Proceedings of the Jangjeon Mathematical Society
24 (2021), No. 3, pp. 389 – 402

www.jangjeon.or.kr
http://dx.doi.org/10.17777/pjms2021.24.3.389

SYMMETRIC DIVISION DEG (SDD) INDEX, SDD AND RANDIĆ MATRICES

K. SRINIVASA RAO AND B. AMUDHA

Abstract. In this paper, the symmetric division deg index of a graph is studied and several bounds for this index are obtained. Also relations between SDD and Randić indices are obtained by means of SDD and Randić matrices.

2020 Mathematics Subject Classification. 05C92, 05C09

Keywords and phrases. Symmetric division deg index, Randić index, bicyclic graphs, second maximum SDD index.

1. Introduction

Let $G = (V(G), E(G))$ be a simple graph with n vertices in the set $V(G)$ and and m edges in the set $E(G)$. For $i = 1, 2, \cdots, n$, the degree of a vertex u_i is denoted by d_{u_i} and assume that $\Delta = d_{u_1} \geq d_{u_2} \geq \cdots d_{u_n} = \delta$. A vertex $u_i \in V(G)$ is said to be pendant vertex if $d_{u_i} = 1$. Molecular descriptors play a remarkable role in mathematical chemistry, especially in QSPR/QSAR investigations. Out of them, a special place is reserved for topological descriptors. Nowadays, there exist hundreds of such topological indices in the literature. One of them is the symmetric division deg index denoted by SDD. This index was determined as a significant predictor of total surface area of polychlorobiphenyls (PCB). Moreover, its extremal graphs obtained with the help of MathChem in [16] have particularly simple and elegant structures. The symmetric division deg index of a connected graph G is defined as

$$SDD(G) = \sum_{uv \in E(G)} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u} \right). \tag{1}$$

The hyper-Zagreb index [15] is defined by

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2.$$

In [6], some lower and upper bounds for SDD index were given and the unicyclic graphs and bicyclic graphs with the maximum and the second maximum SDD indices were determined for $n \geq 5$. In this paper, we pointed out some errors and give our counterexamples, comments, and corrections on some results in [6]. Also we establish new bounds for SDD matrix eigenvalues, obtained different bounds in terms of the trace of the SDD matrix to Randić matrix.

2. Main results

2.1. **Errors in lower bounds.** The main results of the paper [6] deal with lower and upper bounds for the symmetric division deg index of connected graphs. Also, some Nordhaus-Gaddum-type relations for the symmetric division deg index of a connected graph were established for unicyclic and bicyclic graphs.

We identified errors in Theorem 3.4, Corollary 3.5 and Corollary 3.6 of [6]. The following is the Theorem 3.4 in [6]:

Theorem 2.1. [6] *Let G be a simple connected graph with order n, size m, p pendant vertices, maximum degree Δ and minimum degree δ_1. Then*

$$SDD(G) \geq p\left(\frac{\delta_1^2+1}{\delta_1}\right) + \sqrt{T} - 2(m-p)$$

where $T = \dfrac{\left(n - p(\Delta + \frac{1}{\Delta})\right)^2 \left(HM(G) - p(1+\Delta^2)\right)}{m-p} - 4(m-p)^2\left(\dfrac{\Delta}{\delta_1} + \dfrac{\delta_1}{\Delta}\right)$.
The equality holds for regular and star graphs.

Note the graphs in Figure 1.

- If G is a star graph, then $m-p=0$ and the number T is not defined.

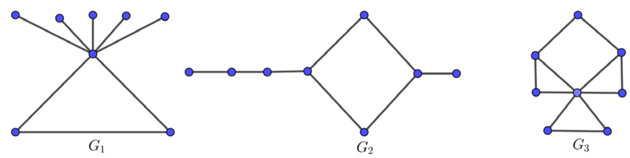

Figure 1. Examples that contradict with Theorem 2.1

- For the graph G_1, substituting $HM(G_1) = 498$, $n = 8$, $\Delta = 7$, $m = 8$, $p = 5$, $\delta_1 = 2$ in the RHS of the above inequality, we get $p\left(\frac{\delta_1^2+1}{\delta_1}\right) + \sqrt{T} - 2(m-p) = 219.1$, whereas $SDD(G) = 45.2875$.
- For the graph G_2, substituting $HM(G_2)$=166, $n = 8$, $\Delta = 3$, $m = 8$, $p = 2$, $\delta_1 = 2$ in T, we get $T = \dfrac{\left(n - p(\Delta + \frac{1}{\Delta})\right)^2 \left(HM(G) - p(1+\Delta^2)\right)}{m-p} - 4(m-p)^2\left(\dfrac{\Delta}{\delta_1} + \dfrac{\delta_1}{\Delta}\right) = -48.2963$. This implies that the RHS of the inequality is an imaginary number.
- For the graph G_3, substituting $HM(G_3)$=534, n=8, $\Delta = 6$, $m = 11$, $p = 0$, $\delta_1 = 2$ in T, we get $T = \dfrac{\left(n - p(\Delta + \frac{1}{\Delta})\right)^2 \left(HM(G) - p(1+\Delta^2)\right)}{m-p} - 4(m-p)^2\left(\dfrac{\Delta}{\delta_1} + \dfrac{\delta_1}{\Delta}\right) = -312.86$. This implies that the RHS of the inequality is an imaginary number.

