $G \circ H$ is defined as the graph obtained from G and H by taking one copy of G and n copies of H and identifying the vertex u_i of G with the vertex v in the ith copy of H for every $1 \leqslant i \leqslant n$ [8]. It is clear that the value of every parameter of the rooted product graph depends on the root of the graph H. The rooted product is especially relevant for trees, as the rooted product of two trees is another tree. For instance, Koh et al. [9] used rooted products to find graceful numberings for a wide family of trees.

Here are some useful properties of rooted product of graphs.

LEMMA 1. *Let G_1 and G_2 be graphs of order n_1 and n_2 and size m_1 and m_2, respectively. Then we have:*

(a) $|V(G_1 \circ G_2)| = |V(G_1)| \times |V(G_2)|$ *and* $|E(G_1 \circ G_2)| = |V(G_1)|\ |E(G_2)| + |E(G_1)|$.

(b) $deg_{G_1 \circ G_2}(u,v) \leqslant deg_{G_1}(u) + deg_{G_2}(v)$, *equality holds, v being a root vertex.*

(c) *The rooted product is associative but not commutative.*

(d) *The rooted product of connected nontrivial graphs is connected.*

Four related graphs $S(G)$, $R(G)$, $Q(G)$, $T(G)$ of a connected and finite graph G are defined as follows:

- The graph $S(G)$, is known as subdivision graph of G and is obtained by inserting an additional vertex in each edge of G.
- The graph $R(G)$, is the graph obtained by adding a new vertex corresponding to each edge of G, then joining each new vertex to the end vertices of the corresponding edge.
- The graph $Q(G)$, is the graph obtained by inserting a new vertex into each edge of G, then joining edges those pairs of new vertices on adjacent edges of G.
- The graph $T(G)$, known as total graph of G, has as its vertices, the edges and vertices of G. Adjacency in $T(G)$ is defined as adjacency or incidence for the corresponding elements of G.

The four operations $S(G)$, $R(G)$, $Q(G)$, $T(G)$ on a graph G are illustrated in Figure 1.

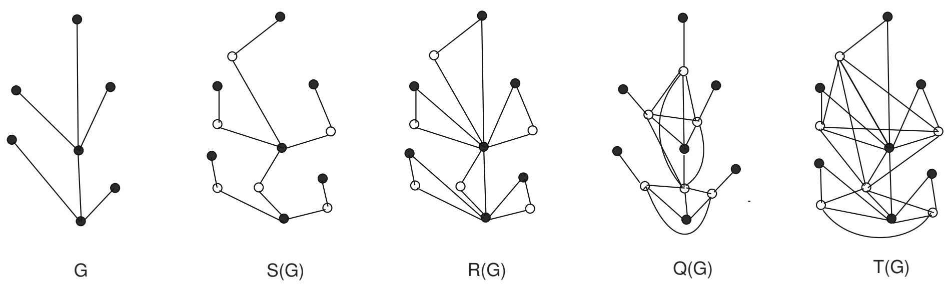

Figure 1: *The graphs G, $S(G)$, $R(G)$, $Q(G)$ and $T(G)$*

Eliasi and Taeri [4] introduced four new operations that are based on $S(G)$, $R(G)$, $Q(G)$, $T(G)$, as follows:

Let F be one of the symbols S, R, Q, T. The F-sum, denoted by $G+_F H$ of graphs G and H, is a graph with the set of vertices $V(G+_F H) = (V(G)\bigcup E(G)) \times V(H))$ and $(u_1,v_1)(u_2,v_2) \in E(G+_F H)$, if and only if $[u_1 = u_2 \in V(G)$ and $v_1v_2 \in E(H)]$ or $[v_1 = v_2 \in V(H)$ and $u_1u_2 \in E(F(G))]$. $G+_F H$ consists of n_2 copies of the graph $F(G)$, and we label these copies by vertices of H. The vertices in each copy have two types, the vertices in $V(G)$ (black vertices) and the vertices in $E(G)$ (white vertices). Now we join only black vertices with the same name in $F(G)$ in which their corresponding labels are adjacent in H. The graphs $C_4+_S P_2$, $C_4+_R P_2$, $C_4+_Q P_2$ and $C_4+_T P_2$ are shown in Figure 2.

