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Bounds for Symmetric Division Deg Index of Graphs

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Abstract. Let $G = (V, E)$ be a simple connected graph of order $n\,(\geq 2)$ and size m, where $V(G) = \{1, 2, \ldots, n\}$. Also let $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(i)$, be a sequence of its vertex degrees with maximum degree Δ and minimum degree δ. The symmetric division deg index, *SDD*, was defined in [D. Vukičević, Bond additive modeling 2. Mathematical properties of max-min rodeg index, *Croat. Chem. Acta* **83** (2010) 261–273] as $SDD = SDD(G) = \sum_{i\sim j} \frac{d_i^2+d_j^2}{d_i d_j}$, where $i \sim j$ means that vertices i and j are adjacent. In this paper we give some new bounds for this topological index. Moreover, we present a relation between topological indices of graph.

1. Introduction

Let $G = (V, E)$ be a simple connected graph with $n\,(\geq 2)$ vertices and m edges, where $V(G) = \{1, 2, \ldots, n\}$ and $E(G) = \{e_1, e_2, \ldots, e_m\}$. The maximum vertex degree is denoted by Δ and the minimum by δ. For the edge e connecting the vertices i and j, the degree of edge is $d(e) = d_i+d_j-2$. Let $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(i)$, and $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m)$, $\Delta_e = d(e_1) + 2$ and $\delta_e = d(e_m) + 2$, be sequences of its vertex and edge degrees, respectively. If vertices v_i and v_j are adjacent, we denote it as $i \sim j$ or $v_iv_j \in E$.

Two vertex–degree–based topological indices, the first and the second Zagreb indices, M_1 and M_2, were defined in [12, 13] as

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad M_2 = M_2(G) = \sum_{i\sim j} d_i d_j.$$

As shown in [19], the first Zagreb index can also be expressed as

$$M_1 = \sum_{i\sim j} (d_i + d_j).$$

Bearing in mind that for the edge e connecting the vertices i and j we have that

$$d(e) = d_i + d_j - 2,$$

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the index M_1 can also be considered as an edge–degree–based topological index [17]

$$M_1 = \sum_{i=1}^{m} (d(e_i) + 2).$$

Multiplicative variants of the Zagreb indices, the first and the second multiplicative Zagreb indices, Π_1 and Π_2, were defined in [15] as

$$\Pi_1 = \Pi_1(G) = \prod_{i=1}^{n} d_i^2 \quad \text{and} \quad \Pi_2 = \Pi_2(G) = \prod_{i \sim j} d_i d_j.$$

One year later, the multiplicative sum Zagreb index, Π_1^*, was introduced in [8]

$$\Pi_1^* = \Pi_1^*(G) = \prod_{i \sim j} (d_i + d_j).$$

Since

$$\Pi_1^* = \prod_{i=1}^{m} (d(e_i) + 2),$$

this index can also be considered as an edge–degree–based topological index.

For an edge $i \sim j$ of G, its weight is defined to be $\frac{2}{d_i + d_j}$. The harmonic index of G is the sum of weights over all its edges. It is denoted by $H(G)$ and is defined in [9] as

$$H = H(G) = \sum_{i \sim j} \frac{2}{d_i + d_j}.$$

For its basic mathematical properties, including lower bound, see, recent paper [2] and the references cited therein.

The general Randić index, R_{-1}, was defined as [22]

$$R_{-1} = R_{-1}(G) = \sum_{i \sim j} \frac{1}{d_i d_j}.$$

The geometric–arithmetic vertex–degree–based topological index, GA, was introduced in [30]. It is defined as

$$GA = GA(G) = \sum_{i \sim j} \frac{2\sqrt{d_i d_j}}{d_i + d_j}.$$

Similarly, in [24], the arithmetic–geometric topological index, AG, was defined as

$$AG = AG(G) = \sum_{i \sim j} \frac{d_i + d_j}{2\sqrt{d_i d_j}}.$$

A family of Adriatic indices was introduced in [28, 29] . An especially interesting subclass of these descriptors consists of 148 discrete Adriatic indices. A so called inverse sum indeg index, ISI, was defined in [29] as a significant predictor of total surface area of octane isomers. The inverse sum indeg index is defined as

$$ISI = ISI(G) = \sum_{i \sim j} \frac{d_i d_j}{d_i + d_j}.$$

The symmetric division deg index, SDD, was defined in [29] as

$$SDD = SDD(G) = \sum_{i\sim j} \frac{d_i^2 + d_j^2}{d_i d_j}.$$

In this paper we are interested in upper and lower bounds on topological index SDD. This problem was considered in [4, 11, 27]. Very recently in [10], the authors studied to test the physico-chemical applicability of SDD on a much wider empirical basis, and to compare it with other, most often used, vertex-degree-based topological indices.

