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BOUNDS ON MODIFIED SYMMETRIC DIVISION DEG INDEX OF GRAPHS

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Abstract. In molecular research, a significant hurdle lies in accurately modeling and predicting the chemical attributes of molecules. To address this challenge, various speculative approaches have been developed by different analysts, with one such approach focusing on topological indices. These indices are numerical representations associated with a molecule's structure graph, utilized to forecast specific chemical and physical characteristics. Degree-based topological indices, a key class within chemical graph theory, play a crucial role in this endeavor. In this article, we introduce a novel degree-based topological index and determine the bounds for the proposed index of general graphs.

Keywords: Chemical graph theory, degree-based topological index, derived graph.

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1. Introduction

Graph theory provides a robust mathematical framework used across various scientific fields, including chemistry. In chemical graph theory, molecules are represented by graphs where atoms are vertices and bonds are edges. This representation allows for the systematic and quantitative analysis of molecular structure, properties, and behavior. A key application of graph theory in chemistry is the development of topological indices. These numerical values, calculated from the graph's structure, are crucial in Quantitative Structure-Property/Activity Relationships (QSPR/QSAR). These indices are essential for predicting a compound's physical, chemical, and biological properties, which is vital for progress in drug discovery, materials science, and environmental chemistry.

Topological indices capture key characteristics such as connectivity, symmetry, and molecular branching, providing insights into reactivity and stability without requiring experimental data. Metrics like the Wiener index, Randic index, and Zagreb indices have been extensively studied and applied to model molecular systems with remarkable accuracy. QSPR models serve as powerful tools for predicting the physical, chemical, and biological properties of molecules based solely on their structural information, eliminating the need for costly experimental procedures. Topological indices, derived from graph representations of molecular structures, provide a numerical approach to encode and quantify molecular connectivity and shape. These indices play a pivotal role in enhancing the predictive power and robustness of QSPR models.

2. PRELIMINARIES AND NOTATION

Topological indices are powerful tools to connect graph theory with other areas. The first degree-based topological indices were introduced by Gutmam et.al. [11, 12] in 1972. They are defined for a connected graph G as

$$M_1(G) = \sum_{ab \in E(G)} (\theta_G(a) + \theta_G(b))$$

and

$$M_2(G) = \sum_{ab \in E(G)} (\theta_G(a)\theta_G(b)).$$

The generalized version of Zagreb indices for a connected graph G are respectively defined as

$$\Lambda^r(G) = \sum_{ab \in E(G)} (\theta_G(a) + \theta_G(b))^r \quad \text{and} \quad \Psi^r(G) = \sum_{ab \in E(G)} (\theta_G(a)\theta_G(b))^r$$

where the parameter $r \in \mathbb{R}$. Similarly, the generalized version of forgotten index of G is defined as $\Gamma^r(G) = \sum_{ab \in E(G)} (\theta_G(a)^2 + \theta_G(b)^2)^r$. Note that if G has n vertices and m edges, then $\Lambda^0(G) = \Psi^0 = m, \Lambda^1(G)$ and Ψ^1 are the first and second Zagreb indices of the graph G. Similarly, $\Psi^{\frac{-1}{2}}$ is the usual Randic index, $\Lambda^{\frac{-1}{2}}$ is the sum-connectivity index, $2\Lambda^{-1}$ is the harmonic index and so on. Hence it is interesting to study Λ^r and Ψ^r.

In this connection, we study the novel index called modified symmetric division deg index of G is defined as $\Omega^{(r,s)}(G) = \sum_{ab \in E(G)} (\theta_G(a)\theta_G(b))^r (\theta_G(a) + \theta_G(b))^s$ where r, s are arbitrary real numbers. Making a suitable choice of the parameters r and s in the above formula, we recover several existing parameters, for example:

- $\Omega^{(0,1)}(G)$ is the forgotten index $F(G)$ [2]
- $\Omega^{(0,\frac{1}{2})}(G)$ is the sombor index $SO(G)$
- $\Omega^{(1,0)}(G)$ is the second Zagreb index $M_2(G)$ [5]
- $\Omega^{(\frac{-1}{2},0)}(G)$ is the Randic index $SO(G)$ [13]
- $\Omega^{(-1,1)}(G)$ is the symmetric devision deg index $SD(G)$ [10] and so on.

The results for F-index of various classes of graphs were studied in [1, 2, 3]. The first and second Zagreb indices of different types of graphs were presented in [4, 5, 6]. Lower and upper bounds for inverse sum indeg index of given graphs were discussed in [7, 8, 9]. In this connection, we obtain several bounds for the modified symmetric division deg index of a general graph.

