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UPPER BOUNDS FOR SYMMETRIC DIVISION DEG INDEX OF GRAPHS

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Abstract: The symmetric division deg index is one of the 148 discrete Adriatic indices introduced several years ago. This index has already been proved a valuable index in the QSAR(Quantitative Structure Activity Relationship) and QSPR(Quantitative Structure Property Relationship) studies. In this paper, we present some new upper bounds for symmetric division deg index of a given Graph.

Keywords and Phrases: Degree, Topological descriptor, Symmetric Division Deg Index.

2010 Mathematics Subject Classification: 05C12, 05C76.

1. Introduction

Molecular descriptors, results of functions mapping molecule's chemical information into a number [5], have found applications in modeling many physicochemical properties in QSAR and QSPR studies [1]. Among the 148 discrete Adriatic indices studied in [6], whose predictive properties were evaluated against the benchmark datasets of the International Academy of Mathematical Chemistry [3], 20 indices were selected as significant predictors of physicochemical properties. One of these useful discrete adriatic indices is the symmetric division deg index which is defined as $SDD(G) = \sum_{xy\in E(G)} \left(\frac{d_x}{d_y} + \frac{d_y}{d_x)}\right)$, where d_x and d_y are the degrees of vertices x and y, respectively. Among all the existing molecular descriptors, SDD index has the best correlating ability for predicting the total surface area of polychlorobiphenys [6]. Vasilyev [7] provided the different types of lower and upper bounds of symmetric division deg index in some classes of graphs and determined the corresponding extremal graphs. In this paper, we present some new lower bounds for symmetric division deg index of a given graph.

2. Preliminaries

Let G be a finite simple connected graph with vertes set $V(G)$ and edge set $E(G)$. Let d_x denote the degree of a vertex x in G. We denote by δ and Δ the maximum and minimum vertex degrees of G, respectively.

The Zagreb indices are among the oldest topological indices introduced by Gutman and Trinajstic in 1972. These indices have since been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. They are defined as $M_1(G) = \sum\limits_{xy\in E(G)} (d_x + d_y)$ and $M_2(G) = \sum\limits_{xy\in E(G)} (d_x d_y)$. A modification Zagreb indices was proposed by Nikolic et al. [2] in 2003. The first and second modified Zagreb indices of G are defined as $M_1^*(G) = \sum\limits_{x\in V(G)} \frac{1}{d_x^2}$ and $M_2^*(G) = \sum\limits_{xy\in E(G)} \frac{1}{d_x d_y}$. The multiplicative version of Zagreb indices were introduced by Todeschini and Consonni [5] in 2010. They are defined as $\pi_1(G) = \prod\limits_{x\in V(G)} d_x^2$ and $\pi_2(G) = \prod\limits_{xy\in E(G)} d_x d_y$.

In 1975, Randić [4] proposed a structure descriptor, based on the end -vertex degrees of edges in a graph, called branching index that later became the well-known Randić connectivity index. The Randić index of G is defined as $R(G) = \sum\limits_{xy\in E(G)} \frac{1}{\sqrt{d_x d_y}}$. It gave rise to a number of generalizations. The most common one arises by varying the exponent α in the edge contribution $(d_x d_y)^\alpha$. The α-Randić index is then defined as $R_\alpha(G) = \sum\limits_{xy\in E(G)} (d_x d_y)^\alpha$. The F-index and multiplicative F-index of a connected graph G are respectively, defined as $F(G) = \sum\limits_{xy\in E(G)} (d_x^2 + d_y^2)$ and $F^*(G) = \prod\limits_{xy\in E(G)} (d_x^2 + d_y^2)$. The α-F-index of G is defined as $F_\alpha(G) = \sum\limits_{xy\in E(G)} (d_x^2 + d_y^2)^\alpha$.

3. Bounds for SDD

Theorem 3.1. *Let G ba a graph with m edges. Then $SDD(G) \leq \frac{4(m\Delta - ISI(G))\delta}{\Delta^2}$ with equality if and only if G is regular.*

Proof. We know that $d_x d_y = \frac{1}{2}\Big[(d_x + d_y)^2 - (d_x^2 + d_y^2)\Big]$ By dividing this expression throughout by $d_x + d_y$, we obtain

$$\frac{d_x d_y}{d_x + d_y} = \frac{1}{2}\Big[(d_x + d_y) - \frac{(d_x^2 + d_y^2)}{(d_x + d_y)}\Big]. \tag{1}$$

Taking summation over all edges in G on both sides, we obtain

$$\begin{aligned}\sum_{xy\in E(G)} \frac{d_x d_y}{d_x + d_y} &= \frac{1}{2}\sum_{xy\in E(G)} \Big[(d_x + d_y) - \frac{(d_x^2 + d_y^2)}{(d_x + d_y)}\Big] \\ &\leq \frac{1}{2}\sum_{xy\in E(G)} \Big[2\Delta - \frac{(d_x^2 + d_y^2)}{2\delta}(\frac{\delta^2}{d_x d_y})\Big] \\ &= m\Delta - \frac{\Delta^2}{4\delta}\sum_{xy\in E(G)} \frac{(d_x^2 + d_y^2)}{d_x d_y}.\end{aligned}$$

Hence $SDD(G) \leq \frac{(m\Delta - ISI(G))4\delta}{\Delta^2}$. Equality holds if and only if $d_x = d_y = \delta = \Delta$, for each edge $xy \in E(G)$, this implies G is regular.