2. Preliminary results

In this section we list some analytical inequalities for real number sequences that will be used in the subsequent considerations. Let $x = (x_i)$ and $a = (a_i)$, $i = 1, 2, \dots, m$, be positive real number sequences. Then for all r, $r \geq 0$, holds [21]

$$\sum_{i=1}^{m} \frac{x_i^{r+1}}{a_i^r} \geq \frac{\left(\sum_{i=1}^{m} x_i\right)^{r+1}}{\left(\sum_{i=1}^{m} a_i\right)^{r}} \tag{1}$$

with equality holding if and only if

$$\frac{x_1}{a_1} = \frac{x_2}{a_2} = \cdots = \frac{x_m}{a_m}.$$

Let $a = (a_i)$, $i = 1, 2, \dots, m$, be a positive real number sequence. In [16] (see also [31]) the following inequalities were proven

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

and

$$\left(\sum_{i=1}^{m} \sqrt{a_i}\right)^2 \geq \sum_{i=1}^{m} a_i + m(m-1)\left(\prod_{i=1}^{m} a_i\right)^{\frac{1}{m}}. \tag{3}$$

Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \dots, m$, be two positive real number sequences with the properties $p_1 + p_2 + \cdots + p_m = 1$ and $0 < r \leq a_i \leq R < +\infty$. In [23] (see also [18]) the following inequality was proven

$$\sum_{i=1}^{m} p_i a_i + rR\sum_{i=1}^{m} \frac{p_i}{a_i} \leq r + R. \tag{4}$$

Moreover, the equality holds in (4) if and only if $R = a_1 = a_2 = \cdots = a_m = r$, or for some k, $1 \leq k \leq m-1$, $R = a_1 = a_2 = \cdots = a_k \geq a_{k+1} = \cdots = a_m = r$.

Let $p = (p_i)$ and $a = (a_i)$, $b = (b_i)$, $i = 1, 2, \dots, m$, be non-negative real number sequences with the properties $r_1 \leq a_i \leq R_1$ and $r_2 \leq b_i \leq R_2$. Further, let S be a subset of $I = \{1, 2, \dots, m\}$ which minimizes the expression

$$\left|\sum_{i\in S} p_i - \frac{1}{2}\sum_{i=1}^{m} p_i\right|. \tag{5}$$

In [1] the following inequality was proven

$$\left|\sum_{i=1}^{m} p_i \sum_{i=1}^{m} p_i a_i b_i - \sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} p_i b_i\right| \le (R_1 - r_1)(R_2 - r_2)\alpha(S)\left(\sum_{i=1}^{m} p_i\right)^2, \tag{6}$$

where

$$\alpha(S) = \frac{\sum_{i\in S} p_i}{\sum_{i=1}^{m} p_i}\left(1 - \frac{\sum_{i\in S} p_i}{\sum_{i=1}^{m} p_i}\right). \tag{7}$$

Moreover, the equality holds in (6) if and only if $R_1 = a_1 = a_2 = \cdots = a_m = r_1$ or $R_2 = b_1 = b_2 = \cdots = b_m = r_2$.

Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real number sequences for which there exist real constants r and R so that for each i, $i = 1, 2, \ldots, n$, holds $r\,a_i \le b_i \le R\,a_i$. Then the following inequality holds [7]:

$$\sum_{i=1}^{n} b_i^2 + r\,R \sum_{i=1}^{n} a_i^2 \le (r + R) \sum_{i=1}^{n} a_i\, b_i \tag{8}$$

with equality holding if and only if for at least one i, $1 \le i \le n$ holds $r\,a_i = b_i = R\,a_i$.

3. Main results

In this section we determine some lower and upper bounds for the *SDD* index in terms of some other topological indices.

In the following theorem we establish lower bound for invariant *SDD* in terms of parameter m and topological indices M_1 and M_2.

Theorem 3.1. *Let G be a connected graph of order n with $m\,(\ge 1)$ edges. Then*

$$SDD \ge \frac{M_1^2}{M_2} - 2m \tag{9}$$

with equality holding if and only if G is a regular graph or a semiregular bipartite graph.

Proof. Define $S = S(G)$ as

$$S = \sum_{i\sim j} \frac{(d_i + d_j)^2}{d_i d_j}.$$

Then we have

$$SDD = \sum_{i\sim j} \frac{d_i^2 + d_j^2}{d_i d_j} = \sum_{i\sim j} \frac{(d_i + d_j)^2 - 2d_i d_j}{d_i d_j} = S - 2m. \tag{10}$$

For $r = 1$, $x_i := d_i + d_j$, $a_i := d_i d_j$, where summation is performed over all edges, the inequality (1) becomes

$$\sum_{i\sim j} \frac{(d_i + d_j)^2}{d_i d_j} \ge \frac{\left(\sum_{i\sim j}(d_i + d_j)\right)^2}{\sum_{i\sim j} d_i d_j}, \quad \text{that is,} \quad S \ge \frac{M_1^2}{M_2} \tag{11}$$

with equality holding if and only if $\frac{1}{d_i}+\frac{1}{d_j}=\frac{1}{d_k}+\frac{1}{d_\ell}$ for any edges $v_iv_j,\ v_kv_\ell \in E(G)$. The inequality (9) follows from equality (10) and inequality (11). The first part of the proof is done.

Suppose that equality holds in (11). Then $\frac{1}{d_i}+\frac{1}{d_j}=\frac{1}{d_k}+\frac{1}{d_\ell}$ for any edges $v_iv_j,\ v_kv_\ell \in E(G)$. For $v_j,\ v_k \in N_G(v_i)$, we have $d_j=d_k$. Since G is connected, one can easily see that G is a regular graph or a semiregular bipartite graph.