3. MAIN RESULTS

In this section, we establish several upper and lower bounds for the proposed novel index $\Omega^{r,s}$ of G.

Theorem 3.1. *Let $r, s \in \mathbb{R}$.*

(i) Let G be a connected graph with $r < 0$. Then

$$\Omega^{(r,s)}(G) \geq \left(\frac{1}{2}\right)^{2r} \Gamma^{2r+s}(G)$$

with equality if and only if $G \cong P_2$

(ii) Let G be a connected graph with $s < 0$ Then $\Omega^{(r,s)}(G) \geq 2^{2s}\Psi^{r+2s}(G)$.

Proof. If $r < 0$ then

$$\text{(i)} \quad (\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s = (\sqrt{\theta(a)\theta(b)})^{2r}(\theta^2(a)+\theta^2(b))^s$$
$$\geq \left(\frac{\theta^2(a)\theta^2(b)}{2}\right)^{2r}(\theta^2(a)+\theta^2(b))^s$$

for every $ab \in E(G)$ we get

$$\sum_{ab\in E(G)} (\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s \geq \left(\frac{1}{2}\right)^{2r} \sum_{ab\in E(G)} (\theta^2(a)+\theta^2(b))^{2r+s}$$

This implies $\Omega^{(r,s)}(G) \geq \left(\frac{1}{2}\right)^{2r} \Gamma^{2r+s}(G)$.

(ii) If $r < 0$ then

$$(\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s \geq (\theta(a)\theta(b))^r((\theta^2(a)+\theta^2(b))^2)^s$$
$$= (\theta(a)\theta(b))^r 2^{2s}(\theta(a)\theta(b))^{2s}$$
$$= 2^{2s}(\theta(a)\theta(b))^{2s+r}.$$

For every $ab \in E(G)$, we have

$$\Omega^{(r,s)}(G) \geq 2^{2s}\Psi^{r+2s}(G).$$

□

Theorem 3.2. *Let G be a graph and $r, s \in \mathbb{R}$. Then*

(i) If $r \geq 0$, then

$$\Omega^{(r,s)}(G) \leq \left(\frac{1}{2}\right)^{2r} \Gamma^{2r+s}(G),$$

with equality if and only if $G \cong P_2$.

(ii) If $s \geq 0$, then

$$\Omega^{(r,s)}(G) \leq 2^{2s}\Psi^{r+2s}(G).$$

Proof. Note that $2\sqrt{ab} \leq a + b$ with equality if and only if $a = b$.

If $\alpha \geq 0$ then

$$(\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s = (\sqrt{\theta(a)\theta(b)})^{2r}(\theta^2(a)+\theta^2(b))^s$$
$$\leq \left(\frac{\theta^2(a)+\theta^2(b)}{2}\right)^{2r}(\theta^2(a)+\theta^2(b)). \tag{1}$$

For every $ab \in E(G)$ Equation (1) gives that

$$\begin{aligned}\sum_{ab\in E(G)} (\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s &\leq \sum_{ab\in E(G)} \left(\frac{\theta^2(a)+\theta^2(b)}{2}\right)^{2r+s} (\theta^2(a)+\theta^2(b))^s \\ \Rightarrow \Omega^{(r,s)}(G) &\leq \left(\frac{1}{2}\right)^{2r} \sum_{ab\in E(G)} (\theta^2(a)+\theta^2(b))^{2r+s} \\ \Rightarrow \Omega^{(r,s)}(G) &\leq \left(\frac{1}{2}\right)^{2r} \Gamma^{2r+s}(G).\end{aligned}$$

Equality in the inequality is true for some values $r > 0$ and s if and only if $\theta(a) = \theta$ for every $ab \in E(G)$ and if G is a connected graph, $G \cong P_2$.

Let $s \geq 0$. We know that $a + b \leq 2a$ for every $ab \geq 1$ with equality if and only if $a = b = 1$. Then

$$\begin{aligned}(\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s &\leq (\theta(a)\theta(b))^r 2^{2s}(\theta^2(a)\theta^2(b))^s \\ \Rightarrow (\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s &\leq 2^{2s}(\theta(a)\theta(b))^{r+2s}\end{aligned}$$

For every edge $ab \in E(G)$ we have

$$\begin{aligned}\sum_{ab\in E(G)} (\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s &\leq 2^{2s} \sum_{ab\in E(G)} (\theta(a)\theta(b))^{r+2s} \\ \Rightarrow \Omega^{(r,s)}(G) &\leq \Psi^{(r+2s)}(G)2^{2s}.\end{aligned}$$

□

Theorem 3.3. *Let $r, s \in \mathbb{R}$*

(i) If $s \geq 0$, and G does not have pendent vertices, then

$$\Omega^{(r,s)}(G) \leq \left(\frac{1}{2}\right)^s \Psi^{r+2s}(G).$$

(ii) If $s < 0$ and G does not have pendent vertices, then $\Omega^{(r,s)}(G) \geq \left(\frac{1}{2}\right)^s \Psi^{r+2s}(G)$.