With these examples, we can conclude that Theorem 3.4, Corollaries 3.5 and 3.6 in [6] have faults. This is due to misutilization of the Cauchy-Schwartz inequality in Ozeki's inequality.

2.2. **Upper bounds-equality cases.** In [6], some upper bounds for SDD index were obtained in Theorem 3.7, Theorem 3.8 and Theorem 3.9 and it was proven that the equalities hold for regular or star graphs. In this section, we prove that the same equalities hold for other classes of graphs, too. The following is Theorem 3.7 in [6]:

Theorem 2.2. [6] *Let G be a simple connected graph of order n, size m, maximum degree Δ and minimum degree δ. Then*

$$SDD(G) \leq m\left(\frac{\Delta^2+\delta^2}{\Delta\delta}\right).$$

The equality holds for the regular and star graphs.

A graph G is called bidegreed if it has two different vertex degrees Δ and δ, with $\Delta \geq \delta \geq 1$ and let $K_{r,n-r}$, $1 \leq r \leq n-1$ denote the bidegreed bipartite graph with r vertices of degree Δ and $n-r$ vertices of degree δ. We can easily observe that the star graph is a special class of bidegreed graphs. If G is a bidegreed bipartite graph, then G has a partition with maximum degree Δ with δ vertices and the other partition with minimum degree δ with Δ vertices. Then, it is easy to compute $SDD(G)$ as $m\left(\frac{\Delta^2+\delta^2}{\Delta\delta}\right)$. Hence we can rewrite the above theorem as below:

Theorem 2.3. *Let G be a simple connected graph with order n, size m, maximum degree Δ and minimum degree δ, then*

$$SDD(G) \leq m\left(\frac{\Delta^2+\delta^2}{\Delta\delta}\right),$$

and the equality holds if and only if G is regular or G is a bidegreed bipartite graph.

The following two theorems and the corollary are Theorem 3.8, Theorem 3.9 and Corollary 3.11 in [6]:

Theorem 2.4. *Let G be a simple connected graph with order n, size m, p pendant vertices, maximimum degree Δ and minimum degree δ_1. Then*

$$SDD(G) \leq p\left(\frac{\Delta^2+1}{\Delta}\right) + (m-p)\left(\frac{\Delta^2+\delta_1^2}{\Delta\delta_1}\right).$$

Equality holds iff the graph is regular or a star graph.

Theorem 2.5. *Let G be a simple connected graph with order n, size m, p pendant vertices, maximum degree Δ and minimum degree δ_1. Then*

$$SDD(G) \leq p\left(\frac{\Delta^2+1}{\Delta}\right) + \frac{1}{\delta_1^2}\left(HM(G) - p(1+\delta_1)^2\right) - 2(m-p)$$

where $HM(G)$ is the hyper-Zagreb index. Equality holds iff the graph is regular or a star graph.

Corollary 2.6. *Let T be a tree of order n, p pendant vertices, maximum degree Δ and minimum degree δ_1. Then*

$$SDD(G) \leq p\left(\frac{\Delta^2+1}{\Delta}\right) + \frac{1}{\delta_1^2}\left(HM(G) - p(1+\delta_1)^2\right) - 2(n-1-p),$$

and the equality holds iff the graph is a star graph.

If G is a bidegreed bipartite graph, then $p = 0$ and we get $SDD(G) = m\left(\frac{\Delta^2+\delta^2}{\Delta\delta}\right)$. From the above result, we conclude that equality holds for bidegreed bipartite graphs. If G is a bidegreed graph with $\delta = 1$ then, G has p vertices of degree one. For p edges, SDD yields $\left(\frac{\Delta^2+1}{\Delta}\right)$ and for the remaining $m-p$ edges, SDD yields 2. Therefore, $SDD(G) = p\left(\frac{\Delta^2+1}{\Delta}\right) + 2(m-p)$. Conversely, if G has $\Delta = \delta_1$, then we get $SDD(G) = p\left(\frac{\Delta^2+1}{\Delta}\right) + 2(m-p)$. Hence we can rewrite the above theorems and corollary as below:

Theorem 2.7. *Let G be a simple connected graph of order n, size m, p pendant vertices, maximum degree Δ and minimum degree δ_1. Then*

$$SDD(G) \leq p\left(\frac{\Delta^2+1}{\Delta}\right) + (m-p)\left(\frac{\Delta^2+\delta_1^2}{\Delta\delta_1}\right),$$

and the equality holds if and only if G is a regular or bidegreed bipartite graph or a bidegreed graph with one pendant vertex.