Conversely, let G be a regular graph. Then

$$SDD=\sum_{i\sim j}\frac{d_i^2+d_j^2}{d_id_j}=2m=\frac{M_1^2}{M_2}-2m.$$

Let G be an $(r,\ s)$-semiregular bipartite graph. Then

$$SDD=\sum_{i\sim j}\frac{d_i^2+d_j^2}{d_id_j}=\frac{r^2+s^2}{rs}\,m=\frac{(r+s)^2}{rs}\,m-2m=\frac{M_1^2}{M_2}-2m.$$

□

Corollary 3.2. *Let G be a connected graph with $m\,(\geq 2)$ edges. Then*

$$\frac{M_1^2}{M_2}\leq SDD+2m\leq m\left(\sqrt{\frac{\Delta}{\delta}}+\sqrt{\frac{\delta}{\Delta}}\right)^2. \tag{12}$$

Remark 3.3. *Since $m\leq\frac{n(n-1)}{2}$, both inequalities in* (12) *are stronger than*

$$\frac{M_1^2}{M_2}\leq\frac{n(n-1)}{2}\left(\sqrt{\frac{\Delta}{\delta}}+\sqrt{\frac{\delta}{\Delta}}\right)^2,$$

which was proven in [20].

Since $M_1^2\geq M_1\delta_e m\geq m^2\delta_e^2$, the following corollary of Theorem 3.1 holds.

Corollary 3.4. *Let G be a connected graph of order n with $m\,(\geq 2)$ edges. Then*

$$SDD\geq\frac{m\delta_eM_1}{M_2}-2m\geq\frac{m^2\delta_e^2}{M_2}-2m.$$

Equalities hold if and only if G is regular or semiregular bipartite graph.

Since $M_1^2\geq\frac{2m^2M_1}{H}\geq\frac{4m^4}{H^2}$ the following corollary of Theorem 3.1 is also valid.

Corollary 3.5. *Let G be a connected graph with $m\,(\geq 2)$ edges. Then*

$$SDD\geq\frac{2m^2M_1}{M_2\,H}-2m\geq\frac{4m^4}{M_2\,H^2}-2m.$$

Equalities hold if and only if G is regular or semiregular bipartite graph.

Since $M_2\leq\Delta_e\,ISI$, the following corollary of Theorem 3.1 holds.

Corollary 3.6. *Let G be a connected graph with $m\,(\geq 2)$ edges. Then*

$$SDD\geq\frac{M_1^2}{\Delta_e\,ISI}-2m.$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Theorem 3.7. *Let G be a connected graph of order n with $m\,(\geq 2)$ edges. Then*

$$SDD \geq \frac{m^2\Delta_e\delta_e}{(\Delta_e+\delta_e)ISI - M_2} - 2m \tag{13}$$

with equality holding if and only if

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k} \text{ for any edges } v_iv_j,\ v_kv_\ell \in E(G),$$

and $d_i+d_j=\Delta_e$ or δ_e for any edge $v_iv_j \in E(G)$.

Proof. Since $\delta_e \leq d_i+d_j \leq \Delta_e$ for any edge $v_iv_j \in E(G)$, we have

$$(\Delta_e-d_i-d_j)(\delta_e-d_i-d_j) \leq 0,$$

$$\text{i.e.,}\quad (d_i+d_j)^2+\Delta_e\,\delta_e-(d_i+d_j)\,(\Delta_e+\delta_e) \leq 0,$$

$$\text{i.e.,}\quad 1+\frac{\Delta_e\,\delta_e}{(d_i+d_j)^2}-\frac{\Delta_e+\delta_e}{d_i+d_j} \leq 0.$$

Moreover, the above equality holds if and only if $d_i+d_j=\Delta_e$ or δ_e for any edge $v_iv_j \in E(G)$. Using the above result, one can easily see that

$$\sum_{i\sim j}\left[1+\frac{\Delta_e\,\delta_e}{(d_i+d_j)^2}-\frac{\Delta_e+\delta_e}{d_i+d_j}\right]d_i\,d_j \leq 0$$

with equality holding if and only if $d_i+d_j=\Delta_e$ or δ_e for any edge $v_iv_j \in E(G)$. Thus we have

$$\sum_{i\sim j} d_i\,d_j+\Delta_e\,\delta_e\sum_{i\sim j}\frac{d_i\,d_j}{(d_i+d_j)^2} \leq (\Delta_e+\delta_e)\sum_{i\sim j}\frac{d_i\,d_j}{d_i+d_j},$$

that is,

$$M_2+\Delta_e\delta_e\sum_{i\sim j}\frac{d_id_j}{(d_i+d_j)^2} \leq (\Delta_e+\delta_e)\,ISI,$$

that is,

$$\sum_{i\sim j}\frac{d_i\,d_j}{(d_i+d_j)^2} \leq \frac{(\Delta_e+\delta_e)\,ISI-M_2}{\Delta_e\delta_e} \tag{14}$$

with equality holding if and only if $d_i+d_j=\Delta_e$ or δ_e for any edge $v_iv_j \in E(G)$.

By Cauchy-Schwarz inequality, we have

$$m^2=\left(\sum_{i\sim j}\frac{\sqrt{d_i\,d_j}}{d_i+d_j}\cdot\frac{d_i+d_j}{\sqrt{d_i\,d_j}}\right)^2 \leq \sum_{i\sim j}\frac{d_id_j}{(d_i+d_j)^2}\sum_{i\sim j}\frac{(d_i+d_j)^2}{d_id_j}=S\sum_{i\sim j}\frac{d_id_j}{(d_i+d_j)^2}$$

with equality holding if and only if

$$\frac{d_i\,d_j}{(d_i+d_j)^2}=\frac{d_k\,d_\ell}{(d_k+d_\ell)^2},\ \text{ that is, }\ \frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}\ \text{ for any edges } v_iv_j,\ v_kv_\ell \in E(G).$$

From the above result with (14), we have

$$\frac{m^2}{S} \leq \frac{(\Delta_e+\delta_e)ISI-M_2}{\Delta_e\delta_e},\ \text{ that is, }\ S \geq \frac{m^2\Delta_e\delta_e}{(\Delta_e+\delta_e)ISI-M_2}$$

with equality holding if and only if

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}\ \text{ for any edges }\ v_iv_j,\, v_kv_\ell\in E(G),$$

and $d_i+d_j=\Delta_e$ or δ_e for any edge $v_iv_j\in E(G)$.