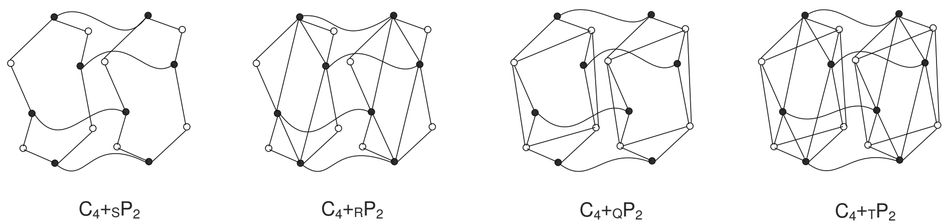

Figure 2: *The graphs $C_4+_S P_2$, $C_4+_R P_2$, $C_4+_Q P_2$ and $C_4+_T P_2$*

Eliasi and Taeri [4] computed the expression for the Wiener index of four graph operations which are based on these graphs $S(G)$, $R(G)$, $Q(G)$, and $T(G)$, in terms of $W(F(G))$ and $W(H)$. Deng et al. [2] computed the first and second Zagreb indices for the graph operations $S(G)$, $R(G)$, $Q(G)$, and $T(G)$. Akhter and Imran computed bounds for the general sum-connectivity index of F-sums of the graphs [1]. We extend their work by applying graph operations on these F-sums.

Computational complexities can be minimized by expressing the formulas for product of F-sum on graphs, in terms of their factor graphs. So, we presented bounds for the first Zagreb index, the second Zagreb index, the third Zagreb index, the augmented Zagreb index, F-index, the first multiple Zagreb index and the second multiple Zagreb index for rooted product on F-sums of graphs in form of their factor graphs.

2. Main results and discussions

In this section we study bounds for the first Zagreb, the second Zagreb, the third Zagreb, the augmented Zagreb, the first multiple Zagreb and the second multiple Zagreb indices of rooted product of F-sum of graphs in terms of their factor graphs. Bounds for F-index are also discussed. Let G_1, G_2, H_1, H_2 be simple, connected graphs such that $|V(G_1)| = n_1$, $|V(G_2)| = n_2$, $|V(H_1)| = \acute{n}_1$, $|V(H_2)| = \acute{n}_2$, $|E(G_1)| = m_1$, $|E(G_2)| = m_2$, $|E(H_1)| = \acute{m}_1$ and $|E(H_2)| = \acute{m}_2$.

In the following lemma we compute size of F-sum on graphs for F=S, in terms of factor graphs.

LEMMA 2. *If* $G = H_1 +_S G_1$ *then size of* G *is* $m_1\acute{n}_1 + 2n_1\acute{m}_1$, *where* $|V(G_1)| = n_1$, $|V(H_1)| = \acute{n}_1$, $|E(G_1)| = m_1$ *and* $|E(H_1)| = \acute{m}_1$.

Proof. We know that $S(H_1)$ is a subdivision of H_1, therefor size of $S(H_1)$ is $2|E(H_1)| = 2\acute{m}_1$.

Hence $|E(G)| = V(H_1)E(G_1) + V(G_1)2E(H_1) = m_1\acute{n}_1 + 2n_1\acute{m}_1$ □

In the following theorem the lower and upper bounds for the first Zagreb, the second Zagreb, the third Zagreb, the augmented Zagreb, the first multiple Zagreb and the second multiple Zagreb indices of rooted product of F-sum on graphs in terms of their factor graphs for F=S are determined.

THEOREM 1. *Let* $G = H_1 +_S G_1$ *and* $H = H_2 +_S G_2$ *then,*

(a). $2\alpha(\delta_G + \delta_H) \leqslant M_1(G \circ H) \leqslant 2\alpha(\Delta_G + \Delta_H)$

(b). $\alpha(\delta_G + \delta_H)^2 \leqslant M_2(G \circ H) \leqslant \alpha(\Delta_G + \Delta_H)$

(c). $4\alpha(\delta_G + \delta_H)^2 \leqslant M_3(G \circ H) \leqslant 4\alpha(\Delta_G + \Delta_H)^2$

(d). $\frac{1}{8}\alpha[\frac{(\delta_G+\delta_H)^2}{\Delta_G+\Delta_H-1}]^3 \leqslant AZI(G \circ H) \leqslant \frac{1}{8}\alpha[\frac{(\Delta_G+\Delta_H)^2}{\delta_G+\delta_H-1}]^3$

(e). $[2(\delta_G + \delta_H)]^\alpha \leqslant PM_1(G \circ H) \leqslant [2(\Delta_G + \Delta_H)]^\alpha$