Theorem 2.8. *Let G be a simple connected graph of order n, size m, p pendant vertices, maximum degree Δ and minimum degree δ_1. Then*

$$SDD(G) \leq p\left(\frac{\Delta^2+1}{\Delta}\right) + \frac{1}{\delta_1^2}\left(HM(G) - p(1+\delta_1)^2\right) - 2(m-p)$$

where the equality holds if and only if G is a regular or bidegreed bipartite graph or a bidegreed graph with one pendant vertex.

Corollary 2.9. *Let T be a tree of order n, p pendant vertices, maximum degree Δ and minimum degree δ_1. Then*

$$SDD(G) \leq p\left(\frac{\Delta^2+1}{\Delta}\right) + \frac{1}{\delta_1^2}\left(HM(G) - p(1+\delta_1)^2\right) - 2(n-1-p),$$

where the equality holds if and only if T is a bidegreed tree.

2.3. **Bicyclic graphs-second maximum SDD index.** Let $B_{n,p}$ be the set of bicyclic graphs with n vertices and p pendant vertices for $0 \leq p \leq n$. Let C_4^* be the bicyclic graph obtained by adding an edge to the cycle C_4. Label the vertices C_4^* by v_1, v_2, v_3, v_4 with $d_{v_1} = d_{v_2} = 3$, $d_{v_3} = d_{v_4} = 2$. Let $C_n^*(p_1, p_2, p_3, p_4)$ be the graph formed from C_4^* by attaching p_i pendant vertices to v_i, where $p_i \geq 0$ for $p_1 \geq p_2 \geq p_3 \geq p_4$ and $\sum_{i=1}^4 p_i = n-4$. In [6], it was proven that among the graphs $B_{n,n-4}$ with $n \geq 5$, the $C_n^*(0,0,n-4,0)$ is the uniqe graph with the second maximum SDD index. But we determined that $C_n^*(0,0,n-4,0)$ does not have the second maximum SDD index. The following are Theorem 6.3 and Corollary 6.4 in [6]:

Theorem 2.10. [6] *Let* $G \in B_{n,n-4}$ *with* $n \geq 5$. *Then*

$$SDD(G) \leq (n-4)\left(\frac{n^2-2n+2}{n-1}\right) + \frac{n^2-2n+10}{3(n-1)} + \frac{n^2-2n+5}{n-1} + \frac{13}{5}$$

with equality if and only if $G \cong C_n^*(n-4,0,0,0)$.

Corollary 2.11. [6] *Among the graphs* $B_{n,n-4}$ *with* $n \geq 5$, $C_n^*(0,0,n-4,0)$ *is the uniqe graph with the second maximum SDD index which is equal to*

$$SDD(C_n^*(0,0,n-4,0)) = (n-4)\left(\frac{n^2-4n+5}{n-2}\right) + 2\left(\frac{n^2-4n+13}{3(n-2)}\right) + \frac{19}{3}.$$

The graph class $C_n^*(n-5,1,0,0)$ contradicts with Corollary 2.11 as shown in Fig. 2:

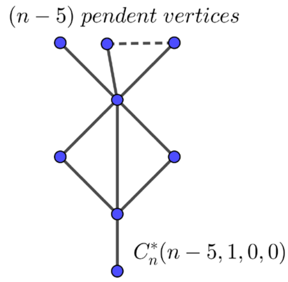

FIGURE 2. Graphs that contradict with Corollary 2.11

We tabulated the values of $SDD(C_n^*(n-5,1,0,0))$ and $SDD(C_n^*(n-5,1,0,0))$ for $n = 5, 6, \cdots, 9$ in Table 1:

n	$SDD(C_n^*(0,0,n-4,0))$	$SDD(C_n^*(n-5,1,0,0))$
5	13.6667	15.6667
6	19	20.5
7	26.4667	27.5
8	36	36.5833
9	47.5714	47.7143

TABLE 1. Values of $SDD(C_n^*(0,0,n-4,0))$ & $SDD(C_n^*(n-5,1,0,0))$

Hence, we can conclude that $SDD(C_n^*(0,0,n-4,0))$ has not the second maximum index.

3. Bounds for SDD index

3.1. **Symmetric division deg matrix-SDD index.** The symmetric division deg matrix [12] of a graph G is denoted by $S(G)$ and defined by

$$S_{ij}(G) = \begin{cases} \dfrac{d_{v_i}}{d_{v_j}} + \dfrac{d_{v_j}}{d_{v_i}} & if\ v_i\ and\ v_j\ are\ adjacent \\ 0 & otherwise \end{cases}$$

