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NEW LOWER BOUNDS FOR SYMMETRIC DIVISION DEGREE INVARIANT OF GRAPHS

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Abstract. Topological invariants are such numbers or set of numbers that describe topology of structures.Virtually 200 topological invariants are calculated so far. The prognostication of physical, chemical, and biological attributes of organic compounds is an important and still unsolved problem of computational chemistry. Topological invariant is the tool to predict the physiochemical properties such as boiling point, melting point, density, viscosity, and polarity of organic compounds. In this paper, a comparative study of the symmetric division degree topological invariant with some well-known and mostly used graph invariants in a given graph is performed.

1. Introduction

Graph theory has played a good role in chemistry in the last decades. Topological invariants investigate the features of graphs that persist constant after continual changing in graphs. They describe symmetry of chemical structures with a number and then work for the improvement of $QSAR$ and $QSPR$ which both are employed to build a connection among the molecular structure and mathematical tools. These invariants are useful to associate physiochemical properties of compounds and they are independent of pictorial representation [**15**]. Among three categories of molecular descriptors, vertex degree-based invariant are considerably more significant. Graph theory and molecular invariants are playing a vital role in analyzing the physiochemical properties of organic compounds.

The symmetric division degree invariant was studied by Vukicevic et al. [**13**] as a remarkable predictor of total surface area of polychlorobiphenyls. It is one of discrete Adriatic indices that showed good predictive properties on the testing sets

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provided by International Academy of Mathematical Chemistry. The symmetric division degree invariant which is defined as $SDD(\Gamma) = \sum_{xy\in E(\Gamma)} \left(\frac{\lambda_\Gamma(x)}{\lambda_\Gamma(y)} + \frac{\lambda_\Gamma(y)}{\lambda_\Gamma(x))}\right)$, where $\lambda_\Gamma(x)$ and $\lambda_\Gamma(y)$ are the degrees of vertices x and y respectively.

Furtula et al. [**1**] established some structural analysis and chemical applicability of the SDD invariant. Some mathematical properties of SDD invariant in terms of structure of a graph are investigated in [**16**]. Vasilev [**14**] and Palacios [**4**] provided the different types of lower and upper bounds of symmetric division deg invariant in some classes of graphs and determined the corresponding extremal graphs. Aguilar-Sanchez et al. [**19**] obtained new inequalities for the variable symmetric division deg invariant and they were characterized extremal graphs with respect to them. The mathematical relations between the symmetric division deg invariant with Sombor invariant and arithmetic-geometric invariant were investigated by Wang et al. [**17**] and Rodríguez et al. [**18**], respectively. Several papers have been appeared in literature addressing the mathematical aspects of this descriptor; for example see [**2, 3, 7, 8**]. In this paper, we investigate some properties of this graph invariant in terms of orbit structure of a graph and then we explore new bounds for symmetric division deg invariant.

Let Γ be a finite simple connected graph with vertex set $V(\Gamma)$ and edge set $E(\Gamma)$. We denote by δ and Δ the minimum and maximum vertex degrees of Γ respectively.

The Zagreb invariants are among the oldest topological invariants 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

$$M_1(\Gamma) = \sum_{xy\in E(\Gamma)} (\lambda_\Gamma(x) + \lambda_\Gamma(y))$$

and

$$M_2(\Gamma) = \sum_{xy\in E(\Gamma)} (\lambda_\Gamma(x)\lambda_\Gamma(y)).$$

A modification Zagreb invariants was proposed by Nikolic et al. [**9**] in 2003. The first and second modified Zagreb invariants of Γ are defined as

$$M_1^*(\Gamma) = \sum_{x\in V(\Gamma)} \frac{1}{\lambda_\Gamma(x)^2}$$

and

$$M_2^*(\Gamma) = \sum_{xy\in E(\Gamma)} \frac{1}{\lambda_\Gamma(x)\lambda_\Gamma(y)}.$$

The multiplicative version of Zagreb invariants were introduced by Todeschini and Consonni [**20**] in 2010. They are defined as

$$\pi_1(\Gamma) = \prod_{x\in V(\Gamma)} \lambda_\Gamma(x)^2$$

and

$$\pi_2(\Gamma) = \prod_{xy \in E(\Gamma)} \lambda_\Gamma(x)\lambda_\Gamma(y).$$

In 1975, Randić [**12**] proposed a structure descriptor, based on the end -vertex degrees of edges in a graph, called branching invariant that later became the well-known Randić connectivity invariant. The Randić invariant of Γ is defined as

$$R(\Gamma) = \sum_{xy \in E(\Gamma)} \frac{1}{\sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)}}.$$

It gave rise to a number of generalizations. The most common one arises by varying the exponent α in the edge contribution $(\lambda_\Gamma(x)\lambda_\Gamma(y))^\alpha$. The α-Randić invariant is then defined as

$$R_\alpha(\Gamma) = \sum_{xy \in E(\Gamma)} (\lambda_\Gamma(x)\lambda_\Gamma(y))^\alpha.$$

The F-invariant and multiplicative F-invariant of a connected graph Γ are respectively, defined as

$$F(\Gamma) = \sum_{xy \in E(\Gamma)} (\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2)$$

and

$$F^*(\Gamma) = \prod_{xy \in E(\Gamma)} (\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2).$$

The α-F-invariant of Γ is defined as $F_\alpha(\Gamma) = \sum\limits_{xy \in E(\Gamma)} (\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2)^\alpha$.

