MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **92** (2024) 643–652
ISSN: 0340–6253
doi: 10.46793/match.92-3.643D

Proof of a Conjecture on Symmetric Division Deg Index of Graphs

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(Received February 1, 2024)

Abstract

Molecular descriptors play a significant role in the quantitative studies on structure-property and structure-activity relationships. One of the popular degree-based topological index, symmetric division deg (SDD) index is a chemically useful descriptor. The SDD index of a graph G is defined as

$$SDD(G) = \sum_{v_i v_j \in E(G)} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right),$$

where d_i is the degree of the vertex $v_i \in V(G)$. Very recently, Ali et al. [Symmetric division deg index: Extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **90** (2023) 263–299] mentioned several open problems on symmetric division deg index of graphs. One of them is as follows:

Characterize graphs attaining the minimum SDD index over the class of all those n-order connected graphs of minimum degree δ that are not δ-regular.

In this paper we completely solved the above problem.

1 Introduction

We only consider simple connected graph throughout this paper. Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. For any vertex $v_i \in V(G)$, let $N_G(v_i)$ be the set of neighbors of v_i in G and $N_G[v_i] = N_G(v_i) \bigcup \{v_i\}$, the *degree* of $v_i \in V(G)$, denoted by d_i, is the cardinality of $N_G(v)$. In particular, the maximum and minimum degree of a graph G will be denoted by $\Delta(G)$ and $\delta(G)$, respectively. We write $v_i v_j \in E(G)$ when the vertices v_i and v_j are adjacent. And a vertex v of degree 1 is called a *pendant vertex* (also known as *leaf*), the edge incident with a pendant vertex is called a *pendant edge*. Other undefined notations and terminology on the graph theory can be found in [4].

Molecular descriptors play a significant role in the quantitative studies on structure-property and structure-activity relationships [9,10]. Vukičević and Gašperov [18] proposed and studied a novel class of molecular descriptors in an effort to improve the quantitative studies that already existed on the specific types of molecular descriptors. They found that only a small number of descriptors from this class are helpful for QSPR (quantitative structure-property relationship) applications. The so-called symmetric division deg (SDD) index is among such chemically useful descriptors. The SDD index of a graph G is defined as

$$SDD(G) = \sum_{v_i v_j \in E(G)} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right),$$

where d_i is the degree of the vertex $v_i \in V(G)$.

Furtula et al. [7] conducted a thorough comparative analysis of the SDD index with regard to several other molecular descriptors of this kind and discovered that the SDD index is a feasible and practicable molecular descriptor that outperforms a number of other descriptors of a similar kind, and hence they concluded that it deserves to be treated as a useful and applicable molecular descriptor, preferable to some of the more widely used ones. The mathematical properties, particularly the extremal problems and bounds, of the SDD index have been studied, see [1–3, 5, 6, 8, 11–17] and the review article [3]. Several open problems related to this molecular descriptor are also given in [3]. In the same paper, the following open problem is mentioned:

Problem 1. Characterize graphs attaining the minimum SDD index over the class of all those n-order connected graphs of minimum degree δ that are not δ-regular.

The path, star and complete graphs of order n are denoted by P_n, S_n and K_n, respectively. We use S'_n to denote the graph obtained by adding an edge to a star S_n. Denote by K'_n the graph obtained by deleting an edge from K_n.

2 Main result

In this section we confirm **Problem 1**.

Let $\Gamma^1_{n,\delta}$ be a class of connected graphs $H = (V, E)$ of order n with $m \, (= \frac{1}{2}\,(n\delta + 1))$ edges and $d_1 = \Delta = \delta + 1$, $d_2 = d_3 = \cdots = d_n = \delta$, where Δ is the maximum degree and δ is the minimum degree. Two graphs $H_1 \in \Gamma^1_{5,3}$ and $H_2 \in \Gamma^1_{9,3}$ (see, Fig. 1). For $G \in \Gamma^1_{n,\delta}$, we obtain

$$SDD(G) = \left(\frac{\delta+1}{\delta} + \frac{\delta}{\delta+1}\right)(\delta+1) + 2(m-\delta-1) = 2m + \frac{1}{\delta} = n\delta + 1 + \frac{1}{\delta}.$$

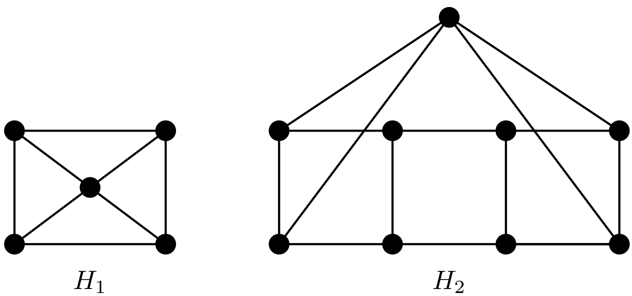

Figure 1. Two graphs H_1 and H_2.

Let $\Gamma^2_{n,\delta}$ be a class of connected graphs $H = (V, E)$ of order n with $m \, (= \frac{1}{2}\,(n\delta + 2))$ edges and $v_1v_2 \in E(G)$ such that $d_1 = \Delta = \delta + 1 = d_2$, $d_3 = d_4 = \cdots = d_n = \delta$, where Δ is the maximum degree and δ is the minimum degree. Two graphs $H_3 \in \Gamma^2_{6,2}$ and $H_4 \in \Gamma^2_{10,2}$ (see, Fig. 2). For

$G \in \Gamma^2_{n,\delta}$, we obtain

$$SDD(G) = \left(\frac{\delta+1}{\delta} + \frac{\delta}{\delta+1}\right) 2\delta + 2(m-2\delta) = 2m + \frac{2}{\delta+1} = n\delta + 2 + \frac{2}{\delta+1}.$$

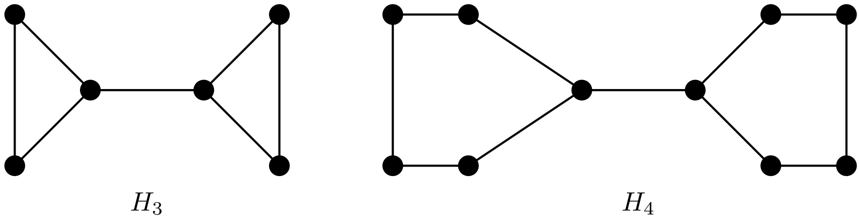

Figure 2. Two graphs H_3 and H_4.