Since the symmetric division deg matrix is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$. Also $\sum_{i=1}^{n} \lambda_i = tr(S(G)) = 0$. The symmetric division deg energy [12] of G is defined as

$$SDDE(G) = \sum_{i=1}^{n} |\lambda_i|.$$

We recall

Lemma 3.1. [12] *If $\lambda_1, \lambda_2, \cdots, \lambda_n$ are the symmetric division deg eigenvalues of $S(G)$, then*

$$\sum_{i=1}^{n} \lambda_i^2 = tr(S^2(G)) = 2 \sum_{uv \in E(G)} \left(\frac{d_u^2 + d_v^2}{d_u d_v} \right)^2.$$

Theorem 3.2. *Let G be a simple graph. For any symmetric division deg eigenvalue λ_j, we have*

$$|\lambda_j| \le \sqrt{\frac{(n-1)tr(S^2(G))}{n}}.$$

Proof. We have $\lambda_j = -\sum_{i=1, i \ne j}^{n} \lambda_i$ and using Cauchy-Schwartz inequality, we get

$$\lambda_j^2 = \left(\sum_{i=1, i \ne j}^{n} \lambda_i \right)^2 \le (n-1) \sum_{i=1, i \ne j}^{n} \lambda_i^2 = (n-1) \left(\sum_{i=1}^{n} \lambda_i^2 - \mu_j^2 \right).$$

We then have

$$n\lambda_j^2 \le (n-1) \sum_{i=1}^{n} \lambda_i^2. \tag{2}$$

Therefore

$$|\lambda_j| \le \sqrt{\frac{(n-1)tr(S^2(G))}{n}}.$$

□

Some graph classes are more frequently used than others. Here we obtain bounds on symmetric division deg eigenvalues for some of such graph classes:

Corollary 3.3. *If G is a path graph P_n, $n \ge 4$, then*

$$|\lambda_j| \le \sqrt{\frac{(n-1)(8n+1)}{n}}.$$

Proof. If G is a path graph P_n, then $tr(S^2(P_n)) = 8n + 1$. Hence we obtain the result. □

Corollary 3.4. *If G is a cycle graph C_n with $n \ge 3$, then*

$$|\lambda_j| \le \sqrt{8(n-1)}.$$

Proof. As $tr(S^2(C_n)) = 4n$ for C_n, the result follows. □

Corollary 3.5. *If G is a complete graph K_n, then*

$$|\lambda_j| \le 2(n-1).$$

Proof. If G is a complete graph K_n, then $tr(S^2(K_n)) = 4n(n-1)$. Hence the result follows. □

Corollary 3.6. *If G is a complete bipartite graph $K_{m,n}$ with $m \geq n$, then*

$$|\lambda_j| \leq (m^2+n^2)\sqrt{\frac{2(m+n-1)}{mn(m+n)}}.$$

Proof. If G is a complete bipartite graph $K_{m,n}$ with $m \geq n$, then $tr(S^2(K_{m,n})) = 2\frac{(m^2+n^2)^2}{mn}$. Hence we obtain the result. □

Corollary 3.7. *If G is a star graph S_n, then*

$$|\lambda_j| \leq \left((n-1)^2+1\right)\sqrt{\frac{2}{n}}.$$

Corollary 3.8. *If G is a crown graph on $2n$ vertices, then*

$$|\lambda_j| \leq 2\sqrt{(n-1)(2n-1)}.$$

Proof. If G is a crown graph on $2n$ vertices, then $tr(S^2(G)) = 8n(n-1)$. This gives the required result. □

Theorem 3.9. *Let G be a simple connected graph. Then*

$$\frac{n\lambda_1^2\delta\Delta}{2(n-1)(\Delta^2+\delta^2)} \leq SDD(G) \leq \frac{n\mu_1}{2}.$$

Proof. By equation (2), we have

$$\begin{aligned}\frac{n}{n-1}\lambda_1^2 &\leq tr(S^2(G))\\ &\leq \frac{2\left(\Delta^2+\delta^2\right)}{\Delta\delta}SDD(G).\end{aligned}$$

Hence,

$$\frac{n\lambda_1^2\delta\Delta}{2(n-1)(\Delta^2+\delta^2)} \leq SDD(G)$$

Let $\mathbf{j} = (1,1,\cdots 1) \in \mathbb{R}^n$. Since G is connected, $S(G)$ is non-negative and irreducible. Perron-Frobenius Theorem gives $\mu \geq |\mu_j|$ for every j and then $\mu_j > 0$. Hence, using the Rayleigh quotient, we obtain

$$\mu_1 = max_{x\neq 0}\frac{< S(G)x, x >}{||x||^2} \geq \frac{< S(G)\mathbf{j}, \mathbf{j} >}{||\mathbf{j}||^2} = \frac{2SDD(G)}{n}.$$

Hence, the required result. □

Now we obtain different bounds for $SDD(G)$ in terms of the trace of $S^2(G)$. We need the following result to establish bounds on $SSD(G)$:

Lemma 3.10. [14] *Let $f(x) = \frac{x^2+y^2}{xy}$ with $0 < a \leq x, y \leq b$. Then*

$$2 \leq f(x,y) \leq \frac{a^2+b^2}{ab}.$$

The equality in the upper bound attained if and only if either $x = a$ and $y = b$, or $x = b$ and $y = a$, and the equality in the lower bound attained if and only if $x = y$.