2. Bounds for SDD

Let $a_1, a_2, \ldots, a_s$ be positive real numbers.
The arithmetic mean of $a_1, a_2, \ldots, a_s$ is equal to $AM(a_1, a_2, \ldots, a_s) = \frac{a_1+a_2+\ldots+a_s}{s}$.
The geometric mean of $a_1, a_2, \ldots, a_s$ is equal to $GM(a_1, a_2, \ldots, a_s) = \sqrt[s]{a_1 a_2 \ldots a_s}$.
The harmonic mean of $a_1, a_2, \ldots, a_s$ is equal to $HM(a_1, a_2, \ldots, a_s) = \frac{s}{\frac{1}{a_1}+\frac{1}{a_2}+\ldots+\frac{1}{a_s}}$.
Related to these means, we have the following lemma.

LEMMA 2.1. *(Arithmetic-Geometric-Harmonic Mean Inequality) Let $a_1, a_2, \ldots, a_s$ be positive real numbers. Then*

$$AM(a_1, a_2, \ldots, a_s) \geqslant GM(a_1, a_2, \ldots, a_s) \geqslant HM(a_1, a_2, \ldots, a_s),$$

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

THEOREM 2.1. *Let Γ be a connected graph with m edges. Then $SDD(\Gamma) \geqslant \frac{2m^2\delta^2}{M_2(\Gamma)}$ with equality if and only if Γ is regular.*

PROOF. Using the arithmetic-harmonic mean inequality, we get

$$\begin{aligned}
\frac{m}{SDD} = \frac{m}{\sum\limits_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}} &\leqslant \frac{m}{\sum\limits_{xy\in E(\Gamma)} \frac{2\delta^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}} \\
&= \frac{1}{2\delta^2}\frac{m}{\sum\limits_{xy\in E(\Gamma)} \frac{1}{\lambda_\Gamma(x)\lambda_\Gamma(y)}} \\
&\leqslant \frac{1}{2m\delta^2}\sum_{xy\in E(\Gamma)} \lambda_\Gamma(x)\lambda_\Gamma(y) \\
&= \frac{1}{2m\delta^2} M_2(\Gamma). \qquad (2.1)
\end{aligned}$$

Equality (2.1) holds if and only if $\lambda_\Gamma(x) = \lambda_\Gamma(y) = \delta$ for any edge $xy \in E(\Gamma)$, this implies that Γ is regular. Equality (2.1) holds if and only if there exists a constant c such that $\lambda_\Gamma(x)\lambda_\Gamma(y) = c$ for each $xy \in E(\Gamma)$. If $xy, xz \in E(\Gamma)$, then $\lambda_\Gamma(x)\lambda_\Gamma(y) = \lambda_x\lambda_z$ which is easily simplified into $\lambda_\Gamma(y) = \lambda_z$. Consequently for each vertex $x \in V(\Gamma)$, every neighbor of x has the same degree, which implies that Γ is regular (or) biregular. □

THEOREM 2.2. *For any connected graph* Γ, $SDD(\Gamma) \geqslant m \sqrt[m]{\frac{F^*(\Gamma)}{\pi_2(\Gamma)}}$ *with equality if and only if* Γ *is regular (or) biregular.*

PROOF. Using the arithmetic-harmonic mean inequality, we obtain

$$\begin{aligned}
\frac{SDD(\Gamma)}{m} &= \frac{1}{m}\sum_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \\
&\geqslant \sqrt[m]{\prod_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}} \\
&= \left(\sqrt[m]{\frac{\prod\limits_{xy\in E(\Gamma)} (\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2)}{\prod\limits_{xy\in E(\Gamma)} \lambda_\Gamma(x)\lambda_\Gamma(y)}}\right).
\end{aligned}$$

$$\frac{SDD(\Gamma)}{m} \geqslant \sqrt[m]{\frac{F^*(\Gamma)}{\pi_2(\Gamma)}}. \qquad (2.2)$$

The equality holds if and only if there exists a constant c such that $\frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} = c$ for each edge $xy \in E(\Gamma)$. Thus Γ is regular (or) biregular. □

THEOREM 2.3. *For any graph* Γ *with atleast two vertices,* $SDD(\Gamma) \geqslant 2\,R_{-1}(\Gamma)$ *with equality if and only if* Γ *is a path on two vertices.*

PROOF. Since for each edge $xy \in E(\Gamma)$, $\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2 \geqslant 2$, we obtain;

$$SDD(\Gamma) = \sum_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \geqslant \sum_{xy\in E(\Gamma)} \frac{2}{\lambda_\Gamma(x)\,\lambda_\Gamma(y)} = 2\,R_{-1}(\Gamma).$$

The equality holds if and only if for each edge $xy \in E(\Gamma)$, $\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2 = 2$, which implies that Γ is a path on two vertices. □