(f). $(\delta_G + \delta_H)^{2\alpha} \leqslant PM_2(G \circ H) \leqslant (\Delta_G + \Delta_H)^{2\alpha}$,

where $\Delta_G = \Delta_{G_1} + \Delta_{H_1}$, $\Delta_H = \Delta_{G_2} + \Delta_{H_2}$, $\delta_G = \delta_{G_1} + \delta_{H_1}$, $\delta_H = \delta_{G_2} + \delta_{H_2}$ *and*

$$\alpha = n_1(\acute{n}_1 + \acute{m}_1)(m_2\acute{n}_2 + 2n_2\acute{m}_2) + (m_1\acute{n}_1 + 2n_1\acute{m}_1)$$

throughout the theorem.

Proof. Let G and H be the graphs with vertex sets $\{u_1, u_2, \ldots, u_{n_1(\acute{n}_1+\acute{m}_1)}\}$ and $\{v_1, v_2, \ldots, v_{n_2(\acute{n}_2+\acute{m}_2)}\}$ respectively. Then by definition,

$$\begin{aligned} M_1(G \circ H) &= \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H)} [deg_{G\circ H}(u_i,v_j) + deg_{G\circ H}(u_k,v_l)] \\ &= \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H), i\neq k} [deg_{G\circ H}(u_i,v_j) + deg_{G\circ H}(u_k,v_l)] \\ &\quad + \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H), j\neq l} [deg_{G\circ H}(u_i,v_j) + deg_{G\circ H}(u_k,v_l)] \end{aligned}$$

$$\begin{aligned} M_1(G \circ H) = &\sum_{u_i\in V(G)} \sum_{v_jv_l\in E(H)} [deg_{G\circ H}(u_i,v_j) + deg_{G\circ H}(u_i,v_l)] \\ &+ \sum_{v_j\in V(H)} \sum_{u_iu_k\in E(G)} [deg_{G\circ H}(u_i,v_j) + deg_{G\circ H}(u_k,v_j)]. \end{aligned} \tag{1}$$

Using Lemma 1, part (b), we get

$$deg_{G\circ H}(u_i,v_j) + deg_{G\circ H}(u_k,v_l) \leqslant deg_G(u_i) + deg_H(v_j) + deg_G(u_k) + deg_H(v_l)$$

Since, for a graph G, for all $u \in V(G)$, $deg_G(u) \leqslant \Delta_G$, and $deg_G(u) \geqslant \delta_G$, Therefore, using these facts, we have

$$deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_l) \leqslant 2(\Delta_G+\Delta_H). \tag{2}$$

Using inequality (2) in equation (1), we have

$$\begin{aligned}
M_1(G\circ H) &= \sum_{u_i\in V(G)}\sum_{v_jv_l\in E(H)}[deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_l)]\\
&\quad+\sum_{v_j\in V(H)}\sum_{u_iu_k\in E(G)}[deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_l)]\\
&\leqslant 2(|V(G)|\;|E(H)|+|E(G)|)(\Delta_G+\Delta_H)\\
&= 2[n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)\\
&\quad+(m_1\acute{n}_1+2n_1\acute{m}_1)][\Delta_{G_1}+\Delta_{H_1}+\Delta_{G_2}+\Delta_{H_2}]
\end{aligned}$$

as

$$|V(G)|=n_1(\acute{n}_1+\acute{m}_1), |V(H)|=n_2(\acute{n}_2+\acute{m}_2)$$

$$|E(G)|=m_1\acute{n}_1+2n_1\acute{m}_1, |E(H)|=m_2\acute{n}_2+2n_2\acute{m}_2$$

$$\Delta_G=\Delta_{G_1}+\Delta_{H_1}, \Delta_H=\Delta_{G_2}+\Delta_{H_2}$$

Putting

$$\alpha=n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+(m_1\acute{n}_1+2n_1\acute{m}_1)$$

we get

$$M_1(G\circ H) \leqslant 2\alpha(\Delta_G+\Delta_H). \tag{3}$$

Using similar arguments with $deg_G(u) \geqslant \delta_G$, we have

$$M_1(G\circ H) \geqslant 2[n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+(m_1\acute{n}_1+2n_1\acute{m}_1)][\delta_{G_1}+\delta_{H_1}]$$

$$M_1(G\circ H) \geqslant 2\alpha(\delta_G+\delta_H). \tag{4}$$

Hence from inequalities 3 and 4, part (a) of the theorem is proved.