From Lemma 3.1, we have

$$tr(S^2(G)) = 2 \sum_{uv \in E(G)} \left(\frac{d_u^2 + d_u^2}{d_u d_v} \right)^2.$$

Theorem 3.11. *Let G be a simple graph. Then*

$$\frac{\Delta\delta}{2\left(\Delta^2+\delta^2\right)} tr(S^2(G)) \le SDD(G) \le \frac{tr(S^2(G))}{4}.$$

The equality in the upper bound is attained if and only if G is regular; the equality in the lower bound is attained if and only if G is either regular or (Δ, δ)-biregular.

Proof. By Lemma 3.10, taking $a = \delta$ and $b = \Delta$, we get

$$\frac{d_u^2 + d_v^2}{d_u d_v} \le \frac{\Delta^2 + \delta^2}{\Delta\delta}. \tag{3}$$

Now

$$\begin{aligned} tr(S^2(G)) &= 2 \sum_{i<j} \left(\frac{d_i^2 + d_j^2}{d_i d_j} \right) \left(\frac{d_i^2 + d_j^2}{d_i d_j} \right) \\ &\le \frac{2\left(\Delta^2+\delta^2\right)}{\Delta\delta} \sum_{i<j} \left(\frac{d_i^2 + d_j^2}{d_i d_j} \right) \\ &= \frac{2\left(\Delta^2+\delta^2\right)}{\Delta\delta} SDD(G). \end{aligned}$$

Again

$$tr(S^2(G)) = 2 \sum_{i<j} \left(\frac{d_i^2 + d_j^2}{d_i d_j} \right) \left(\frac{d_i^2 + d_j^2}{d_i d_j} \right) \ge 4SDD(G).$$

Hence the required inequality. By Lemma 3.10, the equality in the lower bound is attained if and only if either $d_u = \Delta$ and $d_v = \delta$, or vice versa, for each $uv \in E(G)$. Since G is connected, this happens if and only if G is a regular graph; that is, $\Delta = \delta$ or it is a (Δ, δ)-biregular graph otherwise. The equality in the upper bound holds, by Lemma 3.10, if and only if $d_u = d_v$ for every edge $uv \in E(G)$. Since G is a connected graph, this happens if and only if G is regular. □

Let σ^2 be the variance of the sequence $\left\{ \frac{d_u^2 + d_v^2}{d_u d_v} \right\}$ appearing in the definition of $SDD(G)$. Then

Theorem 3.12. *Let G be simple graph. Then*

$$SDD(G) = \sqrt{\frac{m.tr(S^2(G))}{2} - m^2\sigma^2}.$$

Proof. By the definition of σ^2, we have

$$\begin{aligned}\sigma^2 &= \frac{1}{m}\sum_{uv\in E(G)}\left(\frac{d_u^2+d_v^2}{d_ud_v}\right)^2-\left(\frac{1}{m}\sum_{uv\in E(G)}\frac{d_u^2+d_v^2}{d_ud_v}\right)^2\\ &= \frac{1}{2m}tr(S^2(G))-\frac{1}{m^2}SDD(G)^2.\end{aligned}$$

Hence, the required result. □

Theorem 3.13. *Let G be a simple graph. Then*

$$\sqrt{\frac{tr(s^2(G))}{2}+4m(m-1)}\le SDD(G)\le\sqrt{\frac{tr(s^2(G))}{2}+m(m-1)\left(\frac{\Delta^2+\delta^2}{\Delta\delta}\right)^2}.$$

Equality holds iff G is regular.

Proof. We have

$$\begin{aligned}SDD(G)^2 &= \left(\sum_{uv\in E(G)}\frac{d_u^2+d_v^2}{d_ud_v}\right)^2\\ &= \sum_{uv\in E(G)}\left(\frac{d_u^2+d_v^2}{d_ud_v}\right)^2+\sum_{uv\neq xy}\left(\frac{d_u^2+d_v^2}{d_ud_v}\right)\left(\frac{d_x^2+d_y^2}{d_xd_y}\right)\\ &= \frac{tr(s^2(G))}{2}+\sum_{uv\neq xy}\left(\frac{d_u^2+d_v^2}{d_ud_v}\right)\left(\frac{d_x^2+d_y^2}{d_xd_y}\right). \qquad (4)\end{aligned}$$

By Lemma (3.10), taking $a=\delta$ and $b=\Delta$, we get

$$2\le\frac{d_u^2+d_v^2}{d_ud_v}\le\frac{\Delta^2+\delta^2}{\Delta\delta}.$$

$$\begin{aligned}SDD(G)^2 &\ge \frac{tr(s^2(G))}{2}+\sum_{uv\neq xy}4\\ &= \frac{tr(s^2(G))}{2}+4m(m-1).\end{aligned}$$

