

Original Article

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. In this paper, a comparative study of the symmetric division degree topological invariant with some well-known and mostly used graph invariants in a regular (or) biregular graph is performed.

Keywords - Degree, topological invariant, symmetric division deg invariant.

I. 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 [17]. 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. [15] 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 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 S DD invariant. Some mathematical properties of S DD invariant in terms of structure of a graph are investigated in [18]. Vasilev [16] 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. [20] and Rodriguez et al. [21], 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 Trinajstić in 1972. These indices have since been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. They are defined as

$$M_1(\Gamma) = \sum_{xy \in E(\Gamma)} (\lambda_\Gamma(x) + \lambda_\Gamma(y)) \text{ and } M_2(\Gamma) = \sum_{xy \in E(\Gamma)} (\lambda_\Gamma(x)\lambda_\Gamma(y)).$$

The multiplicative version of Zagreb invariants were introduced by Todeschini and Consonni[14] in 2010. They are defined as

$$\pi_1(\Gamma) = \prod_{x \in V(\Gamma)} \lambda_\Gamma(x)^2 \text{ and } \pi_2(\Gamma) = \prod_{xy \in E(\Gamma)} \lambda_\Gamma(x)\lambda_\Gamma(y)$$

In 1975, Randić [13] 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

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

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

II. BOUNDS FOR SDD

Let a_1, a_2, \dots, a_s be positive real numbers.

The arithmetic mean of a_1, a_2, \dots, a_s is equal to $AM(a_1, a_2, \dots, a_s) = \frac{a_1 + a_2 + \dots + a_s}{s}$

The geometric mean a_1, a_2, \dots, a_s is equal to $GM(a_1, a_2, \dots, a_s) = \sqrt[s]{a_1 a_2 \dots a_s}$

The harmonic mean of a_1, a_2, \dots, a_s is equal to $HM(a_1, a_2, \dots, a_s) = \frac{s}{\frac{1}{a_1} + \frac{1}{a_2} + \dots + \frac{1}{a_s}}$

Related to these means, we have the following lemma.

Lemma 2.1. (Arithmetic-Geometric-Harmonic Mean Inequality) Let a_1, a_2, \dots, a_s be positive real numbers. Then $AM(a_1, a_2, \dots, a_s) \geq GM(a_1, a_2, \dots, a_s) \geq HM(a_1, a_2, \dots, a_s)$ with equality if and only if $a_1 = a_2 = \dots = a_s$.

Theorem 2.2. Let Γ be a connected graph with m edges. Then $SDD(\Gamma) \geq \frac{2\delta^2 m^2}{M_2(\Gamma)}$ with equality if and only if Γ is

regular.

Proof:

Using the arithmetic-harmonic mean inequality, we get

$$\frac{m}{SDD(\Gamma)} = \frac{m}{\sum_{xy \in E(\Gamma)} \left(\frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \right)} \leq \frac{m}{\sum_{xy \in E(\Gamma)} \left(\frac{2\delta^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \right)} \tag{1}$$

$$= \frac{1}{2\delta^2} \left(\frac{m}{\sum_{xy \in E(\Gamma)} \left(\frac{1}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \right)} \right) \leq \frac{1}{2m\delta^2} \sum_{xy \in E(\Gamma)} \lambda_\Gamma(x)\lambda_\Gamma(y) \tag{2}$$

$$= \frac{1}{2m\delta^2} M_2(\Gamma) \tag{3}$$

Equality (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 (3) 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 neighbour of x has the same degree, which implies that Γ is regular (or) biregular.

Theorem 2.3. For any connected graph Γ , $SDD(\Gamma) \geq m^m \sqrt{\frac{F^*(\Gamma)}{\pi_2(\Gamma)}}$ with equality if and only if Γ is regular (or)

biregular.

Proof:

Using the arithmetic-harmonic mean inequality, we obtain

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

$$\frac{SDD(\Gamma)}{m} \geq m \sqrt{\frac{F^*(\Gamma)}{\pi_2(\Gamma)}}$$

The equality holds if and only if there exists a constant c such that $\left(\frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \right) = c$ for each edge $xy \in E(\Gamma)$.

Thus Γ is regular (or) biregular.

Theorem 2.4. For any graph Γ with atleast two vertices, $SDD(\Gamma) \geq 2R_{-1}(\Gamma)$ with equality if and only if Γ is a path on two vertices.

Proof:

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

$$SDD(\Gamma) = \sum_{xy \in E(\Gamma)} \left(\frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \right) \geq \sum_{xy \in E(\Gamma)} \left(\frac{2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \right) = 2R_{-1}(\Gamma)$$

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

Proof:

Using the arithmetic-harmonic mean inequality, we obtain

$$\begin{aligned} \frac{m}{R(\Gamma)} &= \frac{m}{\sum_{xy \in E(\Gamma)} \frac{1}{\sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)}}} \\ &\leq \frac{1}{m} \sum_{xy \in E(\Gamma)} \sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)} \\ &= \frac{1}{m} \sum_{xy \in E(\Gamma)} \sqrt{\lambda_\Gamma(x)\lambda_\Gamma(y)} \left(\frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2} \right) \\ &= \frac{1}{m} \sum_{xy \in E(\Gamma)} \left(\frac{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2}{\lambda_\Gamma(x)\lambda_\Gamma(y)} \right) \left(\frac{(\lambda_\Gamma(x)\lambda_\Gamma(y))^{\frac{3}{2}}}{\lambda_\Gamma(x)^2 + \lambda_\Gamma(y)^2} \right) \\ &= \frac{1}{m} SDD(\Gamma) \left(\frac{(\Delta^2)^{\frac{3}{2}}}{2\delta^2} \right) \\ &= \frac{1}{m} SDD(\Gamma) \left(\frac{\Delta^3}{2\delta^2} \right) \end{aligned}$$

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, $SDD(\Gamma) \geq \frac{2\delta^2 m^2}{\Delta^3 R(\Gamma)}$ with equality if and only if Γ is regular (or) biregular.

III. CONCLUSION

In molecular science, one of the key problem is to model a chemical compound and predict its chemical characteristic. Topological invariants consequently determined can assist us with understanding their physical characteristics, synthetic reactivity and natural exercises. Symmetric division deg invariant has productive applications to find heat formation of chemical structures. In this article, the relations between symmetric division deg invariant and other graph invariants of a regular (or) biregular graph are established.

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