$$\begin{aligned}
M_2(G\circ H) &= \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H)}[deg_{G\circ H}(u_i,v_j)\; deg_{G\circ H}(u_k,v_l)]\\
&= \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H), i\neq k}[deg_{G\circ H}(u_i,v_j)\; deg_{G\circ H}(u_k,v_l)]\\
&\quad+\sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H), j\neq l}[deg_{G\circ H}(u_i,v_j)\; deg_{G\circ H}(u_k,v_l)]
\end{aligned}$$

$$\begin{aligned}
M_2(G\circ H) &= \sum_{u_i\in V(G)}\sum_{v_jv_l\in E(H)}[deg_{G\circ H}(u_i,v_j)\; deg_{G\circ H}(u_i,v_l)]\\
&\quad+\sum_{v_j\in V(H)}\sum_{u_iu_k\in E(G)}[deg_{G\circ H}(u_i,v_j)\; deg_{G\circ H}(u_k,v_j)].
\end{aligned} \tag{5}$$

Using Lemma 1, part (b), we get

$$deg_{G\circ H}(u_i,v_j)\; deg_{G\circ H}(u_k,v_l) \leqslant (deg_G(u_i)+deg_H(v_j))(deg_G(u_k)+deg_H(v_l))$$

Since, for a graph G, for all $u \in V(G), deg_G(u) \leqslant \Delta_G$, and $deg_G(u) \geqslant \delta_G$, Therefore, using these facts, we have

$$deg_{G\circ H}(u_i,v_j)\ deg_{G\circ H}(u_k,v_l) \leqslant (\Delta_G+\Delta_H)^2. \tag{6}$$

Using inequality (6) in equation (5), we have

$$\begin{aligned}
M_2(G\circ H) &= \sum_{u_i\in V(G)} \sum_{v_jv_l\in E(H)} [deg_{G\circ H}(u_i,v_j)\ deg_{G\circ H}(u_i,v_l)] \\
&\quad + \sum_{v_j\in V(H)} \sum_{u_iu_k\in E(G)} [deg_{G\circ H}(u_i,v_j)\ deg_{G\circ H}(u_k,v_j)] \\
&\leqslant (|V(G)|\ |E(H)|+|E(G)|)(\Delta_G+\Delta_H)^2 \\
&= [n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+m_1\acute{n}_1+2n_1\acute{m}_1][\Delta_{G_1}+\Delta_{H_1}+\Delta_{G_2}+\Delta_{H_2}]^2
\end{aligned}$$

as

$$|V(G)| = n_1(\acute{n}_1+\acute{m}_1), |V(H)| = n_2(\acute{n}_2+\acute{m}_2)$$

$$|E(G)| = m_1\acute{n}_1+2n_1\acute{m}_1, |E(H)| = m_2\acute{n}_2+2n_2\acute{m}_2$$

$$\Delta_G = \Delta_{G_1}+\Delta_{H_1}, \Delta_H = \Delta_{G_2}+\Delta_{H_2}$$

Substituting

$$n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)m_1\acute{n}_1+2n_1\acute{m}_1 = \alpha$$

we have,

$$M_2(G\circ H) \leqslant \alpha(\Delta_G+\Delta_H)^2. \tag{7}$$

Using similar arguments with $deg_G(u) \geqslant \delta_G$, we have

$$M_2(G\circ H) \geqslant [n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+m_1\acute{n}_1+2n_1\acute{m}_1][\delta_{G_1}+\delta_{H_1}+\delta_{G_2}+\delta_{H_2}]^2$$

$$M_2(G\circ H) \geqslant \alpha(\delta_G+\delta_H)^2. \tag{8}$$

Hence from inequalities 7 and 8, part (b) of the theorem is proved.

$$\begin{aligned}
M_3(G\circ H) &= \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H)} [deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_l)]^2 \\
&= \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H), i\neq k} [deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_i,v_l)]^2 \\
&\quad + \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H), j\neq l} [deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_i,v_l)]^2
\end{aligned}$$

$$\begin{aligned}
M_3(G\circ H) = &\sum_{u_i\in V(G)} \sum_{v_jv_l\in E(H)} [deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_i,v_l)]^2 \\
&+ \sum_{v_j\in V(H)} \sum_{u_iu_k\in E(G)} [deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_j)]^2
\end{aligned} \tag{9}$$

Using Lemma 1, part (b), we get

$$[deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_l)]^2 \leqslant [deg_G(u_i)+deg_H(v_j)+deg_G(u_k)+deg_H(v_l)]^2$$