THEOREM 2.4. *For any graph* Γ, $SDD(\Gamma) \geqslant \frac{2\delta^2 m^2}{\Delta^3\, R(\Gamma)}$ *with equality if and only if* Γ *is regular (or) biregular.*

PROOF. Using the arithmetic-harmonic mean inequality, we obtain

$$\begin{aligned}
\frac{m}{R(\Gamma)} = \frac{m}{\sum\limits_{xy\in E(\Gamma)} \frac{1}{\sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)}}} &\leqslant \frac{1}{m}\sum_{xy\in E(\Gamma)} \sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)} \\
&= \frac{1}{m}\sum_{xy\in E(\Gamma)} \sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big(\frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}\Big) \\
&= \frac{1}{m}\sum_{xy\in E(\Gamma)} \Big(\frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big)\frac{(\lambda_\Gamma(x)\lambda_\Gamma(y))^{\frac{3}{2}}}{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2} \\
&\leqslant \frac{1}{m}SDD(\Gamma)\Big(\frac{(\Delta^2)^{\frac{3}{2}}}{2\delta^2}\Big) \\
&= \frac{1}{m}SDD(\Gamma)\Big(\frac{\Delta^3}{2\delta^2}\Big).
\end{aligned}$$

The first inequality holds if and only if there exists a constant c such that for every edge $xy \in E(\Gamma), \sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)} = c$, this holds if and only if Γ is regular (or) biregular. Also the second equality holds if and only if Γ is regular (or) biregular. Therefore $SDD(\Gamma) \geqslant \frac{2m^2\delta^2}{\Delta^3\, R(\Gamma)}$ with equality if and only if Γ is regular (or) biregular. □

THEOREM 2.5. *Let* Γ *be a graph with* t *pendent vertices and minimal non-pendent vertex degree* δ_1. *Then* $SDD(\Gamma) \geqslant \frac{2(m-t)\delta_1^2 + \Delta\, t(1+\delta_1^2)}{\Delta^2}$ *with equality if and only if* Γ *is regular (or)* $(1,\Delta)$*-biregular.*

PROOF. From the definition of SDD, we have

$$\begin{aligned}
SDD(\Gamma) &= \sum_{xy\in E(\Gamma),\ \lambda_\Gamma(x),\lambda_\Gamma(y)\neq 1} \frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} + \sum_{xy\in E(\Gamma),\, \lambda_\Gamma(x)=1} \frac{1 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(y)} \\
&\geqslant (m-t)\Big(\frac{2\delta_1^2}{\Delta^2}\Big) + t\Big(\frac{1+\delta_1^2}{\Delta}\Big) \\
&= \frac{2(m-t)\delta_1^2 + \Delta\, t(1+\delta_1^2)}{\Delta^2}.
\end{aligned}$$

Equality holds if and only if $\lambda_\Gamma(x) = \Delta = \delta_1$, for each non-pendent vertex $x \in V(\Gamma)$. This implies that Γ is $(1, \Delta)$-biregular if $t > 0$ and Γ is regular if $t = 0$. $\square$

Corollary 2.1. *Let Γ be a graph without pendent vertices. Then $SDD(\Gamma) \geqslant \frac{2m\delta^2}{\Delta^2}$ with equality if and only if Γ is regular.*

Proof. By setting $t = 0$ and $\delta_1 = \delta$ in Theorem 2.5, we can get the required result. $\square$

The inverse sum indeg invariant of Γ is defined as $ISI(\Gamma) = \sum\limits_{xy \in E(\Gamma)} \frac{\lambda_\Gamma(x)\lambda_\Gamma(y)}{\lambda_\Gamma(x)+\lambda_\Gamma(y)}$.

Theorem 2.6. *For any graph Γ, $SDD(\Gamma) \geqslant \frac{4\delta}{\Delta^2} ISI(\Gamma)$. Equality holds if and only if Γ is regular.*

Proof. By geometric-quadratic mean inequality, $\sqrt{xy} \leqslant \sqrt{\frac{x^2+y^2}{2}}$. By squaring it and applying to the numerators of edge contributions, we have

$$\frac{\lambda_\Gamma(x)\lambda_\Gamma(y)}{\lambda_\Gamma(x)+\lambda_\Gamma(y)} \leqslant \frac{1}{2}\Big(\frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)+\lambda_\Gamma(y)}\Big).$$

An upper bound for the right-hand term can be obtained by decreasing the denominators as

$$\begin{aligned}
\frac{1}{2}\Big(\frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)+\lambda_\Gamma(y)}\Big) &\leqslant \frac{1}{4\delta}(\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2)\\
&= \frac{1}{4\delta}\Big(\frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big)(\lambda_\Gamma(x)\lambda_\Gamma(y))\\
&\leqslant \frac{\Delta^2}{4\delta}\Big(\frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big).
\end{aligned}$$

By summing over all edges of Γ, we get

$$\sum_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)\lambda_\Gamma(y)}{\lambda_\Gamma(x)+\lambda_\Gamma(y)} \leqslant \sum_{xy\in E(\Gamma)} \frac{\Delta^2}{4\delta}\Big(\frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big).$$

Hence, $SDD(\Gamma) \geqslant \frac{4\delta}{\Delta^2} ISI(\Gamma)$.