Theorem 3.2. *Let G ba a graph with s pendent vertices and minimal non-pendant vertex degree δ_1. Then $SDD(G) \leq \frac{2\Delta^2(m-s)+s(1+\Delta^2)\delta_1}{\delta_1^2}$ with equality if and only if G is regular (or) G is $(1, \Delta)$-semiregular.*

Proof. From the definition of SDD, we have

$$\begin{aligned}SDD(G) &= \sum_{xy\in E(G),\ d_x,d_y\neq 1} \frac{d_x^2 + d_y^2}{d_x d_y} + \sum_{xy\in E(G),\ d_x=1} \frac{1 + d_y^2}{d_y} \\ &\leq (m-s)\frac{2\Delta^2}{\delta_1^2} + s\frac{1+\Delta^2}{\delta_1} \\ &= \frac{2\Delta^2(m-s) + s(1+\Delta^2)\delta_1}{\delta_1^2}.\end{aligned}$$

Equality holds above if and only if $d_x = d_y = \delta_1$, for each non-pendent vertex $x \in V(G)$, this implies G is $(1, \Delta)$-semiregular if $s \geq 0$ and G is regular if $s = 0$.

Corollary 3.3. *Let G ba a graph without pendent vertices. Then $SDD(G) \leq \frac{2\Delta^2 m}{\delta^2}$ with equality if and only if G is regular.*

Proof. By setting $s = 0$ and $\delta_1 = \delta$ in above theorem, we get the required result.

Theorem 3.4. *Let G be a graph with m edges. Then $SDD(G) \leq \left(\frac{\delta+\Delta}{\sqrt{\delta\Delta}}\right)^2 - 2m$*

with equality if and only if G is regular.
Proof. From the definition of SDD, we have

$$\begin{aligned} SDD(G)+2m &= \sum_{xy\in E(G)} \Big(\frac{d_x^2+d_y^2}{d_xd_y}+2\Big) \\ &= \sum_{xy\in E(G)} \Big(\frac{d_x^2+d_y^2+2d_xd_y}{d_xd_y}\Big) = \sum_{xy\in E(G)} \Big(\frac{(d_x+d_y)}{\sqrt{d_xd_y}}\Big)^2. \quad (2) \end{aligned}$$

For each edge $xy \in E(G)$, we have

$$\begin{aligned} \Big(\frac{(d_x+d_y)}{\sqrt{d_xd_y}}\Big)^2 &= \Big(\sqrt{\frac{d_x}{d_y}}-\sqrt{\frac{d_y}{d_x}}\Big)^2+4 \\ &\leq \Big(\sqrt{\frac{\Delta}{\delta}}-\sqrt{\frac{\delta}{\Delta}}\Big)^2+4 = \Big(\frac{\Delta+\delta}{\sqrt{\delta\Delta}}\Big)^2. \end{aligned}$$

Hence $\frac{(d_x+d_y)}{\sqrt{d_xd_y}} \leq \frac{\Delta+\delta}{\sqrt{\delta\Delta}}$. Equality if and only if $\frac{d_x}{d_y} = \frac{\Delta}{\delta}$ for each edge $xy \in E(G)$ with $d_x \geq d_y$, which implies that $d_x = \Delta$ and $d_y = \delta$, this holds if and only if G is regular (or) biregular. Thus (2) implies that $SDD(G) + 2m \leq m\frac{\Delta+\delta}{\sqrt{\delta\Delta}}$.

Hence $SDD(G) \leq m\frac{\Delta+\delta}{\sqrt{\delta\Delta}} - 2m$ with equality if and only if G is regular.

Theorem 3.5. *For any graph G,* $SDD(G) \leq \frac{2\Delta^2\sqrt{m}}{\delta}M_2^*(G)$. *Equality holds if and only if G is regular (or) biregular.*
Proof. From the definition of SDD, we have

$$\Big(SDD(G)\Big)^2 = \Big(\sum_{xy\in E(G)} \frac{d_x^2+d_y^2}{d_xd_y}\Big)^2 = \Big(\sum_{xy\in E(G)} \frac{d_x^2+d_y^2}{\sqrt{d_xd_y}}\frac{1}{\sqrt{d_xd_y}}\Big)^2.$$

By Cauchy-Schwarz inequality, we have

$$\begin{aligned} \Big(SDD(G)\Big)^2 &\leq \sum_{xy\in E(G)} \Big(\frac{d_x^2+d_y^2}{\sqrt{d_xd_y}}\Big)^2 \sum_{xy\in E(G)} \Big(\frac{1}{\sqrt{d_xd_y}}\Big)^2 \\ &= m\frac{4\Delta^4}{\delta^2} \sum_{xy\in E(G)} \Big(\frac{1}{\sqrt{d_xd_y}}\Big)^2 = m\frac{4\Delta^4}{\delta^2}(M_2^*(G))^2. \end{aligned}$$

Hence $SDD(G) \leq \frac{2\Delta^2\sqrt{m}}{\delta}M_2^*(G)$.