Again using the facts that for a graph G, for all $u \in V(G)$, $deg_G(u) \leqslant \Delta_G$, and $deg_G(u) \geqslant \delta_G$, we have

$$[deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_l)]^2 \leqslant 4(\Delta_G+\Delta_H)^2. \tag{10}$$

Using inequality (10) in equation (9) and adopting the same procedure as in part (a) of this theorem,

$$M_3(G\circ H) \leqslant 4[n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+m_1\acute{n}_1+2n_1\acute{m}_1][(\Delta_{G_1}+\Delta_{H_1}+\Delta_{G_2}+\Delta_{H_2}]^2$$

$$M_3(G\circ H) \leqslant 4\alpha(\Delta_G+\Delta_H)^2. \tag{11}$$

and

$$M_3(G\circ H) \geqslant 4[n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+m_1\acute{n}_1+2n_1\acute{m}_1][\delta_{G_1}+\delta_{H_1}+\delta_{G_2}+\delta_{H_2}]^2$$

$$M_3(G\circ H) \geqslant 4\alpha(\delta_G+\delta_H)^2. \tag{12}$$

Inequalities (11) and (12) complete the proof of part (c) of the theorem.

$$\begin{aligned} AZI(G\circ H) &= \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H)} \left[\frac{deg_{G\circ H}(u_i,v_j)deg_{G\circ H}(u_i,v_l)}{deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_i,v_l)-2}\right]^3 \\ &= \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H), i\neq k} \left[\frac{deg_{G\circ H}(u_i,v_j)deg_{G\circ H}(u_i,v_l)}{deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_i,v_l)-2}\right]^3 \\ &+ \sum_{(u_i,v_j)(u_k,v_l)\in E(G\circ H), j\neq l} \left[\frac{deg_{G\circ H}(u_i,v_j)\, deg_{G\circ H}(u_k,v_l)}{deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_l)-2}\right]^3 \end{aligned}$$

$$\begin{aligned} AZI(G\circ H) = &\sum_{u_i\in V(G)}\sum_{v_jv_l\in E(H)} \left[\frac{deg_{G\circ H}(u_i,v_j)deg_{G\circ H}(u_i,v_l)}{deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_i,v_l)-2}\right]^3 \\ &+\sum_{v_j\in V(H)}\sum_{u_iu_k\in E(G)} \left[\frac{deg_{G\circ H}(u_i,v_j)deg_{G\circ H}(u_i,v_l)}{deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_i,v_l)-2}\right]^3. \end{aligned} \tag{13}$$

Using inequality (2) and (6) in equation (13), we have

$$\begin{aligned} AZI(G\circ H) = &\sum_{u_i\in V(G)}\sum_{v_jv_l\in E(H)} \left[\frac{deg_{G\circ H}(u_i,v_j)\, deg_{G\circ H}(u_i,v_l)}{deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_i,v_l)-2}\right]^3 \\ &+\sum_{v_j\in V(H)}\sum_{u_iu_k\in E(G)} \left[\frac{deg_{G\circ H}(u_i,v_j)\, deg_{G\circ H}(u_k,v_j)}{deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_j)-2}\right]^3 \\ &\leqslant (|V(G)|\,|E(H)|+|E(G)|)\left[\frac{(\Delta_G+\Delta_H)^2}{2(\Delta_G+\Delta_H-1)}\right]^3 \end{aligned}$$

as

$$|V(G)| = n_1(\acute{n}_1+\acute{m}_1), |V(H)| = n_2(\acute{n}_2+\acute{m}_2)$$

$$|E(G)| = m_1\acute{n}_1+2n_1\acute{m}_1, |E(H)| = m_2\acute{n}_2+2n_2\acute{m}_2$$

$$\Delta_G = \Delta_{G_1}+\Delta_{H_1}, \Delta_H = \Delta_{G_2}+\Delta_{H_2}$$

$$AZI(G\circ H)\leqslant \frac{1}{8}[n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+m_1\acute{n}_1+2n_1\acute{m}_1]\Big[\frac{(\Delta_G+\Delta_H)^2}{\delta_G+\delta_H-1}\Big]^3$$

Using

$$\alpha = n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+m_1\acute{n}_1+2n_1\acute{m}_1$$

we get,

$$AZI(G\circ H)\leqslant \frac{1}{8}\alpha\Big[\frac{(\Delta_G+\Delta_H)^2}{\delta_G+\delta_H-1}\Big]^3. \tag{14}$$

Using similar arguments with $deg_G(u)\geqslant \delta_G$, we have

$$AZI(G\circ H)\geqslant \frac{1}{8}[n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+m_1\acute{n}_1+2n_1\acute{m}_1]\Big[\frac{(\delta_G+\delta_H)^2}{\Delta_G+\Delta_H-1}\Big]^3$$

$$AZI(G\circ H)\leqslant \frac{1}{8}\alpha\Big[\frac{(\delta_G+\delta_H)^2}{\Delta_G+\Delta_H-1}\Big]^3. \tag{15}$$

Hence from inequalities 14 and 15, part (d) of the theorem is proved.