Again from (4), we have

$$\begin{aligned}SDD(G)^2 &= \frac{tr(s^2(G))}{2}+\sum_{uv\neq xy}\left(\frac{d_u^2+d_v^2}{d_ud_v}\right)\left(\frac{d_x^2+d_y^2}{d_xd_y}\right)\\ &\le \frac{tr(s^2(G))}{2}+\sum_{uv\neq xy}\left(\frac{\Delta^2+\delta^2}{\Delta\delta}\right)^2\\ &= \frac{tr(s^2(G))}{2}+m(m-1)\left(\frac{\Delta^2+\delta^2}{\Delta\delta}\right)^2.\end{aligned}$$

Hence, the required result. □

Theorem 3.14. *If G is a simple graph, then*

$$SDD(G)\ge\frac{(n-1)tr(S^2(G))}{2(n^2-2n+2)}.$$

Equality is attained iff G is a star graph.

Proof. By Lemma (3.10), taking $a = 1$ and $b = n - 1$, we get

$$2 \leq \frac{d_u^2 + d_v^2}{d_u d_v} \leq \frac{n^2 - 2n + 2}{n - 1}.$$

We have

$$\begin{aligned} tr(S^2(G)) &= 2\sum_{i<j} \left(\frac{d_i^2 + d_j^2}{d_i d_j}\right)\left(\frac{d_i^2 + d_j^2}{d_i d_j}\right) \\ &\leq \frac{2(n^2 - 2n + 2)}{n - 1} \sum_{i<j} \left(\frac{d_i^2 + d_j^2}{d_i d_j}\right) \\ &= \frac{2(n^2 - 2n + 2)}{n - 1} SDD(G). \end{aligned}$$

Hence, the required result. □

3.2. **Randić matrix-SDD index.** In 1975, the chemist Milan Randić proposed a topological index $R_{-1/2}$ under the name "branching index" suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons in [13]. Later in 1998, Bollobas and Erdös [3] generalised this index by replacing -$\frac{1}{2}$ with any real number α, which is called the general Randić index. It is denoted by $R_\alpha(G)$ and defined by

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$$

where α is an arbitrary real number.

The Randić matrix of a graph G for α =-$\frac{1}{2}$ is denoted by $R(G)$ and is defined by

$$R_{ij}(G) = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & if\ v_i\ and\ v_j\ are\ adjacent \\ 0 & otherwise. \end{cases}$$

Since the Randić matrix is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\rho_1 \leq \rho_2 \leq \cdots \leq \rho_n$. Also $\sum_{i=1}^n \rho_i = tr(R(G)) = 0$; $\sum_{i=1}^n \rho_i^2 = tr(R^2(G)) = 2\sum_{uv\in E(G)} \frac{1}{d_u d_v}$.

The Randić energy of G is defined as

$$RE(G) = \sum_{i=1}^n |\rho_i|.$$

Theorem 3.15. *Let G be a simple graph. For any Randić eigenvalue ρ_j,*

$$|\rho_j| \leq \sqrt{\frac{(n-1)}{n} tr(R^2(G))}.$$

Now we can easily obtain bounds on Randić eigenvalues for some graph classes:

- If G is a path graph P_n $(n \geq 4)$, then $|\rho_j| \leq \sqrt{\frac{n^2-1}{2n}}$;
- If G is a cycle graph C_n with $n \geq 3$, then $|\rho_j| \leq \sqrt{\frac{n-1}{2}}$;
- If G is a complete graph K_n, then $|\rho_j| \leq 1$;
- If G is a complete bipartite graph $K_{m,n}$, $m \geq n$, then $|\rho_j| \leq \sqrt{\frac{2(m+n-1)}{m+n}}$;
- If G is a crown graph on $2n$ vertices, then $|\rho_j| \leq \sqrt{\frac{2n-1}{n-1}}$.

Theorem 3.16. *Let G be a simple graph: Then*

$$\delta^2\, tr(R^2(G)) \leq SDD(G) \leq \Delta^2\, tr(R^2(G)).$$

Equality holds if and only if G is regular.

Proof. We have

$$SDD(G) = \sum_{uv\in E(G)} \left(\frac{d_u^2+d_v^2}{d_ud_v}\right) \geq \delta^2 \sum_{uv\in E(G)} \left(\frac{2}{d_ud_v}\right) = \delta\, tr(R^2(G))$$

$$SDD(G) = \sum_{uv\in E(G)} \left(\frac{d_u^2+d_v^2}{d_ud_v}\right) \leq \Delta \sum_{uv\in E(G)} \left(\frac{2}{d_ud_v}\right) = \Delta^2\, tr(R^2(G))$$

If $SDD(G) = \delta^2\, tr(R^2(G)$, (respectively, $SDD(G) = \Delta^2\, tr(R^2(G)))$, then $d_u^2 + d_v^2 = 2\delta^2$ for every edge $uv \in E(G)$ and we conclude that $d_u = \delta$, (respectively $d_v = \Delta$) for every $u \in V(G)$. Conversely, if G is regular, then lower bound and upper bounds are the same and they are equal to $SDD(G)$. □

Theorem 3.17. *Let G be a simple graph. Then*

$$SDD(G) \leq \frac{\Delta^2}{\delta}\sqrt{2m\, tr(R^2(G))}.$$

Equality holds iff G is a regular graph.