Equality holds for both (i) and (ii) if and only if G is 2-regular.

Proof. (i) If G does not have pendent vertices, then $\theta(G) \geq 2$ for every $a \in V(G)$. We observe that $2(x^2 + y^2) \leq x^2y^2$ for every $x, y \geq 2$ with equality if and only if $x = y = 2$. Hence

$$\begin{aligned}(\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s &\leq (\theta(a)\theta(b))^r \left(\frac{(\theta(a)\theta(b))^2}{2}\right) \\ &= (\theta(a)\theta(b))^r(\theta(a)\theta(b))^{2s} \left(\frac{1}{2}\right)^s.\end{aligned}$$

For an edge $ab \in E(G)$, we get

$$\Omega^{(r,s)}(G) \leq \left(\frac{1}{2}\right)^s \Psi^{r+2s}(G)$$

with an equality if and only if G is 2-regular graph.

(ii) If $s < 0$ and G does not have pendent vertices, then

$$(\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s \geq \left(\frac{1}{2}\right)^s (\theta(a)\theta(b))^{r+2s}$$

For an edge $ab \in E(G)$ we have

$$\Omega^{(r,s)}(G) \geq \left(\frac{1}{2}\right)^s \Psi^{r+2s}(G)$$

with equality if and only if G is 2-regular. □

Theorem 3.4. *Let $r, s, t \in \mathbb{R}$ If G is a graph with m edges, then*

$$(\Omega^{(r,s)}(G))^t \leq \Omega^{t-1}\Omega^{(rt,st)}(G) \quad \textit{if } t \geq 1 \textit{ or } t \leq 0 \textit{ and}$$

$$(\Omega^{(r,s)}(G))^t \geq \Omega^{t-1}\Omega^{(rt,st)}(G) \quad \textit{if } 0 < t < 1.$$

Proof. Let $f(x) = x^t$ is a convex function on $\mathbb{R}$, for every $t \geq 1$ or $t \leq 0$. Then

$$\left(\frac{\sum_{ab\in E(G)}(\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s}{m}\right)^t \leq \frac{1}{m}\sum_{ab\in E(G)}((\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s)^t$$

$$\Rightarrow \left(\frac{1}{m}\right)^t \Omega^{(r,s)}(G) \leq \frac{1}{m}\Omega^{(rt,st)}(G)$$

$$\Rightarrow (\Omega^{(r,s)}(G))^t \leq \Omega^{t-1}\Omega^{(rt,st)}(G).$$

Let $f(x) = -x^t$, $0 < t < 1$ be the convex function. Then

$$\left(\frac{\sum_{ab\in E(G)}(\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s}{m}\right)^t \geq \frac{1}{m}\sum_{ab\in E(G)}((\theta(a)\theta(b))^r(\theta^2(a)+\theta^2(b))^s)^t$$

$$\Rightarrow (\Omega^{(r,s)}(G))^t \geq \Omega^{t-1}\Omega^{(rt,st)}(G).$$

□

Theorem 3.5. *For $r, s, t > 0$,*

$$\Omega^{(r,s)}(G) \geq (\Gamma^{\frac{s}{t+1}}(G))^{t+1}(\Psi^{\frac{-r}{t}}(G))^{-t} \quad \textit{and} \quad \Omega^{(r,s)}(G) \geq (\Psi^{\frac{r}{t+1}}(G))^{t+1}(\Gamma^{\frac{-s}{t}}(G))^{-t}.$$

Proof. Let $r > 0$ and $p_1, \ldots, p_n, q_1, \ldots, q_n > 0$ be the real numbers. Then by Radon's inequality, we have

$$\sum_{i=1}^n \frac{q_i^{t+1}}{p_i^t} \geq \frac{\left(\sum_{i=1}^n q_i\right)^{t+1}}{\left(\sum_{i=1}^n p_i\right)^t}$$