(e). By definition

$$PM_1(G\circ H)=\prod_{(u_i,v_j)(u_k,v_l)\in E(G\circ H)}[deg_{G\circ H}(u_i,v_j)+deg_{G\circ H}(u_k,v_l)]. \tag{16}$$

Using inequality (2) in equation (16) and adopting the same procedure as in part (a) of this theorem,

$$PM_1(G\circ H)\leqslant 2^{\alpha}(\Delta_G+\Delta_H)^{\alpha} \tag{17}$$

and

$$PM_1(G\circ H)\geqslant 2^{\alpha}(\delta_G+\delta_H)^{\alpha}. \tag{18}$$

Hence from inequalities 17 and 18, part (e) of the theorem is proved.

(f). By definition

$$PM_2(G\circ H)=\prod_{(u_i,v_j)(u_k,v_l)\in E(G\circ H)}[deg_{G\circ H}(u_i,v_j)\ deg_{G\circ H}(u_k,v_l)]. \tag{19}$$

Using inequality (6) in equation (19) and adopting the same procedure as in part (b) of this theorem,

$$PM_2(G\circ H)\leqslant (\Delta_G+\Delta_H)^{2\alpha} \tag{20}$$

and

$$PM_2(G\circ H)\geqslant (\delta_G+\delta_H)^{2\alpha}. \tag{21}$$

Hence from inequalities 20 and 21, part (e) of the theorem is proved. □

COROLLARY 1. *Let* $G=H_1+_S G_1$ *and* $H=H_2+_S G_2$ *then,*

$$2\alpha(\delta_G+\delta_H)^2\leqslant F(G\circ H)\leqslant 2\alpha(\Delta_G+\Delta_H)^2,$$

where

$$\Delta_G=\Delta_{G_1}+\Delta_{H_1},\quad \Delta_H=\Delta_{G_2}+\Delta_{H_2},\quad \delta_G=\delta_{G_1}+\delta_{H_1},\quad \delta_H=\delta_{G_2}+\delta_{H_2}$$

and $\alpha = n_1(\acute{n}_1+\acute{m}_1)(m_2\acute{n}_2+2n_2\acute{m}_2)+m_1\acute{n}_1+2n_1\acute{m}_1$

Proof. Using relation $F(G) = M_3(G) - 2M_2(G)$, in Theorem 1, we get the required result. □

In the following lemma we compute size of F-sum of graphs for F=R, in terms of factor graphs.

LEMMA 3. *If $G = H_1 +_R G_1$ then size of G is $m_1\acute{n}_1 + 3n_1\acute{m}_1$, where $|V(G_1)| = n_1$, $|V(H_1)| = \acute{n}_1$, $|E(G_1)| = m_1$ and $|E(H_1)| = \acute{m}_1$.*

Proof. We know that the size of $R(H_1)$ is equal to three times the size of H_1, therefor size of $R(H_1)$ is $3|E(H_1)| = 3\acute{m}_1$.

Hence

$$|E(G)| = V(H_1)E(G_1) + V(G_1)3E(H_1) + = m_1\acute{n}_1 + 3n_1\acute{m}_1. \quad \square$$

In the following theorem the lower and upper bounds for the first Zagreb, the second Zagreb, the third Zagreb, the augmented Zagreb, the first multiple Zagreb and the second multiple Zagreb indices of rooted product of F-sum on graphs in terms of their factor graphs for F=R are determined.