From the above with identity (10), we arrive at (13). This completes the proof of the theorem. □

Example 3.8. *Let $H=(V,E)$ be a graph with vertex set $V(H)=\{v_1,v_2,\ldots,v_{33}\}$ and $|E(H)|=72$ such that $v_1v_i\in E(H)$ $(i=2,3,\ldots,13)$ and $v_{j+1}v_{k+13}\in E(H)$ $(j=1,2,\ldots,12;\ k=(5j-4\ mod\ 20),(5j-3\ mod\ 20),(5j-2\ mod\ 20),(5j-1\ mod\ 20),(5j\ mod\ 20))$. For graph H,*

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{5}{2}\ \textit{for any edge } v_iv_j\in E(H),$$

and $\Delta_e=18$, $\delta_e=9$. Moreover, $d_i+d_j=18$ or 9 for any edge $v_iv_j\in E(H)$. This graph H is neither regular graph nor semiregular bipartite graph.

The following result is the corollary of Theorem 3.7.

Corollary 3.9. *Let G be a connected graph with $m\,(\geq 2)$ edges. Then*

$$SDD\geq\frac{m^2\delta_e}{ISI}-2m.$$

Equality holds if and only if G is a regular graph or a semiregular bipartite graph.

Proof. Since $d_i+d_j\geq\delta_e$, we have

$$ISI=\sum_{i\sim j}\frac{d_i\,d_j}{d_i+d_j}\leq\frac{1}{\delta_e}\sum_{i\sim j}d_i\,d_j=\frac{M_2}{\delta_e}$$

with equality holding if and only if $d_i+d_j=\delta_e$ for any edge $v_iv_j\in E(G)$, that is, if and only if G is a regular graph or a semiregular bipartite graph [3].

The above result with Theorem 3.7, we get the required result. Moreover, the equality holds if and only if G is a regular graph or a semiregular bipartite graph. □

In the following theorem we determine lower bound for the invariant SDD depending on parameter m and topological index GA.

Theorem 3.10. *Let G be a simple graph of order n with $m\,(\geq 1)$ edges. Then*

$$SDD\geq\frac{4m^3}{(GA)^2}-2m \tag{15}$$

with equality holding if and only if

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}\ \textit{for any edges }\ v_iv_j,\, v_kv_\ell\in E(G).$$

Proof. By Cauchy-Schwarz inequality, we have

$$\left(\sum_{i\sim j}\frac{d_i+d_j}{2\sqrt{d_id_j}}\right)^2\leq m\sum_{i\sim j}\frac{(d_i+d_j)^2}{4d_id_j},\ \text{ that is, }\ \frac{m}{4}S\geq(AG)^2 \tag{16}$$

with equality holding if and only if

$$\frac{d_i+d_j}{2\sqrt{d_id_j}}=\frac{d_k+d_\ell}{2\sqrt{d_kd_\ell}},\quad \text{that is,}\quad \sqrt{\frac{d_i}{d_j}}+\sqrt{\frac{d_j}{d_i}}=\sqrt{\frac{d_k}{d_\ell}}+\sqrt{\frac{d_\ell}{d_k}},$$

$$\text{that is,}\qquad \frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}\ \text{ for any edges } v_iv_j,\ v_kv_\ell\in E(G).$$

Using the arithmetic-harmonic mean inequality for real numbers (see e.g. [18]), we have

$$(AG)(GA)\geq m^2 \tag{17}$$

with equality holding if and only if

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}\ \text{ for any edges } v_iv_j,\ v_kv_\ell\in E(G).$$

From this inequality and inequality (16) follows

$$S\geq\frac{4m^3}{(GA)^2}$$

with equality holding if and only if

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}\ \text{ for any edges } v_iv_j,\ v_kv_\ell\in E(G).$$

According to this inequality and (10), we obtain (15). Moreover, the equality holds in (15) if and only if

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}\ \text{ for any edges } v_iv_j,\ v_kv_\ell\in E(G).$$

□

In the next theorem we establish lower and upper bounds for SDD in terms of parameter m and invariants GA, AG, Π_1^* and Π_2.

Theorem 3.11. *Let G be a connected graph with m (≥ 2) edges. Then*

$$SDD\geq\frac{4m^4}{(m-1)(GA)^2}-\frac{m\left(\Pi_1^*\right)^{\frac{2}{m}}}{(m-1)\left(\Pi_2\right)^{\frac{1}{m}}}-2m \tag{18}$$

with equality holding if and only if

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}\ \textit{ for any edges } v_iv_j,\ v_kv_\ell\in E(G),$$

and

$$SDD\leq 4(AG)^2-\frac{m(m-1)\left(\Pi_1^*\right)^{\frac{2}{m}}}{\left(\Pi_2\right)^{\frac{1}{m}}}-2m. \tag{19}$$

Moreover, the equality holds in (19) for

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}\ \textit{ for any edges } v_iv_j,\ v_kv_\ell\in E(G).$$