The equality holds if and only if $\delta = \lambda_\Gamma(x) = \lambda_\Gamma(y) = \Delta$, for each edge $xy \in E(\Gamma)$. This implies that Γ is regular. $\square$

Theorem 2.7. *Let Γ be a graph with m edges. Then $SDD(\Gamma) \geqslant \frac{4\Delta}{\delta^2}(m\delta - ISI(\Gamma))$ with equality if and only if Γ is regular.*

Proof. We start from $\lambda_\Gamma(x)\lambda_\Gamma(y) = \frac{1}{2}\Big[(\lambda_\Gamma(x)+\lambda_\Gamma(y))^2 - (\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2)\Big]$. By dividing this expression for the contribution throughout $\lambda_\Gamma(x)+\lambda_\Gamma(y)$, we get following expression for the contribution of edges to SDD,

$$\frac{\lambda_\Gamma(x)\lambda_\Gamma(y)}{\lambda_\Gamma(x)+\lambda_\Gamma(y)} = \frac{1}{2}\Big[(\lambda_\Gamma(x)+\lambda_\Gamma(y)) - \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)+\lambda_\Gamma(y)}\Big].$$

Since $2\delta \leqslant \lambda_\Gamma(x) + \lambda_\Gamma(y) \leqslant 2\Delta$, for any edge xy in Γ. Therefore

$$\sum_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)\lambda_\Gamma(y)}{\lambda_\Gamma(x)+\lambda_\Gamma(y)} \geqslant \frac{1}{2}\Big[2m\delta - \sum_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big(\frac{\delta^2}{2\Delta}\Big)\Big].$$

This implies $ISI(\Gamma) \geqslant m\delta - \Big(\frac{\delta^2}{4\Delta}\Big)SDD(\Gamma)$. Equality holds if and only if $\delta = \lambda_\Gamma(x) = \lambda_\Gamma(y) = \Delta$, for each edge $xy \in E(\Gamma)$. This implies that Γ is regular. □

Lemma 2.2. *(Cauchy-Schwarz inequality) Let* $X = (x_1, x_2 \ldots x_n)$ *and* $Y = (y_1, y_2, \ldots, y_n)$ *be two sequences of real numbers. Then* $\Big(\sum\limits_{i=1}^{n} x_i y_i\Big)^2 \leqslant \sum\limits_{i=1}^{n} x_i^2 \sum\limits_{i=1}^{n} y_i^2$ *with equality if and only if the sequences* X *and* Y *are proportional, that is, there exists a constant* c *such that* $x_i = cy_i$*, for each* $1 \leqslant i \leqslant n$.

As a special case of the Cauchy-Schwarz inequality, when $y_1 = y_2 = \ldots = y_n$*, we get the following result.*

Corollary 2.2. *Let* $x_1, x_2, \ldots, x_n$ *be real numbers. Then* $\Big(\sum\limits_{i=1}^{n} x_i\Big)^2 \leqslant n\sum\limits_{i=1}^{n} x_i^2$ *with equality if and only if* $x_1 = x_2 = \ldots = x_n$.

Theorem 2.8. *For any graph* Γ, $SDD(\Gamma) \geqslant \frac{(R(\Gamma))^2}{F_{-1}(\Gamma)}$ *with equality if and only if* Γ *is regular (or) biregular.*

Proof. Using Cauchy-Schwarz inequality, we obtain;

$$\begin{aligned} (R(\Gamma))^2 &= \Big(\sum_{xy\in E(\Gamma)} \frac{1}{\sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)}}\Big)^2 \\ &= \Big(\sum_{xy\in E(\Gamma)} \frac{\sqrt{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}}{\sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)}} \frac{1}{\sqrt{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}}\Big)^2 \\ &\leqslant \sum_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \sum_{xy\in E(\Gamma)} \frac{1}{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2} \\ &= SDD(\Gamma)F_{-1}(\Gamma). \end{aligned} \tag{2.3}$$

Equality holds if and only if there exists a constant c such that for every edge xy in Γ,

$$\frac{\sqrt{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}}{\sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)}} = \frac{c}{\sqrt{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}},$$

this implies that

$$c^2 = \frac{(\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}.$$

If $xy, yz \in E(\Gamma)$, then $\frac{(\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} = \frac{(\lambda_\Gamma(x)^2+\lambda_z^2)^2}{\lambda_x\lambda_z}$, which is easily simplified into

$$\lambda_z(\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2)^2 - \lambda_\Gamma(y)(\lambda_\Gamma(x)^2+\lambda_z^2)^2 = 0.$$

By direct calculation, we get $(\lambda_z - \lambda_\Gamma(y))\Big(\lambda_\Gamma(x)^4 - \lambda_z\lambda_y(\lambda_z^2 + \lambda_\Gamma(y)^2 + 2\lambda_x^2 + \lambda_z\lambda_y)\Big) = 0$. since $\lambda_\Gamma(x)^4 - \lambda_z\lambda_y(\lambda_z^2 + \lambda_\Gamma(y)^2 + 2\lambda_x^2 + \lambda_z\lambda_y) \neq 0$, so $\lambda_z = \lambda_\Gamma(y)$.