THEOREM 2. *Let $G = G_1 +_R H_1$ and $H = G_2 +_R H_2$ then,*

(a). $2\beta(\delta_G + \delta_H) \leqslant M_1(G \circ H) \leqslant 2\beta(\Delta_G + \Delta_H)$

(b). $\beta(\delta_G + \delta_H)^2 \leqslant M_2(G \circ H) \leqslant \beta(\Delta_G + \Delta_H)^2$

(c). $4\beta(\delta_G + \delta_H)^2 \leqslant M_3(G \circ H) \leqslant 4\beta(\Delta_G + \Delta_H)^2$

(d). $\frac{1}{8}\beta[\frac{(\delta_G+\delta_H)^2}{\Delta_G+\Delta_H-1}]^3 \leqslant AZI(G \circ H) \leqslant \frac{1}{8}\beta[\frac{(\Delta_G+\Delta_H)^2}{\delta_G+\delta_H-1}]^3$

(e). $2^\beta(\delta_G + \delta_H)^\beta \leqslant PM_1(G \circ H) \leqslant 2^\beta(\delta_G + \delta_H + \delta_G\delta_H)^\beta$

(f). $(\delta_G + \delta_H + \delta_G\delta_H)^{2\beta} \leqslant PM_2(G \circ H) \leqslant (\delta_G + \delta_H)^{2\beta}$*, where*

$$\Delta_G = \Delta_{G_1} + \Delta_{H_1}, \ \Delta_H = \Delta_{G_2} + \Delta_{H_2}, \ \delta_G = \delta_{G_1} + \delta_{H_1}, \ \delta_H = \delta_{G_2} + \delta_{H_2}$$

and $\beta = n_1(\acute{n}_1 + \acute{m}_1)(m_2\acute{n}_2 + 3n_2\acute{m}_2) + m_1\acute{n}_1 + 3n_1\acute{m}_1$, throughout the theorem.

Proof. Let G and H be the graphs with vertex sets $\{u_1, u_2, \ldots, u_{n_1(\acute{n}_1+\acute{m}_1)}\}$ and $\{v_1, v_2, \ldots, v_{n_2(\acute{n}_2+\acute{m}_2)}\}$ respectively. Clearly orders of G and H are $n_1(\acute{n}_1 + \acute{m}_1)$ and $n_2(\acute{n}_2 + \acute{m}_2)$, respectively. $m_1\acute{n}_1 + 3n_1\acute{m}_1$ and $m_2\acute{n}_2 + 3n_2\acute{m}_2$ are sizes of G and H, respectively. Also

$$\Delta_G = \Delta_{G_1} + \Delta_{H_1}, \ \Delta_H = \Delta_{G_2} + \Delta_{H_2}, \ \delta_G = \delta_{G_1} + \delta_{H_1} \text{ and } \delta_H = \delta_{G_2} + \delta_{H_2}.$$

The proof is completed by using these facts and proceeding as in Theorem 1, setting

$$\beta = n_1(\acute{n}_1 + \acute{m}_1)(m_2\acute{n}_2 + 3n_2\acute{m}_2) + m_1\acute{n}_1 + 3n_1\acute{m}_1. \quad \square$$

COROLLARY 2. *Let $G = H_1 +_R G_1$ and $H = H_2 +_R G_2$ then,*

$$2\beta(\delta_G + \delta_H^2 \leqslant F(G \circ H) \leqslant 2\beta(\Delta_G + \Delta_H)^2,$$

where

$$\Delta_G = \Delta_{G_1} + \Delta_{H_1}, \quad \Delta_H = \Delta_{G_2} + \Delta_{H_2}, \quad \delta_G = \delta_{G_1} + \delta_{H_1}, \quad \delta_H = \delta_{G_2} + \delta_{H_2}$$

and $\beta = n_1(\acute{n}_1 + \acute{m}_1)(m_2\acute{n}_2 + 3n_2\acute{m}_2) + m_1\acute{n}_1 + 3n_1\acute{m}_1)$.

Proof. Using relation $F(G) = M_3(G) - 2M_2(G)$, in Theorem 2, we get the required result. □

In the following theorem the lower and upper bounds for the first Zagreb, the second Zagreb, the third Zagreb, the augmented Zagreb, the first multiple Zagreb and the second multiple Zagreb indices of rooted rooted of F-sum of graphs in terms of their factor graphs for F=S and F=R are determined.

THEOREM 3. *Let $G = H_1 +_S G_1$ and $H = H_2 +_R G_2$ then,*

(a). $2\gamma(\delta_G + \delta_H) \leqslant M_1(G \circ H) \leqslant 2\gamma(\Delta_G + \Delta_H)$

(b). $\gamma(\delta_G + \delta_H)^2 \leqslant M_2(G \circ H) \leqslant \gamma(\Delta_G + \Delta_H)^2$.

