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NEW BOUNDS ON SDD INVARIANT OF GRAPHS

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ABSTRACT. The SDD invariant is one of the 148 discrete Adriatic indices contributed many years ago. In this paper, we obtain several new upper bounds for SDD invariant of a given graph in terms of other graph parameters.

1. INTRODUCTION

Molecular descriptors have found applications in modeling several physicochemical properties in $QSAR$ and $QSPR$ studies [2, 4]. A particularly many type of molecular descriptors are defined as functions of the structure of the underlying molecular graph, such as the Wiener invariant [10], the Zagreb invariants [3] and Balaban invariant [1]. Damir Vukicević et al. [9] proved that many of these descriptors are defined the sum of individual bond contributions. Among the 148 discrete Adriatic invariants studied in [9], whose predictive properties were evaluated against the benchmark datasets of the Internation Academy of Mathematical Chemistry [8], 20 invariants were selected as significant predictors of physicochemical properties. One of these useful discrete adriatic indices is the symmetric division deg (SDD) invariant which is defined as $SDD(\Gamma) = \sum\limits_{xy \in E(\Gamma)} \left(\frac{\eta_x}{\eta_y} + \frac{\eta_y}{\eta_x)} \right)$, where η_x and η_y are the degrees of vertices x and y, respectively. Among all the existing molecular descriptors, SDD invariant has the best correlating ability for predicting the total surface area of

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polychlorobiphenys [9]. In this paper, several new upper bounds for symmetric division deg invariant of a given graph are established.

2. Preliminaries

The minimum and minimum vertex degrees of Γ, respectively, denoted by δ and Δ.

- First and second Zagreb invariants:
  $M_1(\Gamma) = \sum\limits_{xy \in E(\Gamma)} (\eta_x + \eta_y)$ and $M_2(\Gamma) = \sum\limits_{xy \in E(\Gamma)} (\eta_x \eta_y)$.
- The first and second modified Zagreb invariants:
  $M_1^*(\Gamma) = \sum\limits_{x \in V(\Gamma)} \frac{1}{\eta_x^2}$ and $M_2^*(\Gamma) = \sum\limits_{xy \in E(\Gamma)} \frac{1}{\eta_x \eta_y}$.
- The multiplicative version of Zagreb invariant:
  $\pi_1(\Gamma) = \prod\limits_{x \in V(\Gamma)} \eta_x^2$,$\pi_2(\Gamma) = \prod\limits_{xy \in E(\Gamma)} \eta_x \eta_y$ and $\pi_1^*(\Gamma) = \prod\limits_{xy \in E(\Gamma)} (\eta_x + \eta_y)$.
- The α-Randić invariant is then defined as $R_\alpha(\Gamma) = \sum\limits_{xy \in E(\Gamma)} (\eta_x \eta_y)^\alpha$.
- The α-sum-connectivity invariant of Γ is defined as
  $\chi_\alpha(\Gamma) = \sum\limits_{xy \in E(\Gamma)} (\eta_x + \eta_y)^\alpha$.
- The sum and product F-invariants:
  $F(\Gamma) = \sum\limits_{xy \in E(\Gamma)} (\eta_x^2 + \eta_y^2)$ and $F^*(\Gamma) = \prod\limits_{xy \in E(\Gamma)} (\eta_x^2 + \eta_y^2)$.
- The α-F-invariant: $F_\alpha(\Gamma) = \sum\limits_{xy \in E(\Gamma)} (\eta_x^2 + \eta_y^2)^\alpha$.
- The (r,t)-Zagreb invariant: $Z'_{r,t}(\Gamma) = \sum\limits_{xy \in E(\Gamma)} (\eta_x^r \eta_y^t + \eta_x^t \eta_y^r)$.

3. Bounds for SDD

Let Γ be a connected graph with s vertices and m edges and let $\Delta = \eta_1 \geq \eta_2 \geq \ldots \geq \eta_s = \delta > 0,\ \eta_i = \eta(i)$ and $\eta(e_1) \geq \eta(e_2) \geq \ldots \geq \eta((e_m)$ be sequences of its vertex and edge degrees, respectively. We denote $\Delta_{e_1} = \eta(e_1) + 2$ and $\delta_{e_1} = \eta(e_m) + 2$. If the vertices x and y are adjacent, we write $x \sim y$.

Let $p = (p_i)$ and $a = (a_i),\ i = 1, 2, \ldots, m$ be positive real number sequences with the properties $p_1 + p_2 + \ldots + p_m = 1$ and $0 < a \leq a_i \leq A < \infty$. Rennie [6] proved

$$\sum_{i=1}^{m} p_i a_i + aA\sum_{i=1}^{m}\frac{p_i}{a_i} \le a + A, \tag{3.1}$$

with equality if and only if $a_i = A(\text{or})a_i = a$, for every $i = 1, 2, \ldots, m$.