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

LEMMA 2.3. *(Pólya-Szego inequality* [**21**]*) Let* $0 < m_1 \leqslant x_i \leqslant M_1$ *and* $0 < m_2 \leqslant y_i \leqslant M_2$, *for* $1 \leqslant i \leqslant n$. *Then*

$$\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i^2 \leqslant \frac{1}{4}\Big(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\Big)^2 (\sum_{i=1}^{n} x_iy_i)^2.$$

THEOREM 2.9. *Let* Γ *be a simple connected graph on s vertices and* m *edges and let* t, Δ *and* δ_1 *denote the number of pendent vertices, maximum vertex degree and minimum nonpendant vertex degree of* Γ, *respectively. Then*$SDD(\Gamma) \geqslant \frac{16(m-t)\delta_1^6}{\Big(\delta_1^4+\Delta^4\Big)^2} + \frac{t\delta_1^2+1}{\Delta}$ *with equality if and only if* Γ *is regular.*

PROOF. For $2 \leqslant \delta_1 \leqslant \lambda_\Gamma(x) \leqslant \Delta$, we have $\frac{2{\delta_1}^2}{\Delta^2} \leqslant \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \leqslant \frac{2\Delta^2}{\delta_1^2}$ for any edge xy in Γ. Setting $m_1 = \frac{2\delta_1^2}{\Delta^2}$,$x_i = \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}$, $1 \leqslant i \leqslant m$, $M_1 = \frac{2\Delta^2}{\delta_1^2}$ and $m_2 = y_i = M_2 = 1$, $1 \leqslant i \leqslant m$ in Polya-Szego inequality (Lemma 2.3), we obtain

$$\sum_{xy\in E(\Gamma),\lambda_\Gamma(x),\ \lambda_\Gamma(y)\neq 1} \Big(\frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big)^2 \sum_{xy\in E(\Gamma),\lambda_\Gamma(x),\ \lambda_\Gamma(y)\neq 1} \Big(1\Big)^2$$

$$\leqslant \frac{1}{4}\left(\sqrt{\frac{\frac{2\Delta^2}{\delta_1^2}}{\frac{2\delta_1^2}{\Delta^2}}} + \sqrt{\frac{\frac{2\delta_1^2}{\Delta^2}}{\frac{2\Delta^2}{\delta_1^2}}}\right)^2 \left(\sum_{xy\in E(\Gamma),\lambda_\Gamma(x),\ \lambda_\Gamma(y)\neq 1} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\right)^2.$$

$$(m-t)\sum_{\substack{xy\in E(\Gamma),\\ \lambda_\Gamma(x),\ \lambda_\Gamma(y)\neq 1}} \Big(\frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big)^2 \leqslant \frac{1}{4}\Big(\frac{\delta_1^2}{\Delta^2} + \frac{\Delta^2}{\delta_1^2}\Big)^2 \left(\sum_{\substack{xy\in E(\Gamma),\\ \lambda_\Gamma(x),\ \lambda_\Gamma(y)\neq 1}} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\right)^2.$$

$$\frac{16(m-t)\delta_1^6}{\Big(\delta_1^4+\Delta^4\Big)^2} \leqslant \left(\sum_{\substack{xy\in E(\Gamma),\\ \lambda_\Gamma(x),\ \lambda_\Gamma(y)\neq 1}} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\right)^2. \tag{2.4}$$

It is easy to see that

$$\begin{aligned} SDD(\Gamma) &= \sum_{\substack{xy\in E(\Gamma),\\ \lambda_\Gamma(x),\ \lambda_\Gamma(y)\neq 1}} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} + \sum_{\substack{xy\in E(\Gamma),\\ \lambda_\Gamma(y)=1}} \frac{\lambda_\Gamma(x)^2+1}{\lambda_\Gamma(x)} \\ &\geqslant \sum_{\substack{xy\in E(\Gamma),\\ \lambda_\Gamma(x),\ \lambda_\Gamma(y)\neq 1}} \frac{\lambda_\Gamma(x)^2+\lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} + \frac{t\Big(\delta_1^2+1}{\Delta}\Big). \qquad (2.5) \end{aligned}$$

From (2.4) and (2.5), we have $SDD(\Gamma) \geqslant \frac{16(m-t)\delta_1^6}{\left(\delta_1^4+\Delta^4\right)^2} + \frac{t\delta_1^2+1}{\Delta}$ with equality if and only if Γ is regular. $\square$

THEOREM 2.10. *Let Γ be a graph on s vertices and m edges. Then $SDD(\Gamma) \geqslant \frac{M_2^*(\Gamma)F(\Gamma)}{m}$ with equality if and only if Γ is regular.*