Proof. Lower bound: For $a_i := \frac{(d_i+d_j)^2}{d_i d_j}$, where summation goes over all edges in graph G, the inequality (2) becomes

$$\left(\sum_{i\sim j}\frac{d_i+d_j}{\sqrt{d_i d_j}}\right)^2 \leq (m-1)\sum_{i\sim j}\frac{(d_i+d_j)^2}{d_i d_j} + m\left(\prod_{i\sim j}\frac{(d_i+d_j)^2}{d_i d_j}\right)^{\frac{1}{m}},$$

that is,

$$4(AG)^2 \leq (m-1)S + m\frac{\left(\Pi_1^*\right)^{\frac{2}{m}}}{(\Pi_2)^{\frac{1}{m}}}.$$

According to this and inequality (17) we get

$$\frac{4m^4}{(GA)^2} \leq (m-1)S + m\frac{\left(\Pi_1^*\right)^{\frac{2}{m}}}{(\Pi_2)^{\frac{1}{m}}}.$$

The inequality (18) is obtained from the above inequality and equality (10). The first part of the proof is done.

Suppose that equality holds in (18). Then all the above inequalities must be equalities. From the equality in (17), we have

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k} \text{ for any edges } v_iv_j,\ v_kv_\ell \in E(G).$$

Conversely, let

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_k}{d_\ell}+\frac{d_\ell}{d_k}=p \text{ for any edges } v_iv_j,\ v_kv_\ell \in E(G).$$

Then one can easily see that

$$\sqrt{\frac{d_i}{d_j}}+\sqrt{\frac{d_j}{d_i}}=\sqrt{p+2} \text{ for any edge } v_iv_j \in E(G).$$

Now,

$$\begin{aligned}
&\frac{4m^4}{(m-1)(GA)^2}-\frac{m\left(\Pi_1^*\right)^{\frac{2}{m}}}{(m-1)\,(\Pi_2)^{\frac{1}{m}}}-2m\\
=\;&\frac{m^2\,(p+2)}{(m-1)}-\frac{m}{(m-1)}\left(\prod_{i\sim j}\frac{(d_i+d_j)^2}{d_i d_j}\right)^{\frac{1}{m}}-2m\\
=\;&\frac{m^2\,(p+2)}{(m-1)}-\frac{m\,(p+2)}{(m-1)}-2m\\
=\;&mp=SDD.
\end{aligned}$$

Upper bound: For $a_i := \frac{(d_i+d_j)^2}{d_i d_j}$, where summation goes over all edges in graph G, the inequality (3) becomes

$$\left(\sum_{i\sim j}\frac{d_i+d_j}{\sqrt{d_i d_j}}\right)^2 \geq \sum_{i\sim j}\frac{(d_i+d_j)^2}{d_i d_j} + m(m-1)\left(\prod_{i\sim j}\frac{(d_i+d_j)^2}{d_i d_j}\right)^{\frac{1}{m}},$$

that is,

$$4(AG)^2 \geq S + m(m-1)\frac{\left(\Pi_1^*\right)^{\frac{2}{m}}}{(\Pi_2)^{\frac{1}{m}}}.$$

From this inequality and equality (10) we arrive at (19). Let

$$\frac{d_i}{d_j} + \frac{d_j}{d_i} = \frac{d_k}{d_\ell} + \frac{d_\ell}{d_k} = p \text{ for any edges } v_iv_j,\ v_kv_\ell \in E(G).$$

Then

$$\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}} = \sqrt{p+2} \quad \text{for any edge } v_iv_j \in E(G).$$

Now,

$$\begin{aligned} & 4(AG)^2 - \frac{m(m-1)\left(\Pi_1^*\right)^{\frac{2}{m}}}{(\Pi_2)^{\frac{1}{m}}} - 2m \\ = \quad & m^2\,(p+2) - m\,(m-1)\,(p+2) - 2m \\ = \quad & mp = SDD. \end{aligned}$$

This completes the proof of the theorem. □

Corollary 3.12. *Let G be a connected graph with m (≥ 2) edges. Then*

$$SDD \geq \frac{m}{m-1}\left(2(m+1) - \frac{\left(\Pi_1^*\right)^{\frac{2}{m}}}{(\Pi_2)^{\frac{1}{m}}}\right).$$

Equality holds if and only if G is a regular graph.

Proof. In [5], we have that $GA \leq m$ with equality holding if and only if G is a regular graph as G is connected. Using this result with Theorem 3.11, we get the required result. Moreover, the equality holds if and only if G is a regular graph. □

In the following theorem we determine an upper bound for SDD in terms of parameters n, m, Δ_e, δ_e and topological index R_{-1}.

Theorem 3.13. *Let G be a connected graph with n (≥ 2) vertices and m edges. Then*

$$SDD \leq n(\delta_e + \Delta_e) - \delta_e\Delta_e R_{-1} - 2m. \tag{20}$$

Equality holds if and only if G is a regular graph or a semiregular bipartite graph, or $d_i + d_j = \Delta_e$ or δ_e for any edge $v_iv_j \in E(G)$ $(\Delta_e \neq \delta_e)$.

Proof. For $p_i := \frac{d_i+d_j}{nd_id_j}$, $a_i := d_i + d_j$, $r = \delta_e$, $R = \Delta_e$, where summation goes over all edges in graph G, the inequality (4) becomes

$$\sum_{i\sim j}\frac{(d_i+d_j)^2}{nd_id_j} + \delta_e\Delta_e\sum_{i\sim j}\frac{1}{nd_id_j} \leq \delta_e + \Delta_e,$$

that is,

$$S + \delta_e\Delta_e R_{-1} \leq n(\delta_e + \Delta_e). \tag{21}$$

The inequality (20) is obtained from this inequality and equality (10).