Let $x = (x_i)$ and $a = (a_i),\ i = 1, 2, \ldots, m$ be positive real number sequences. Then by [7],

$$\sum_{i=1}^{m}\frac{x_i^{r+1}}{a_i^r} \ge \frac{\left(\sum\limits_{i=1}^{m} x_i\right)^{r+1}}{\left(\sum\limits_{i=1}^{m} a_i\right)^{r}}$$

with equality if and only if $\frac{a_1}{x_1} = \frac{a_2}{x_2} = \ldots = \frac{a_m}{x_m}$.

If $a = (a_i),\ i = 1, 2, \ldots, m$ is a positive real number sequences, then by [5], we write

$$\Big(\sum_{i=1}^{m}\sqrt{a_i}\Big)^2 \ge \sum_{i=1}^{m} a_i + m(m-1)\Big(\prod_{i=1}^{m} a_i\Big)^{\frac{1}{m}} \tag{3.2}$$

with equality if and only if $a_1 = a_2 = \ldots = a_m$.

Theorem 3.1. *For a connected graph* Γ, $SDD(\Gamma) \le \dfrac{(\Delta_e + \delta_e)F(\Gamma) - 2\,Z'_{3,1}(\Gamma)}{\Delta_e\delta_e}$. *Equality holds if and only if* Γ *is regular (or) semiregular bipartite graph.*

Proof. For $p_i = \dfrac{\eta_x^2 + \eta_y^2}{\sum\limits_{x\sim y}(\eta_x^2 + \eta_y^2)}$, $a_i = \eta_x\eta_y$, $r = \delta_e$, $R = \Delta_e$ where summation is performed over all edges in a graph Γ, the inequality (3.1) becomes

$$\frac{\sum\limits_{x\sim y}(\eta_x^2 + \eta_y^2)\eta_x\eta_y}{\sum\limits_{x\sim y}(\eta_x^2 + \eta_y^2)} + \Delta_e\delta_e\frac{\sum\limits_{x\sim y}\frac{\eta_x^2+\eta_y^2}{\eta_x\eta_y}}{\sum\limits_{x\sim y}(\eta_x^2 + \eta_y^2)} \le \Delta_e + \delta_e$$

$$\Rightarrow\ \sum_{x\sim y}(\eta_x^2 + \eta_y^2)\eta_x\eta_y + \Delta_e\delta_e\sum_{x\sim y}\frac{\eta_x^2 + \eta_y^2}{\eta_x\eta_y} \le (\Delta_e + \delta_e)\sum_{x\sim y}(\eta_x^2 + \eta_y^2)$$

$$\Rightarrow\ \sum_{x\sim y}(\eta_x^2 + \eta_y^2)\eta_x\eta_y + \Delta_e\delta_e\,SDD(\Gamma) \le (\Delta_e + \delta_e)F(\Gamma). \tag{3.3}$$

By the definition of (r,t)-Zagreb invariant, we obtain

$$2\,Z'_{3,1}(\Gamma) + \Delta_e\delta_e SDD(\Gamma) \le (\Delta_e + \delta_e)F(\Gamma).$$

Therefore

$$SDD(\Gamma) \leq \frac{(\Delta_e + \delta_e)F(\Gamma) - 2\, Z'_{3,1}(\Gamma)}{\Delta_e \delta_e}.$$

Equality in (3.1) holds if and only if $a_1 = a_2 = \ldots = a_m$ (or) $a_1 = a_2 = \ldots = a_s \geq a_{s+1} = \ldots = a_m$ for some s,$1 \leq s \leq m-1$. This means that equality in (3.3) is attained if and only if either $\Delta_e = \eta(e_1) + 2 = \ldots = \eta(e_m) + 2 = \delta_e$ (or) $\Delta_e = \eta(e_1) + 2 = \ldots = \eta(e_s) + 2 \geq \eta(e_{s+1}) + 2 = \ldots = \eta(e_m) + 2 = \delta_e$for some s,$1 \leq s \leq m-1$. This implies Γ is regular (or) semiregular bipartite graph. □

Theorem 3.2. *Let Γ be a connected graph with m edges. Then*

$$SDD(\Gamma) \leq \Big[(\Delta_e + \delta_e)F(\Gamma) - \frac{F(\Gamma) + m(m-1)(F^*(\Gamma))^{\frac{1}{m}}}{M_2^*(\Gamma)}\Big]\Big(\frac{1}{\Delta_e \delta_e}\Big),$$

with equality if and only if Γ is regular (or) semiregular bipartite graph.