PROOF. One can observe that $\delta^2 \leqslant \lambda_\Gamma(x)\lambda_\Gamma(y) \leqslant \Delta^2$ for any edge xy in Γ and setting $m_1 = \frac{1}{\delta^2}$,$x_i = \frac{1}{\lambda_\Gamma(x)\lambda_\Gamma(y)}$, $1 \leqslant i \leqslant m$, $M_1 = \frac{1}{\Delta^2}$ and $m_2 = 2\delta^2$,$y_i = \lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2$,$M_2 = 2\Delta^2$, $1 \leqslant i \leqslant m$ in Polya-Szego inequality (Lemma 2.3), we obtain

$$\sum_{xy\in E(\Gamma)} \Big(\frac{1}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big)^2 \sum_{xy\in E(\Gamma)} \Big(\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2\Big)^2 \leqslant \Big(\sum_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big)^2.$$

By Cauchy inequality, we have

$$\sum_{xy\in E(\Gamma)} \Big(\frac{1}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big)^2 \sum_{xy\in E(\Gamma)} \Big(\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2\Big)^2$$

$$\geqslant \frac{1}{m^2}\Big(\sum_{xy\in E(\Gamma)} \frac{1}{\lambda_\Gamma(x)\lambda_\Gamma(y)}\Big)^2\Big(\sum_{xy\in E(\Gamma)} \Big(\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2\Big)^2 = \frac{1}{m^2}\Big(M_2^*(\Gamma)F(\Gamma)\Big)^2.$$

Combining the above two inequality, we obtain

$$SDD(\Gamma) \geqslant \frac{M_2^*(\Gamma)F(\Gamma)}{m}.$$

The equality holds if and only if $\lambda_\Gamma(x)) = \lambda_\Gamma(y) = \delta = \Delta$ for each $xy \in E(\Gamma)$ which implies that Γ is regular. $\square$

The (a, b)-eccentric Zagreb invariant is defined for a connected graph Γ as

$$\xi_{a,b}(\Gamma) = \frac{1}{2} \sum_{xy\in E(\Gamma)} \Big(\epsilon_x^a\epsilon_y^b + \epsilon_x^b\epsilon_y^a\Big).$$

Note that $\xi_{0,0}(\Gamma) = E(\Gamma)$,$2\xi_{1,0}(\Gamma) = \xi(\Gamma)$ and $\xi_{1,1}(\Gamma) = \xi_2(\Gamma)$.

LEMMA 2.4. [**5**] *Let Γ be a nontrivial connected graph of order s. For each vertex $x \in V(\Gamma)$, $\epsilon_x \leqslant (s - \lambda_\Gamma(x))$ with equality if and only if $\Gamma \cong P_4$ or $\Gamma \cong K_s - iK_2$,$0 \leqslant i \leqslant \left\lfloor \frac{s}{2} \right\rfloor$, where P_4 denotes the path on 4 vertices and $K_s - iK_2$ denotes the graph obtained from the complete graph K_s by removing i independent edges.*

THEOREM 2.11. *Let Γ be a graph on s vertices and m edges. Then $SDD(\Gamma) \geqslant \frac{1}{2\delta^2}\sqrt{\frac{m}{\sigma}}$, where $\sigma = ms^4 + 2s^2\xi_{2,0}(\Gamma) - 4s^3\xi_{1,0}(\Gamma) - 4s\xi_{2,1}(\Gamma) + 4s^2\xi(\Gamma) + \xi^2(\Gamma)$. Equality holds if and only if $\Gamma \cong P_4$ or $\Gamma \cong K_s - iK_2$,$0 \leqslant i \leqslant \left\lfloor \frac{s}{2} \right\rfloor$.*

PROOF. Let Γ be a nontrivial connected graph on s vertices. Then

$$\begin{aligned}
\Big(\frac{m}{SDD(\Gamma)}\Big)^2 &= \Big(\frac{m}{\sum\limits_{xy\in E(\Gamma)} \frac{\lambda_\Gamma^2(x)+\lambda_\Gamma^2(y)}{\lambda_\Gamma(x)\lambda_\Gamma(y)}}\Big)^2 \\
&\leqslant \Big(\frac{1}{m}\sum_{xy\in E(\Gamma)} \frac{\lambda_\Gamma(x)\lambda_\Gamma(y)}{\lambda_\Gamma^2(x)+\lambda_\Gamma^2(y)}\Big)^2 \\
&\leqslant \frac{1}{m}\sum_{xy\in E(\Gamma)} \Big(\frac{\lambda_\Gamma(x)\lambda_\Gamma(y)}{\lambda_\Gamma^2(x)+\lambda_\Gamma^2(y)}\Big)^2 \\
&\leqslant \frac{1}{4\delta^4 m}\sum_{xy\in E(\Gamma)} (\lambda_\Gamma(x)\lambda_\Gamma(y))^2
\end{aligned}$$

For each vertex $y \in V(\Gamma)$, we have $\epsilon_y \leqslant s - \lambda_\Gamma(y)$. Thus

$$\begin{aligned}
\Big(\frac{m}{SDD(\Gamma)}\Big)^2 &\leqslant \frac{1}{4\delta^4 m}\sum_{xy\in E(\Gamma)} \Big((s-\epsilon_x)(s-\epsilon_y)\Big)^2 \\
&= \frac{1}{4\delta^4 m}\sum_{xy\in E(\Gamma)} \Big(s^4 + s^2(\epsilon_x^2+\epsilon_y^2) - 2s^3(\epsilon_x+\epsilon_y) \qquad (2.6) \\
&- 2s(\epsilon_x^2\epsilon_y + \epsilon_x\epsilon_y^2) + 4s^2\epsilon_x\epsilon_y + \epsilon_x^2\epsilon_y^2\Big) \\
&= \frac{1}{4\delta^4 m}\Big(ms^4 + 2s^2\xi_{2,0}(\Gamma) - 4s^3\xi_{1,0}(\Gamma) \\
&- 4s\xi_{2,1}(\Gamma) + 4s^2\xi(\Gamma) + \xi^2(\Gamma)\Big).
\end{aligned}$$