Let us choose $p_i = (\theta(a)\theta(b))^{\frac{-r}{t}}$ and $q_i = (\theta^2(a) + \theta^2(b))^{\frac{s}{t+1}}$ in Radon's inequality, we obtain

$$\sum_{ab\in E(G)} (\theta(a)\theta(b))^r(\theta^2(a) + \theta^2(b))^s \geq \frac{\left(\sum_{ab\in E(G)} \left(\theta^2(a) + \theta^2(b)\right)^{\frac{s}{t+1}}\right)^{t+1}}{\left(\sum_{ab\in E(G)} (\theta(a)\theta(b))^{\frac{-r}{t}}\right)^{t}}.$$

This gives

$$\Omega^{(r,s)}(G) \geq (\Gamma^{\frac{s}{t+1}}(G))^{t+1}(\Psi^{\frac{-r}{t}}(G))^{-t}.$$

Let us consider $p_i = (\theta^2(a) + \theta^2(b))^{\frac{-s}{t}}$ and $q_i = (\theta(a)\theta(b))^{\frac{r}{t+1}}$ in Radon's inequality, we obtain

$$\sum_{ab\in E(G)} (\theta(a)\theta(b))^r(\theta^2(a) + \theta^2(b))^s \geq \frac{\left(\sum_{ab\in E(G)} (\theta(a)\theta(b))^{\frac{r}{t+1}}\right)^{t+1}}{\left(\sum_{ab\in E(G)} (\theta^2(a) + \theta^2(b))^{\frac{-s}{t}}\right)^{t}}.$$

This implies that

$$\Omega^{(r,s)}(G) \geq (\Psi^{\frac{r}{t+1}}(G))^{t+1}(\Gamma^{\frac{-s}{t}}(G))^{-t}$$

□

Theorem 3.6. *For a graph G with $t \in \mathbb{R}$,*

$$\Omega^{(r,s+1)}(G) + t^2\Omega^{(r,s)}(G) \geq 2t\delta(G)\Omega^{(r,s)}(G) + \Omega^{(r+1,s)}(G).$$

Proof. One can easily check that

$$(\theta(a) - \theta(b))^2 + (\theta(a) - t)^2 + (\theta(b) - t)^2 \geq 0.$$

This gives that

$$(\theta^2(a) + \theta^2(b)) + t^2 \geq t(\theta(a) + \theta(b)) + \theta(a)\theta(b),$$

$$\begin{aligned}(\theta(a)\theta(b))^r(\theta^2(a) + \theta^2(b))^{s+1} \quad &+t^2(\theta(a) + \theta(b))^r(\theta^2(a) + \theta^2(b))^s \\ &\geq t(\theta(a) + \theta(b))(\theta(a)\theta(b))^r(\theta^2(a) + \theta^2(b))^s \\ &+(\theta(a)\theta(b))^{r+1}(\theta^2(a) + \theta^2(b))^s.\end{aligned}$$

Taking summation over all edges $ab \in E(G)$ we obtain

$$\Omega^{(r,s+1)}(G) + t^2\Omega^{(r,s)}(G) \geq 2t\delta(G)\Omega^{(r,s)}(G) + \Omega^{(r+1,s)}(G).$$

Equality holds if and only if G is t-regular. □

Corollary 3.7. *For $r, s, t \in \mathbb{R}$,*

$$4\delta^2(G)(\Omega^{(r,s)}(G))^2 - 4\Omega^{(r,s)}(G)(\Omega^{(r,s+1)}(G) - \Omega^{(r+1,s)}(G)) \leq 0.$$

Proof. By the previous Theorem, for every $t \in \mathbb{R}$

$$\Omega^{(r,s)}(G)t^2 - 2\delta(G)\Omega^{(r,s)}(G)t + \Omega^{(r,s+1)}(G) - \Omega^{(r+1,s)}(G) \geq 0 \tag{2}$$

We know that if Equation (2) is non-negative, then its discriminant is non-positive, that is,

$$4\delta^2(G)(\Omega^{(r,s)}(G))^2 - 4\Omega^{(r,s)}(G)(\Omega^{(r,s+1)}(G) - \Omega^{(r+1,s)}(G)) \leq 0.$$

□

Theorem 3.8. *For $r, s \in \mathbb{R}$,*

$$(\triangle^{2r} + \delta^{2r})\Omega^{(r,s)}(G) \geq (\triangle\delta)^{2r}\Gamma^s(G) + \Omega^{(r,s)}(G)$$

with equality, $r \neq 0$ if and only if G is regular.