Proof. One can see that

$$\sum_{x\sim y}(\eta_x^2 + \eta_y^2)\eta_x\eta_y = \sum_{x\sim y}\frac{(\sqrt{\eta_x^2 + \eta_y^2})^2}{\frac{1}{\eta_x\eta_y}} \geq \frac{(\sum\limits_{x\sim y}\sqrt{\eta_x^2 + \eta_y^2})^2}{\sum\limits_{x\sim y}\frac{1}{\eta_x\eta_y}}. \tag{3.4}$$

Setting $a_i = \eta_x^2 + \eta_y^2$ in (3.2), we have

$$\begin{aligned}(\sum_{x\sim y}\sqrt{\eta_x^2 + \eta_y^2})^2 &\geq \sum_{x\sim y}(\eta_x^2 + \eta_y^2) + m(m-1)\Big(\prod_{x\sim y}(\eta_x^2 + \eta_y^2)\Big)^{\frac{1}{m}} \\ &= F(\Gamma) + m(m-1)(F^*(\Gamma))^{\frac{1}{m}}. \end{aligned} \tag{3.5}$$

From the Equations (3.4) and (3.5) we obtain

$$\sum_{x\sim y}(\eta_x^2 + \eta_y^2)\eta_x\eta_y \geq \frac{F(\Gamma) + m(m-1)(F^*(\Gamma))^{\frac{1}{m}}}{M_2^*(\Gamma)}. \tag{3.6}$$

Substitute (3.6) in (3.3), we get

$$\frac{F(\Gamma) + m(m-1)(F^*(\Gamma))^{\frac{1}{m}}}{M_2^*(\Gamma)} + \Delta_e\delta_e SDD(\Gamma) \leq (\Delta_e + \delta_e)F(\Gamma).$$

Hence

$$SDD(\Gamma) \leq \Big[(\Delta_e + \delta_e)F(\Gamma) - \frac{F(\Gamma) + m(m-1)(F^*(\Gamma))^{\frac{1}{m}}}{M_2^*(\Gamma)}\Big]\Big(\frac{1}{\Delta_e \delta_e}\Big).$$

Equality holds if and only if Γ is regular (or) semiregular bipartite graph. □

Theorem 3.3. *For a connected graph Γ with m edges,*

$$SDD(\Gamma) \leq \Big[(\Delta_e + \delta_e)F(\Gamma) - m(F^*\Gamma)^{\frac{1}{m}}(\pi_2(\Gamma))^{\frac{1}{m}}\Big]\Big(\frac{1}{\Delta_e\delta_e}\Big).$$

Equality holds if and only if Γ is regular (or) semiregular bipartite graph.

Proof. One can observe that

$$\sum_{x\sim y}(\eta_x^2+\eta_y^2)^2\eta_x\eta_y \geq m\Big(\prod_{x\sim y}(\eta_x^2+\eta_y^2)\eta_x\eta_y\Big)^{\frac{1}{m}} = m(F^*\Gamma)^{\frac{1}{m}}(\pi_1^*)^{\frac{1}{m}}. \tag{3.7}$$

By the Equations (3.3) and (3.7), we have

$$m(F^*\Gamma)^{\frac{1}{m}}(\pi_2(\Gamma))^{\frac{1}{m}} + \Delta_e\delta_e SDD(\Gamma) \leq (\Delta_e+\delta_e)F(\Gamma).$$

Therefore $SDD(\Gamma) \leq \Big[(\Delta_e + \delta_e)F(\Gamma) - m(F^*\Gamma)^{\frac{1}{m}}(\pi_2(\Gamma))^{\frac{1}{m}}\Big]\Big(\frac{1}{\Delta_e\delta_e}\Big)$.

The equality sign holds throughtout in (3.7) if and only if $(\eta_x^2+\eta_y^2)^2\eta_x\eta_y = k$, constant, for every edge of Γ. Therefore equality holds in (3.7) if and only if Γ is regular (or) semiregular bipartite graph. Hence $SDD(\Gamma) \leq \Big[(\Delta_e + \delta_e)F(\Gamma) - m(F^*\Gamma)^{\frac{1}{m}}(\pi_2(\Gamma))^{\frac{1}{m}}\Big]\Big(\frac{1}{\Delta_e\delta_e}\Big)$ with equality if and only if Γ is regular (or) semiregular bipartite graph. □

Theorem 3.4. *Let Γ be a connected graph with m edges. Then $SDD(\Gamma) \leq \dfrac{(\Delta_e+\delta_e)F(\Gamma) - 2m\delta^4}{\Delta_e\delta_e}$ with equality if and only if Γ is regular (or) semiregular bipartite graph.*

Proof. Since $\delta \leq \eta_x \leq \Delta$, for every vertex $x \in V(\Gamma)$ with equality if and only if Γ is regular. Hence $\sum\limits_{x\sim y}(\eta_x^2+\eta_y^2)\eta_x\eta_y \geq 2m\delta^4$. From the Equation (3.3), we get

$$\begin{aligned} & 2m\delta^4 + \Delta_e\delta_e\, SDD(\Gamma) \leq (\Delta_e+\delta_e)F(\Gamma) \\ \Rightarrow\quad & \Delta_e\delta_e\, SDD(\Gamma) \leq (\Delta_e+\delta_e)F(\Gamma) - 2m\delta^4 \\ \Rightarrow\quad & SDD(\Gamma) \leq \frac{(\Delta_e+\delta_e)F(\Gamma) - 2m\delta^4}{\Delta_e\delta_e}. \end{aligned}$$

□

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