By Lemma 2.4, the equality holds if and only if $\lambda_\Gamma(y) = s - \epsilon_x$ for each vertex $x \in V(\Gamma)$, which by Lemma 2.4, implies that $\Gamma \cong P_4$ or $\Gamma \cong K_s - iK_2, 0 \leqslant i \leqslant \lfloor \frac{s}{2} \rfloor$. $\square$

Let Γ be a connected graph with s vertices and m edges and let $\Delta = \lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_s = \delta > 0,\ \lambda_i = \lambda(i)$ and $\lambda(e_1) \geqslant \lambda(e_2) \geqslant \ldots \geqslant \lambda(e_m)$ be sequences of its vertex
and edge degrees, respectively. We denote $\Delta_{e_1} = \lambda(e_1) + 2$ and $\delta_{e_1} = \lambda(e_m) + 2$. If the vertices x and y are adjacent, we write $x \sim y$.

The first and second Zagreb indices are recalled as $M_1(\Gamma) = \sum\limits_{i=1}^{s} \lambda_i^2 = \sum\limits_{i\sim j}(\lambda_i + \lambda_j)$ and $M_2(\Gamma) = \sum\limits_{i\sim j} \lambda_i\lambda_j$. Bearing in mind that for the edge e connecting the vertices x and y, $\lambda(e) = \lambda_\Gamma(x) + \lambda_\Gamma(y) + 2$, the F-invariant and multiplicative F-invariant are respectively defined as $F(\Gamma) = \sum\limits_{i\sim j}(\lambda_i^2 + \lambda_j^2)$ and $F^*(\Gamma) = \prod\limits_{i\sim j}(\lambda_i^2 + \lambda_j^2)$.

The α- F-invariant and α- Randić invariant are respectively, defined as $F_\alpha(\Gamma) = \sum\limits_{i\sim j}(\lambda_i^2 + \lambda_j^2)^\alpha$ and $R_\alpha(\Gamma) = \sum\limits_{i\sim j}(\lambda_i\lambda_j)^\alpha$, where α is an arbitrary real number.

THEOREM 2.12. *Let Γ be a connected graph. Then* $SDD(\Gamma) \geqslant \frac{1}{\delta_{e_1}+\Delta_{e_1}}\Big(F(\Gamma)F_{-1}(\Gamma) + 4\delta_{e_1}\Delta_{e_1}(R_{-1}(\Gamma))^2\Big)$. *Equality holds if and only if Γ is regular (or) biregular.*

PROOF. 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 $0 < a \leqslant a_i \leqslant A < \infty$. Rennie [**10**] proven

$$\sum_{i=1}^{m} p_i a_i + aA\sum_{i=1}^{m}\frac{p_i}{a_i} \leqslant a + A \tag{2.7}$$

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

By setting $p_i = \frac{\lambda_i^2+\lambda_j^2}{\lambda_i\lambda_j\, SDD(\Gamma)}$,$a_i = \lambda_i\lambda_j$,$a = \delta_{e_1}$ and $A = \Delta_{e_1}$ in (2.7), then

$$\sum_{i=1}^{m}\frac{\lambda_i^2+\lambda_j^2}{\lambda_i\lambda_j\, SDD(\Gamma)}\lambda_i\lambda_j + \delta_{e_1}\Delta_{e_1}\sum_{i=1}^{m}\frac{\lambda_i^2+\lambda_j^2}{\lambda_i\lambda_j\, SDD(\Gamma)}\Big(\frac{1}{\lambda_i\lambda_j}\Big) \leqslant \delta_{e_1} + \Delta_{e_1}$$

$$\Rightarrow \sum_{i=1}^{m}\Big(\lambda_i^2+\lambda_j^2\Big) + \delta_{e_1}\Delta_{e_1}\sum_{i=1}^{m}\frac{\lambda_i^2+\lambda_j^2}{\lambda_i^2\lambda_j^2} \leqslant \Big(\delta_{e_1}+\Delta_{e_1}\Big)SDD(\Gamma)$$

$$\Rightarrow\ F(\Gamma) + \delta_{e_1}\Delta_{e_1}\sum_{i\sim j}\frac{\lambda_i^2+\lambda_j^2}{\lambda_i^2\lambda_j^2} \leqslant \Big(\delta_{e_1}+\Delta_{e_1}\Big)SDD(\Gamma). \tag{2.8}$$

Let $x = (x_i)$ and $a = (a_i),\ i = 1, 2, \ldots, m$ be positive real number sequences. Then by [**11**],

$$\sum_{i=1}^{m}\frac{x_i^{r+1}}{a_i^r} \geqslant \frac{\Big(\sum\limits_{i=1}^{m} x_i\Big)^{r+1}}{\Big(\sum\limits_{i=1}^{m} a_i\Big)^{r}} \tag{2.9}$$