Proof. Using the Cauchy-Schwartz inequality,

$$\begin{aligned} SDD(G)^2 &= \left(\sum_{uv\in E(G)} \frac{d_u^2+d_v^2}{d_ud_v}\right)^2 \\ &\leq \sum_{uv\in E(G)} (d_u^2+d_v^2)^2 \sum_{uv\in E(G)} \left(\frac{1}{d_ud_v}\right)^2 \\ &\leq \frac{2m\Delta^4}{\delta^2} tr(R^2(G)) \end{aligned}$$

□

In order to obtain few more relations between $SDD(G)$ and $tr(S^2(G))$ we need the following result, [7]:

Lemma 3.18. *If* $0 < n_1 \leq a_j \leq N_1$ *and* $0 < n_2 \leq b_j \leq N_2$ *for* $1 \leq j \leq k$, *then*

$$\left(\sum_{j=1}^{k} a_j^2\right)^{1/2} \left(\sum_{j=1}^{k} b_j^2\right)^{1/2} \leq \frac{1}{2}\left(\sqrt{\frac{N_1N_2}{n_1n_2}} + \sqrt{\frac{n_1n_2}{N_1N_2}}\right)\left(\sum_{j=1}^{k} a_jb_j\right).$$

Theorem 3.19. *Let* G *be a simple graph. Then*

$$SDD(G) \geq \frac{2\delta^4\Delta}{\Delta^4+\delta^4}\sqrt{2m\,tr(R^2(G))}.$$

Equality holds iff G *is a regular graph.*

Proof. Since $2\delta^2 \leq d_u^2 + d_v^2 \leq 2\Delta^2$ and $\frac{1}{\Delta^2} \leq \frac{1}{d_ud_v} \leq \frac{1}{\delta^2}$, using Lemma 3.18, we get

$$\begin{aligned} SDD(G) &= \sum_{uv\in E(G)} \left(\frac{d_u^2+d_v^2}{d_ud_v}\right) \\ &\geq \frac{\left(\sum_{uv\in E(G)} (d_u^2+d_v^2)^2\right)^{1/2} \left(\sum_{uv\in E(G)} \left(\frac{1}{d_ud_v}\right)^2\right)^{1/2}}{\frac{1}{2}\left(\frac{\Delta^2}{\delta^2}+\frac{\delta^2}{\Delta^2}\right)} \\ &\geq \frac{\left(2\sqrt{m}\delta^2\right)\frac{1}{\Delta}\sqrt{\frac{tr(R^2(G))}{2}}}{\frac{1}{2}\left(\frac{\Delta^4+\delta^4}{\Delta^2\delta^2}\right)} \\ &= \frac{2\delta^4\Delta}{\Delta^4+\delta^4}\sqrt{2m\,tr(R^2(G))}. \end{aligned}$$

□

Theorem 3.20. *Let* G *be a simple graph. Then*

$$SDD(G) \geq \frac{4\delta^2\sqrt{m\Delta\delta(\Delta^2+\delta^2)tr(R^2(G))}}{\Delta^2(\Delta+\delta)}.$$

Equality holds iff G *is regular.*

Proof. Using Lemma 3.10, we can write

$$2 \leq \frac{d_u^2+d_v^2}{d_ud_v} \leq \frac{\Delta^2+\delta^2}{\Delta\delta}$$

Using Lemma 3.18, we have

$$\begin{aligned}
SDD(G) &= \sum_{uv\in E(G)} \left(\frac{d_u^2+d_v^2}{d_ud_v}\right) \\
&\geq \frac{\left(\sum_{uv\in E(G)} \left(\frac{d_u^2+d_v^2}{d_ud_v}\right)^2\right)^{1/2} \left(\sum_{uv\in E(G)} 1\right)^{1/2}}{\frac{1}{2}\left(\sqrt{\frac{\Delta^2+\delta^2}{2\delta\Delta}}+\sqrt{\frac{2\delta\Delta}{\Delta^2+\delta^2}}\right)} \\
&\geq \frac{\frac{2\delta^2}{\Delta^2}\sqrt{\frac{tr(R^(G))}{2}}\sqrt{m}}{\frac{1}{2}\left(\frac{(\Delta+\delta)}{\sqrt{2\Delta\delta(\Delta^2+\delta^2)}}\right)} \\
&= \frac{4\delta^2\sqrt{m\Delta\delta(\Delta^2+\delta^2)tr(R^2(G))}}{\Delta^2(\Delta+\delta)}.
\end{aligned}$$