Moreover, the equality holds in (4) if and only if $R = a_1 = a_2 = \cdots = a_m = r$, or for some k, $1 \le k \le m-1$, $R = a_1 = a_2 = \cdots = a_k \ge a_{k+1} = \cdots = a_m = r$. It follows that equality holds in (21) if and only if $d_i + d_j = \Delta_e = \delta_e$ for any edge $v_iv_j \in E(G)$, or $d_i + d_j = \Delta_e$ or δ_e for any edge $v_iv_j \in E(G)$ ($\Delta_e \neq \delta_e$). Consequently, the equality holds in (20) if and only if G is a regular graph or a semiregular bipartite graph [3], or $d_i + d_j = \Delta_e$ or δ_e for any edge $v_iv_j \in E(G)$ ($\Delta_e \neq \delta_e$). □

Corollary 3.14. *Let G be a connected graph with n (≥ 2) vertices and m edges. Then*

$$SDD \le n(\delta_e + \Delta_e) - \frac{m^2 \delta_e \Delta_e}{M_2} - 2m. \tag{22}$$

Equality holds if and only if G is a regular graph or a semiregular bipartite graph.

Proof. By Cauchy-Schwarz inequality, we have

$$m^2 = \left(\sum_{i \sim j} \sqrt{d_i\, d_j} \frac{1}{\sqrt{d_i\, d_j}} \right)^2 \le \sum_{i \sim j} d_i d_j \sum_{i \sim j} \frac{1}{d_i d_j}, \text{ that is, } m^2 \le M_2\, R_{-1} \tag{23}$$

with equality holding if and only if $d_id_j = d_kd_\ell$, for any edges v_iv_j, $v_kv_\ell \in E(G)$. By Theorem 3.13 with (23), we get the required result in (22). The first part of the proof is done.

We have to prove that $d_id_j = d_kd_\ell$, for any edges v_iv_j, $v_kv_\ell \in E(G)$ if and only if G is a regular graph or a semiregular bipartite graph. For this we suppose that $d_id_j = d_kd_\ell$, for any edges v_iv_j, $v_kv_\ell \in E(G)$. From the equality $d_id_j = d_id_k$, $v_iv_j \in E(G)$ and $v_iv_k \in E(G)$, follows $d_j = d_k$. Similarly, from the equality $d_jd_i = d_jd_t$, $v_iv_j \in E(G)$ and $v_jv_t \in E(G)$, it follows that $d_i = d_t$. Hence all the vertices adjacent to any vertex v_i ($i = 1, 2, \ldots, n$) have the same degree. First we assume that G contains an odd cycle. Since G is connected, then using the above result, we conclude that $d_1 = d_2 = \cdots = d_n$, that is, G is a regular graph. Next we assume that G contains only even cycles. In this case G is semiregular bipartite graph as G is connected. Hence G is a regular graph or a semiregular bipartite graph. Conversely, one can easily see that $d_id_j = d_kd_\ell$, for any edges v_iv_j, $v_kv_\ell \in E(G)$ holds for regular graph or semiregular bipartite graph.

By Theorem 3.13 with the above result, we conclude that the equality holds in (22) if and only if G is a regular graph or a semiregular bipartite graph. □

Corollary 3.15. *Let G be a connected graph with n (≥ 2) vertices and m edges. Then*

$$SDD \le \frac{n^2}{4R_{-1}} \frac{(\Delta_e + \delta_e)^2}{\Delta_e \delta_e} - 2m, \tag{24}$$

with equality holding if and only if G is a regular graph or a semiregular bipartite graph, or $d_i + d_j = \Delta_e$ or δ_e for any edges $v_iv_j \in E(G)$ ($\Delta_e \neq \delta_e$) with

$$\Delta_e \sum_{v_iv_j \in S} \frac{1}{d_id_j} = \delta_e \sum_{v_iv_j \in W} \frac{1}{d_id_j},$$

where $S = \{v_iv_j \in E(G) : d_i + d_j = \Delta_e\}$ and $W = \{v_iv_j \in E(G) : d_i + d_j = \delta_e\}$.

Moreover,

$$SDD \le \frac{n^2 M_2}{4m^2} \frac{(\Delta_e + \delta_e)^2}{\Delta_e \delta_e} - 2m. \tag{25}$$

Equality in (25) *holds if and only if G is a regular graph or a semiregular bipartite graph.*

Proof. Using the arithmetic-geometric mean inequality for real numbers (see e.g. [18]), according to (21) we have that

$$2\sqrt{S\,\Delta_e\delta_e\,R_{-1}} \le S + \delta_e\Delta_e\,R_{-1} \le n(\Delta_e + \delta_e), \ \text{ that is, } \ S \le \frac{n^2(\Delta_e+\delta_e)^2}{4\Delta_e\delta_e R_{-1}}.$$

According to this inequality and equality (10) we obtain (24).