Proof. If $r \geq 0$ then $\delta^{2r} \leq (\theta(a)\theta(b))^r \leq \triangle^{2r}$ and if $r < 0$ then $\triangle^{2r} \leq (\theta(a)\theta(b))^r \leq \delta^{2r}$. Thus, $(\triangle^{2r} - (\theta(a)\theta(b))^r)((\theta(a)\theta(b))^r - \delta^{2r}) \geq 0$ This implies that

$$(\triangle^{2r} + \delta^{2r})\Omega^{(r,s)}(G)(\theta(a)\theta(b))^r = (\triangle^{2r} + \delta^{2r})(\theta(a)\theta(b))^r(\theta^2(a) + \theta^2(b))^s$$

$$\geq (\triangle\delta)^{2r}(\theta(a)\theta(b))^{2r}(\theta^2(a) + \theta^2(b))^s.$$

Taking summation over all edges $ab \in E(G)$, we obtain

$$(\triangle^{2r} + \delta^{2r})\Omega^{(r,s)}(G) \geq (\triangle\delta)^{2r}\Gamma^s(G)\Omega^{(2r,s)}(G) \tag{3}$$

If $r \neq 0$, the equality holds if and only if $(\theta(a)\theta(b))^r = \triangle^{2r}$ or $(\theta(a)\theta(b))^r = \delta^{2r}$ for every $ab \in E(G)$. That is, $\theta(a) = \theta(b) = \triangle$ or $\theta(a) = \theta(b) = \delta$ for every $ab \in E(G)$. This gives that G is regular graph. □

Lemma 3.9. *If $p_i \geq 0$ for $1 \leq i \leq k$ and $q \in \mathbb{R}$, then*

$$k^{1-q}\left(\sum_{i=1}^{k} p_i\right)^q \leq \sum_{i=1}^{k} p_i^q \leq \left(\sum_{i=1}^{k} p_i\right)^q \tag{4}$$

whenever $q \leq 0$ or $q \geq 1$ and

$$\left(\sum_{i=1}^{k} p_i\right)^q \leq \sum_{i=1}^{k} p_i^q \leq k^{1-q}\left(\sum_{i=1}^{k} p_i\right)^q \tag{5}$$

whenever $0 < q < 1$. If $q \neq 0$, then equalities hold for Equations (4) and (5) if and only if $p_1 = p_2 = \cdots = p_k$.

Theorem 3.10. *For $r \in \mathbb{R}$ $n^r\Omega^{1-r} \leq \Omega^{(-r,r)}(G) \leq (SD(G))^r$ if $r \geq 0$ or $r \geq 1$ and $n^r \leq \Omega^{(-r,r)}(G) \leq (SD(G))^r\Omega^{1-r}$ if $0 < r < 1$.*

Proof. If $r \leq 0$ or $r \geq 1$, then by previous Lemma,

$$\sum_{ab\in E(G)}\left(\frac{\theta^2(a) + \theta^2(b)}{\theta(a)\theta(b)}\right)^r \leq \left(\sum_{ab\in E(G)}\frac{\theta^2(a) + \theta^2(b)}{\theta(a)\theta(b)}\right)^r$$

$$\leq \Omega^{r-1} \sum_{ab \in E(G)} \left(\frac{\theta^2(a) + \theta^2(b)}{\theta(a)\theta(b)} \right)^r$$

$$\Rightarrow \Omega^{(-r,r)}(G) \leq (SD(G))^r \leq \Omega^{r-1}\Omega^{(-r,r)}(G).$$

If $0 < r < 1$, then by previous Lemma,

$$\Omega^{r-1} \sum_{ab \in E(G)} \left(\frac{\theta^2(a) + \theta^2(b)}{\theta(a)\theta(b)} \right)^r \leq \left(\sum_{ab \in E(G)} \frac{\theta^2(a) + \theta^2(b)}{\theta(a)\theta(b)} \right)^r$$

$$\leq \sum_{ab \in E(G)} \left(\frac{\theta^2(a) + \theta^2(b)}{\theta(a)\theta(b)} \right)^r$$

This implies that $\Omega^{r-1}\Omega^{(-r,r)}(G) \leq (SD(G))^r \leq \Omega^{(-r,r)}(G)$. □

Corollary 3.11. *For* $0 < r \leq 1$, $\Omega^{(-r,r)}(G) \geq (4\delta(G))^r$.

Proof. By previous Theorem, $\Omega^{(-r,r)}(G) \geq n^r$ for any graph G with n vertices and $0 < r \leq 1$ We know that if G is connected graph, then $\delta(G) \leq \frac{n}{4}$ This gives that $n \geq 4\delta(G)$. Hence $\Omega^{(-r,r)}(G) \geq n^r \geq (4\delta(G))^r$. □

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