□

The Randić matrix of a graph G for α =-1 is denoted by $R_{-1}(G)$ and defined by

$$R_{-1}(ij) \;=\; \begin{cases} \dfrac{1}{d_id_j} & if\ v_i\ and\ v_j\ are\ adjacent \\ 0 & otherwise \end{cases}$$

Since the matrix $R_{-1}(G)$ is real and symmetric, its eigenvalues are real numbers we label them in a non-increasing order $\gamma_1 \leq \gamma_2 \leq \cdots \leq \gamma_n$. Also $\sum_{i=1}^{n}\gamma_i = tr(R_{-1}(G)) = 0$; $\sum_{i=1}^{n}\gamma_i^2 = tr(R_{-1}^2(G)) = 2\sum_{uv\in E(G)}\left(\frac{1}{d_ud_v}\right)^2$ and we can establish the following results.

Theorem 3.21. *Let G be a simple graph. Then*

$$SDD(G) \leq \Delta^2\sqrt{2m\,tr(R_{-1}^2(G))}.$$

Equality holds iff G is a regular graph.

Theorem 3.22. *Let G be a simple graph. Then*

$$SDD(G) \geq \frac{2\delta^4\Delta^2}{\Delta^4+\delta^4}\sqrt{\frac{1}{2}m\,tr(R_{-1}^2(G))}.$$

Equality holds iff G is a regular graph.

Theorem 3.23. *Let G be a simple graph. Then*

$$SDD(G) \geq \frac{4\delta^2\sqrt{m\Delta\delta(\Delta^2+\delta^2)tr(R_{-1}^2(G))}}{(\Delta+\delta)}.$$

Equality holds iff G is reqular.

References

[1] V. Alexander, *Upper and lower bounds of symmetric division deg index*, Iranian J. Math. Chem. 5 (2) (2014), 91-98.

[2] A. Ali, S. Elumalai, T. Mansour, *On the symmetric division deg index of molecular graphs*, MATCH Commun. Math. Comput. Chem. 83 (2020), 205-220.

[3] B. Bollobas and P. Erdos, *Graphs of extremal weights*, Ars Combin. 50 (1998), 225-233.

[4] H. Deng, S. Elumalai, S. Balachandran, *Maximum and second maximum of geometric-arithmetic index of tricyclicgraphs*, MATCH Commun. Math. Comput. Chem. 79 (2018), 467-475.

[5] B. Furtula, K. C. Das, I. Gutman, *Comparative analysis of symmetric division deg index as potentially useful molecular descriptor*, Int. J. Quantum Chem. 118 (17) (2018), e25659.

[6] C. K. Gupta, V. Lokesha et al., *On the symmetric division degree index of graph*, South East Asian Bulletin of Mathematics 40 (2016), 59-80.

[7] G. H. Hardy, J. E. Littlewood, G. Polya, *Inequalities*, Cambridge University Press, 1952.

[8] C. Liu, Y. Pan, J. Li, *Tricyclic graphs with the minimum symmetric division deg index*, Discrete Math. Lett. 3 (2020), 14-18.

[9] V. Lokesha, T. Deepika, *Symmetric division deg index of tricyclic and tetracyclic graphs*, Int. J. Sci. Eng. Res. 7 (5) (2016), 53-55.

[10] G. Mohanappriya, D. Vijayalakshmi, *Symmetric division degree index and inverse sum index of transformation graph*, IOP Conf. Series: Journal of Physics: Conf. Series 1139 (2018), 012048.

[11] Y. Pan, J. Li, *Graphs that minimizing symmetric division deg index*, MATCH Commun. Math. Comput. Chem. 82 (2019), 43-55.

[12] K. N. Prakasha, P. S. K. Reddy, I. N. Cangul, *Symmetric Division Deg Energy of a Graph*, Turkish Journal of Analysis and Number Theory, 5 (6) (2017), 202-209.

[13] M. Randić, *On characterization of molecular branching*, J. Amer. Chem. Soc. 97 (1975), 6609-6615.

[14] J. M. Rodriguez, J. M. Sigarreta, *On the geometric-arithmetic index*, MATCH Commun. Math. Comput. Chem. 74 (2015), 103-120.

[15] G. H. Shirdel, H. Rezapour, A. M. Sayadi, *The Hyper-Zagreb index of graph operations*, Iranian Journal of Mathematical Chemistry 4 (2) (2013), 213-220.

[16] A. Vasilyev and D. Stevanovic, *MathChem: a Python package for calculating topological indices*, MATCH Commun. Math. Comput. Chem. 71 (2014), 657-680.

Department of Mathematics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya, Kanchipuram, Tamilnadu, India
Email address: raokonda@yahoo.com[1]

Department of Mathematics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya, Kanchipuram, Tamilnadu, India
Email address: amudhamaths@gmail.com

[1]corresponding author
Date of paper submission: 12-02-2021