By Theorem 3.13 with the above results, we conclude that the equality holds in (24) if and only if G is a regular graph or a semiregular bipartite graph, or $d_i + d_j = \Delta_e$ or δ_e for any edges $v_iv_j \in E(G)$ ($\Delta_e \neq \delta_e$) with $S = \delta_e\Delta_e\,R_{-1}$, that is, if and only if G is a regular graph or a semiregular bipartite graph, or $d_i + d_j = \Delta_e$ or δ_e for any edges $v_iv_j \in E(G)$ ($\Delta_e \neq \delta_e$) with

$$\Delta_e^2 \sum_{v_iv_j\in S} \frac{1}{d_i\,d_j} + \delta_e^2 \sum_{v_iv_j\in W} \frac{1}{d_i\,d_j} = \sum_{i\sim j} \frac{(d_i+d_j)^2}{d_i\,d_j} = S = \delta_e\Delta_e \sum_{i\sim j} \frac{1}{d_i\,d_j} = \Delta_e\,\delta_e \sum_{v_iv_j\in S} \frac{1}{d_i\,d_j} + \Delta_e\,\delta_e \sum_{v_iv_j\in W} \frac{1}{d_i\,d_j},$$

that is, if and only if G is a regular graph or a semiregular bipartite graph, or $d_i + d_j = \Delta_e$ or δ_e for any edges $v_iv_j \in E(G)$ ($\Delta_e \neq \delta_e$) with

$$\Delta_e \sum_{v_iv_j\in S} \frac{1}{d_i\,d_j} = \delta_e \sum_{v_iv_j\in W} \frac{1}{d_i\,d_j},$$

where $S = \{v_iv_j \in E(G) :\ d_i + d_j = \Delta_e\}$ and $W = \{v_iv_j \in E(G) :\ d_i + d_j = \delta_e\}$.

The inequality (25) is obtained from (24) and $R_{-1}M_2 \ge m^2$. Since $R_{-1}M_2 = m^2$ if and only if G is a regular graph or a semiregular bipartite graph (see proof of the Corollary 3.14). Hence the equality in (25) is attained if and only if G is a regular graph or a semiregular bipartite graph. $\square$

In the following theorem we determine lower bound for *SDD* in terms of parameters n, m and invariant R_{-1}.

Theorem 3.16. *Let G be a connected graph with $n\,(\ge 2)$ vertices and m edges. Then*

$$SDD \ge \frac{n^2}{R_{-1}} - 2m. \tag{26}$$

Equality holds if and only if G is a regular graph or a bipartite semiregular graph.

Proof. By Cauchy-Schwarz inequality, we have

$$\sum_{i\sim j} \frac{1}{d_id_j} \sum_{i\sim j} \frac{(d_i+d_j)^2}{d_id_j} \ge \left(\sum_{i\sim j} \frac{d_i+d_j}{d_id_j} \right)^2$$

with equality holding if and only if $d_i + d_j = d_k + d_\ell$ for any edges v_iv_j, $v_kv_\ell \in E(G)$.
Since

$$\sum_{i\sim j} \frac{d_i+d_j}{d_id_j} = \sum_{i\sim j} \left(\frac{1}{d_i} + \frac{1}{d_j} \right) = \sum_{i=1}^{n} 1 = n,$$

the inequality becomes

$$R_{-1}S \ge n^2.$$

According to this inequality and equality (10), we obtain the inequality (26). Moreover, the equality holds in (26) if and only if $d_i + d_j = d_k + d_\ell$ for any edges v_iv_j, $v_kv_\ell \in E(G)$. Since G is connected, the equality holds in (26) if and only if G is a regular graph or a bipartite semiregular graph [3]. $\square$

In the following theorem we prove an inequality opposite to the inequality (26).

Theorem 3.17. *Let G be a connected graph with n vertices and m (≥ 2) edges. Let S be a subset of $I = \{e_1, e_2, \ldots, e_m\}$ which minimizes the expression*

$$\left| \sum_{e \in S} \frac{1}{d_i d_j} - \frac{1}{2} R_{-1} \right|. \tag{27}$$

Then

$$SDD \leq \frac{n^2}{R_{-1}} - 2m + (\Delta_e - \delta_e)^2 \alpha(S) R_{-1}, \tag{28}$$

where

$$\alpha(S) = \frac{\sum\limits_{e \in S} \frac{1}{d_i d_j}}{R_{-1}} \left(1 - \frac{\sum\limits_{e \in S} \frac{1}{d_i d_j}}{R_{-1}} \right). \tag{29}$$

Equality holds in (28) *if and only if G is a regular graph or a semiregular bipartite graph.*

Proof. For $p_i := \frac{1}{d_i d_j}$ the expressions (5) and (7) become (27) and (29). Now, for $p_i := \frac{1}{d_i d_j}$, $a_i = b_i := d_i + d_j$, $R_1 = R_2 = \Delta_e$, $r_1 = r_2 = \delta_e$, where summation goes over all adjacent vertices in graph G, i.e., over all edges, the inequality (6) becomes

$$\sum_{i \sim j} \frac{1}{d_i d_j} \sum_{i \sim j} \frac{(d_i + d_j)^2}{d_i d_j} - \left(\sum_{i \sim j} \frac{d_i + d_j}{d_i d_j} \right)^2 \leq (\Delta_e - \delta_e)^2 \alpha(S) \left(\sum_{i \sim j} \frac{1}{d_i d_j} \right)^2,$$

i.e.

$$R_{-1} S - n^2 \leq (\Delta_e - \delta_e)^2 \alpha(S) R_{-1}^2. \tag{30}$$

According to this inequality and (10) we obtain (28).