(c). $4\gamma(\delta_G + \delta_H)^2 \leqslant M_3(G \circ H) \leqslant 4\gamma(\Delta_G + \Delta_H)^2$.

(d). $\frac{1}{8}\gamma[\frac{(\delta_G+\delta_H)^2}{\Delta_G+\Delta_H-1}]^3 \leqslant AZI(G \circ H) \leqslant \frac{1}{8}\gamma[\frac{(\Delta_G+\Delta_H)^2}{\delta_G+\delta_H-1}]^3$.

(e). $[2(\delta_G + \delta_H)]^\gamma \leqslant PM_1(G \circ H) \leqslant [2(\delta_G + \delta_H)]^\gamma$.

(f). $(\delta_G + \delta_H)^{2\gamma} \leqslant PM_2(G \circ H) \leqslant (\delta_G + \delta_H)^{2\gamma}$.

For, $\gamma = n_1(\acute{n}_1 + \acute{m}_1)(m_2\acute{n}_2 + 3n_2\acute{m}_2) + m_1\acute{n}_1 + 2n_1\acute{m}_1$,

$$\Delta_G = \Delta_{G_1} + \Delta_{H_1}, \quad \Delta_H = \Delta_{G_2} + \Delta_{H_2}, \quad \delta_G = \delta_{G_1} + \delta_{H_1} \quad \textit{and} \quad \delta_H = \delta_{G_2} + \delta_{H_2},$$

throughout the theorem.

Proof. Let G and H be the graphs with vertex sets $\{u_1, u_2, \ldots, u_{n_1(\acute{n}_1+\acute{m}_1)}\}$ and $\{v_1, v_2, \ldots, v_{n_2(\acute{n}_2+\acute{m}_2)}\}$ respectively. Then $|V(G)| = n_1(\acute{n}_1 + \acute{m}_1)$, $|V(H)| = n_2(\acute{n}_2 + \acute{m}_2)$, $|E(G)| = m_1\acute{n}_1 + 2n_1\acute{m}_1$ and $|E(H)| = m_2\acute{n}_2 + 3n_2\acute{m}_2$.

Also

$$\Delta_G = \Delta_{G_1} + \Delta_{H_1}, \quad \Delta_H = \Delta_{G_2} + \Delta_{H_2}, \quad \delta_G = \delta_{G_1} + \delta_{H_1} \quad \text{and} \quad \delta_H = \delta_{G_2} + \delta_{H_2}.$$

The proof is completed by using these facts and proceeding as in Theorem 1, setting

$$\gamma = n_1(\acute{n}_1 + \acute{m}_1)(m_2\acute{n}_2 + 3n_2\acute{m}_2) + m_1\acute{n}_1 + 2n_1\acute{m}_1. \quad \square$$

COROLLARY 3. *Let $G = H_1 +_S G_1$ and $H = H_2 +_R G_2$ then,*

$$2\gamma(\delta_G + \delta_H)^2 \leqslant F(G \circ H) \leqslant 2\gamma(\Delta_G + \Delta_H)^2,$$

where $|V(G)| = n_1(\acute{n}_1 + \acute{m}_1)$, $|V(H)| = n_2(\acute{n}_2 + \acute{m}_2)$, $|E(G)| = m_1\acute{n}_1 + 2n_1\acute{m}_1$, $|E(H)| = m_2\acute{n}_2 + 3n_2\acute{m}_2$,

$$\Delta_G = \Delta_{G_1} + \Delta_{H_1}, \ \ \Delta_H = \Delta_{G_2} + \Delta_{H_2}, \ \ \delta_G = \delta_{G_1} + \delta_{H_1}, \ \ \delta_H = \delta_{G_2} + \delta_{H_2}$$

and $\gamma = n_1(\acute{n}_1 + \acute{m}_1)(m_2\acute{n}_2 + 3n_2\acute{m}_2) + m_1\acute{n}_1 + 2n_1\acute{m}_1$.

Proof. Using relation $F(G) = M_3(G) - 2M_2(G)$, in Theorem 3, we get the required result. □

3. Conclusion and general remarks

In this paper, we conducted the study of Zagreb type indices of rooted product of F-sum on connected, simple and finite graphs. We found expressions for the exact formulas for lower and upper bounds of first, second, third, augmented, first multiple and second multiple indices of rooted product of F-sums on graphs in form of the maximum and minimum degrees, orders and sizes of their factor graphs, for the first time. Also the equality holds if the under lying graphs are regular. Some other products and topological indices can be considered for future study.

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