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

By setting $r = 1, x_i = \frac{1}{\lambda_i\lambda_j}$ and $a_i = \frac{1}{\lambda_i^2+\lambda_j^2}$ in (2.9), we obtain;

$$\sum_{i\sim j}\frac{\lambda_i^2+\lambda_j^2}{\lambda_i^2\lambda_j^2} \geqslant \frac{\Big(\sum\limits_{i\sim j}\frac{1}{\lambda_i\lambda_j}\Big)^2}{\Big(\sum\limits_{i\sim j}\frac{1}{\lambda_i^2+\lambda_j^2}\Big)} \geqslant \frac{\Big(R_{-1}(\Gamma)\Big)^2}{F_1(\Gamma)} \tag{2.10}$$

Using (2.10) in (2.8), we have

$$SDD(\Gamma) \geqslant \frac{1}{\delta_{e_1}+\Delta_{e_1}}\Big(F(\Gamma)F_{-1}(\Gamma) + \delta_{e_1}\Delta_{e_1}(R_{-1}(\Gamma))^2\Big).$$

The equality in (2.10) holds if and only if for any pair of adjacent vertices $i \sim j$ and $x \sim y$ such that $\frac{1}{\lambda_i} + \frac{1}{\lambda_j} = \frac{1}{\lambda_\Gamma(x)} + \frac{1}{\lambda_\Gamma(y)}$. Let j and x be two vertices adjacent to i, that is, $i \sim j$ and $i \sim x$. Then $\lambda_j = \lambda_\Gamma(x)$. Since Γ is a connected, equality in 2.10 holds if and only if Γ is reqular (or) biregular. Similarly, equality in (2.8) holds if and only if $\lambda_i + \lambda_j = \Delta_{e_1}$ (or) $\lambda_i + \lambda_j = \delta_{e_1}$, for every edge of Γ, that is, Γ is regular or biregular. $\square$

Theorem 2.13. *Let Γ be a connected graph with m edges. Then* $SDD(\Gamma) \geqslant \frac{F(\Gamma)+m(m-1)(F^*(\Gamma))^{\frac{1}{m}}}{M_2(\Gamma)}$ *Equality holds if and only if for any two pair of vertices $i \sim j$ and $x \sim y$ the identity $\frac{\lambda_i}{\lambda_j} + \frac{\lambda_j}{\lambda_i} = \frac{\lambda_\Gamma(x)}{\lambda_\Gamma(y)} + \frac{\lambda_\Gamma(y)}{\lambda_\Gamma(x)}$ and $\lambda_i^2 + \lambda_j^2 = \lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2$ holds.*

Proof. For $r = 1, x_i = \sqrt{\lambda_i^2 + \lambda_j^2}$ and $a_i = \lambda_i\lambda_j$ in (2.9), we obtain;

$$\sum_{i\sim j} \frac{\sqrt{\lambda_i^2 + \lambda_j^2}}{\lambda_i\lambda_j} \geqslant \frac{\left(\sum\limits_{i\sim j} \sqrt{\lambda_i^2 + \lambda_j^2}\right)^2}{\left(\sum\limits_{i=1}^{m} \lambda_i\lambda_j\right)}. \tag{2.11}$$

If $a = (a_i),\ i = 1, 2, \dots, m$ is a positive real number sequences, then by [**6**], we write

$$\left(\sum_{i=1}^{m} \sqrt{a_i}\right)^2 \geqslant \sum_{i=1}^{m} a_i + m(m-1)\left(\prod_{i=1}^{m} a_i\right)^{\frac{1}{m}} \tag{2.12}$$

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

Setting $a_i = \lambda_i^2 + \lambda_j^2$ in (2.12), we have

$$\begin{aligned} \left(\sum_{i=1}^{m} \sqrt{\lambda_i^2 + \lambda_j^2}\right)^2 &\geqslant \sum_{i=1}^{m}(\lambda_i^2 + \lambda_j^2) + m(m-1)\left(\prod_{i=1}^{m}(\lambda_i^2 + \lambda_j^2)\right)^{\frac{1}{m}} \\ &= F(\Gamma) + m(m-1)(F^*(\Gamma))^{\frac{1}{m}}. \end{aligned} \tag{2.13}$$

Using (2.13) in (2.11), we have

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

Equality holds in (2.11) if and only if for any two pair of adjacent vertices $i \sim j$ and $x \sim y$ the identity $\frac{\lambda_i}{\lambda_j} + \frac{\lambda_j}{\lambda_i} = \frac{\lambda_\Gamma(x)}{\lambda_\Gamma(y)} + \frac{\lambda_\Gamma(y)}{\lambda_\Gamma(x)}$ and $\lambda_i^2 + \lambda_j^2 = \lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2$ holds. Equality holds in (2.12) if and only if for any two pair of adjacent vertices $i \sim j$ and $x \sim y$ the identity $\lambda_i^2 + \lambda_j^2 = \lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2$ holds. $\square$

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