Moreover, the equality holds in (6) if and only if $R_1 = a_1 = a_2 = \cdots = a_m = r_1$ or $R_2 = b_1 = b_2 = \cdots = b_m = r_2$. It follows that equality holds in (30) if and only if $\Delta_e = d(e_1) + 2 = \cdots = d(e_m) + 2 = \delta_e$, that is, if and only if G is a regular graph or a semiregular bipartite graph [3]. Consequently, the equality holds in (28) if and only if G is a regular graph or a semiregular bipartite graph. □

Using the arithmetic-geometric mean inequality for real numbers (see e.g. [18]), we have that $\alpha(S) \leq \frac{1}{4}$ for every subset $S \subset I$. Therefore, we have the following corollary of Theorem 3.17.

Corollary 3.18. *Let G be a connected graph with n vertices and m (≥ 2) edges. Then*

$$SDD \leq \frac{n^2}{R_{-1}} - 2m + \frac{(\Delta_e - \delta_e)^2 R_{-1}}{4}.$$

Equality holds if and only if G is a regular graph or a semiregular bipartite graph.

We now give a relation between different topological indices of graphs:

Theorem 3.19. *Let G be a graph of order n with m edges and maximum degree Δ, minimum degree δ. Then*

$$SDD + 2m + R \cdot r \cdot ISI \leq (r + R) \sqrt{(m-1) M_1 + m \left(\Pi_1^* \right)^{1/m}}, \tag{31}$$

where

$$r = \sqrt{\frac{8}{\Delta}}, \qquad R = \sqrt{\frac{\Delta}{\delta^2} + \frac{1}{\Delta} + \frac{6}{\delta}}.$$

Moreover, the equality holds if and only if G is a regular graph.

Proof. We have

$$\begin{aligned}
\sqrt{\frac{(d_i+d_j)^3}{d_i^2\,d_j^2}} &= \sqrt{\frac{1}{d_i}\left(3+\frac{d_j}{d_i}\right)+\frac{1}{d_j}\left(3+\frac{d_i}{d_j}\right)}\\
&\le \frac{1}{\sqrt{\delta}}\sqrt{6+\frac{d_j}{d_i}+\frac{d_i}{d_j}}\\
&= \frac{1}{\sqrt{\delta}}\sqrt{8+\left(\sqrt{\frac{d_i}{d_j}}-\sqrt{\frac{d_j}{d_i}}\right)^2}\\
&\le \frac{1}{\sqrt{\delta}}\sqrt{8+\left(\sqrt{\frac{\Delta}{\delta}}-\sqrt{\frac{\delta}{\Delta}}\right)^2} = \sqrt{\frac{\Delta}{\delta^2}+\frac{1}{\Delta}+\frac{6}{\delta}} = R, \text{ (say)}
\end{aligned} \tag{32}$$

and

$$\sqrt{\frac{(d_i+d_j)^3}{d_i^2\,d_j^2}} \ge \frac{1}{\sqrt{\Delta}}\sqrt{6+\frac{d_j}{d_i}+\frac{d_i}{d_j}} \ge \sqrt{\frac{8}{\Delta}} = r, \text{ (say)}, \quad \text{as } \frac{d_j}{d_i}+\frac{d_i}{d_j} \ge 2. \tag{33}$$

Setting $a_i := d_i + d_j$, where summation is performed over all edges, the inequality (2) becomes

$$\left(\sum_{i\sim j}\sqrt{d_i+d_j}\right)^2 \le (m-1)\sum_{i\sim j}(d_i+d_j) + m\left(\prod_{i\sim j}(d_i+d_j)\right)^{1/m},$$

that is,

$$\sum_{i\sim j}\sqrt{d_i+d_j} \le \sqrt{(m-1)\,M_1 + m\left(\Pi_1^*\right)^{1/m}}. \tag{34}$$

Setting $a_i := \sqrt{\frac{d_i\,d_j}{d_i+d_j}}$ and $b_i := \sqrt{\frac{(d_i+d_j)^2}{d_i\,d_j}}$ with $r \le \frac{b_i}{a_i} \le R$, where summation is performed over all edges, the inequality (8) becomes

$$\sum_{i\sim j}\frac{(d_i+d_j)^2}{d_i\,d_j} + r\,R\sum_{i\sim j}\frac{d_i\,d_j}{d_i+d_j} \le (r+R)\sum_{i\sim j}\sqrt{d_i+d_j},$$

that is,

$$SDD + 2m + R\cdot r\cdot ISI \le (r+R)\sqrt{(m-1)\,M_1 + m\left(\Pi_1^*\right)^{1/m}},$$

where

$$r = \sqrt{\frac{8}{\Delta}}, \quad R = \sqrt{\frac{\Delta}{\delta^2}+\frac{1}{\Delta}+\frac{6}{\delta}}, \quad \text{by (32), (33) and (34).}$$

The first part of the proof is done.

Suppose that equality holds in (31). Then all the above inequalities must be equalities. From the equality in (8), we have that there exists at least one i, $r = \frac{b_i}{a_i} = R$, that is, $\sqrt{\frac{8}{\Delta}} = \sqrt{\frac{\Delta}{\delta^2} + \frac{1}{\Delta} + \frac{6}{\delta}}$, that is, $\Delta = \delta$. Hence G is a regular graph.

Conversely, let G be a d-regular graph. Then $SDD = m$, $ISI = md/2$, $M_1 = nd^2$ and $\Pi_1^* = 2^m\, d^m$ and hence

$$SDD + 2m + R \cdot r \cdot ISI = 8m = (r + R)\, \sqrt{(m-1)\, M_1 + m\left(\Pi_1^*\right)^{1/m}}.$$

Hence the equality holds in (31). □

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