By Cauchy-Schwarz inequality, the equality holds if and only if there exists a constant k such that for every edge $xy \in E(G)$, $\frac{d_x^2+d_y^2}{\sqrt{d_x d_y}} = \frac{k}{\sqrt{d_x d_y}}$, this implies $d_x^2 + d_y^2 = k$. If $xy, yz \in E(G)$, then $d_x^2 + d_y^2 = d_y^2 + d_z^2$, this implies that $d_y = d_z$.

Consequently, for each vertex $x \in V(G)$, every neighbor of x has the same degree. This holds if and only if G is regular (or) biregular.

Theorem 3.6. *Let G be (n, m) graph. Then $SDD(G) \leq \frac{2mn^2+\chi_3(G)-2n\chi^c(G)}{\delta^2}$ with equality holds if and only if G is regular (or) biregular.*

Proof. From the definition of SDD, we have

$$\begin{aligned} SDD(G) &= \sum_{xy\in E(G)} \frac{d_x^2 + d_y^2}{d_x d_y} \\ &\leq \frac{1}{\delta^2} \sum_{xy\in E(G)} \Big((n-\epsilon(x))^2 + (n-\epsilon(y))^2\Big) \\ &= \frac{1}{\delta^2} \sum_{xy\in E(G)} \Big((n^2+\epsilon(x)^2 - 2n\epsilon(x)) + (n^2+\epsilon(y)^2-2n\epsilon(y))\Big) \\ &= \frac{1}{\delta^2} \sum_{xy\in E(G)} \Big(2n^2 + (\epsilon(x)^2+\epsilon(y)^2) - 2n(\epsilon(x)+\epsilon(y))\Big) \\ &= \frac{2n^2 m}{\delta^2} + \frac{1}{\delta^2}\sum_{xy\in E(G)} \Big(\epsilon(x)^2+\epsilon(y)^2\Big) - \frac{2n}{\delta^2}\sum_{xy\in E(G)}\Big(\epsilon(x)+\epsilon(y)\Big) \\ &= \frac{2n^2 m}{\delta^2} + \frac{1}{\delta^2}\chi_3(G) - \frac{2n}{\delta^2}\chi^c(G). \end{aligned}$$

Lemma 3.7. *Suppose a_i and b_i, $1 \leq i \leq n$ are positive real numbers, then*

$$\left| n\sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \beta(n)(A-a)(B-b),$$

where a, b, A and B are real constants, that for each i, $1 \leq i \leq n$, $a \leq a_i \leq A$ and $b \leq b_i \leq B$. Further, $\beta(n) = n\left\lceil \frac{n}{2} \right\rceil (1 - \frac{1}{n}\left\lceil \frac{n}{2} \right\rceil)$.

Theorem 3.8. *Let G be (n, m) graph. The $SDD(G) \leq \frac{F(G)M_2^*(G)}{m} - \frac{2\beta(m)(\Delta^2-\delta^2)^2}{\delta^2\Delta^2 m}$ with equality holds if and only if G is regular, where $\beta(m) = m\left\lceil \frac{m}{2} \right\rceil \left(1 - \frac{1}{m}\left\lceil \frac{m}{2} \right\rceil\right)$.*

Proof. By setting $a_i = \frac{1}{d_x d_y}$, $b_i = d_x^2 + d_y^2$, $a = \frac{1}{\delta^2}$, $A = \frac{1}{\Delta^2}$, $b = 2\delta^2$ and $B = 2\Delta^2$, in

Lemma 3.7, we obtain

$$\left| m \sum_{xy \in E(G)} \frac{(d_x^2 + d_y^2)}{d_x d_y} - \sum_{xy \in E(G)} \frac{1}{d_x d_y} \sum_{xy \in E(G)} (d_x^2 + d_y^2) \right| \leq \beta(m) \Big(\frac{1}{\Delta^2} - \frac{1}{\delta^2} \Big) (2\Delta^2 - 2\delta^2).$$

This implies, $m\, SDD(G) - M_2^*(G)F(G) \leq 2\beta(m)\Big(\frac{\delta^2 - \Delta^2}{\delta^2\Delta^2}\Big)(\Delta^2 - \delta^2)$. Hence $SDD(G) \leq \frac{M_2^*(G)F(G)}{m} - 2\beta(m)\frac{(\Delta^2-\delta^2)^2}{m\delta^2\Delta^2}$ with equality if and only if $\delta = \Delta$. Thus G is regular.

4. Conclusion

symmetric division deg index is recently devolved topological index which is used in chemistry. In this article, we have found some new upper bounds for above index for a given connected graph.

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