We solve the **Problem 1** in the following. Without loss of generality, we can assume that $d_1 \geq d_2 \geq \cdots \geq d_n$.

Theorem 1. *Let G be a connected non-regular graph of order $n > 3$ with minimum degree δ. If both n and δ are odd, then*

$$SDD(G) \geq n\delta + 1 + \frac{1}{\delta} \tag{1}$$

with equality if and only if $G \in \Gamma^1_{n,\delta}$. Otherwise,

$$SDD(G) \geq n\delta + 2 + \frac{2}{\delta+1} \tag{2}$$

with equality if and only if $G \in \Gamma^2_{n,\delta}$.

Proof. Let v_iv_j be any edge in G such that $d_i \geq d_j$. Also let Δ be the maximum degree in G. Since G is not regular and δ is the minimum degree in G, we have $\Delta \geq \delta + 1$. Now,

$$\frac{d_i}{d_j} + \frac{d_j}{d_i} = \left(\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}}\right)^2 + 2.$$

Let m_1 be the number of edges $v_iv_j \in E(G)$ such that $d_i = d_j$. Thus we have

$$SDD(G) = \sum_{v_i v_j \in E(G)} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right)$$

$$= \sum_{\substack{v_i v_j \in E(G), \\ d_i = d_j}} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right) + \sum_{\substack{v_i v_j \in E(G), \\ d_i > d_j}} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right)$$

$$= 2m_1 + \sum_{\substack{v_i v_j \in E(G), \\ d_i > d_j}} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right). \tag{3}$$

Let $v_k v_\ell$ be an edge in G such that $d_k > d_\ell$. Then one can easily check that

$$\frac{d_k}{d_\ell} \geq \frac{d_k}{d_k - 1} \quad \text{and} \quad \frac{d_\ell}{d_k} \leq \frac{d_k - 1}{d_k}.$$

From the above, we obtain

$$\sqrt{\frac{d_k}{d_\ell}} - \sqrt{\frac{d_\ell}{d_k}} \geq \sqrt{\frac{d_k}{d_k - 1}} - \sqrt{\frac{d_k - 1}{d_k}} = \frac{1}{\sqrt{(d_k - 1)\, d_k}},$$

that is,

$$\left(\sqrt{\frac{d_k}{d_\ell}} - \sqrt{\frac{d_\ell}{d_k}} \right)^2 \geq \frac{1}{(d_k - 1)\, d_k},$$

that is,

$$\frac{d_k}{d_\ell} + \frac{d_\ell}{d_k} \geq 2 + \frac{1}{(d_k - 1)\, d_k}.$$

Since G is non-regular, using the above result in (3), we obtain

$$SDD(G) = \sum_{v_i v_j \in E(G)} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right) \geq 2m_1 + \sum_{\substack{v_i v_j \in E(G), \\ d_i > d_j}} \left(2 + \frac{1}{(d_i - 1)\, d_i} \right)$$

$$\geq 2m + \frac{1}{(\Delta - 1)\, \Delta} \tag{4}$$

as $d_i\,(d_i - 1) \leq \Delta\,(\Delta - 1)$ and $\sum_{\substack{v_i v_j \in E(G), \\ d_i > d_j}} 1 = m - m_1$, where m is the number of edges in G.

Again since G is non-regular, $2m \geq n\,\delta + 1$. Let k be the number of vertices of degree Δ in G. We consider the following cases:

Case 1. Both n and δ are odd. Since $\Delta \geq \delta + 1$, we consider the following two subcases.

Case 1.1. $\Delta = \delta{+}1$. If $k = 1$, then $d_1 = \Delta = \delta{+}1$, $d_2 = d_3 = \cdots = d_n = \delta$, that is, $G \in \Gamma^1_{n,\delta}$ with

$$SDD(G) = n\delta + 1 + \frac{1}{\delta}$$

and hence the equality holds in (1). Otherwise, $k \geq 2$. We have

$$2m = k(\delta + 1) + (n - k)\,\delta = n\,\delta + k \geq n\,\delta + 3$$

as both n and δ are odd. Using this result in (4), we obtain

$$SDD(G) \geq n\delta + 3 + \frac{1}{(\Delta - 1)\,\Delta} > n\delta + 1 + \frac{1}{\delta}.$$

The result (1) strictly holds.

Case 1.2. $\Delta \geq \delta + 2$. In this case $2m \geq n\,\delta + 3$ as both n and δ are odd. From (4), we obtain

$$SDD(G) \geq n\delta + 3 + \frac{1}{(\Delta - 1)\,\Delta} > n\delta + 1 + \frac{1}{\delta}.$$

Again the result (1) strictly holds.

Case 2. n and/or δ are even. In this case $2m \geq n\,\delta + 2$ as G is non-regular. First we assume that $\delta = 1$. Then n must be even and $2m \geq n + 2$. We have $n \geq 4$. If $n = 4$, then $G \cong P_4$ or $G \cong S_4$ or $G \cong S'_4$ or $G \cong K'_4$. One can easily check that

$$SDD(P_4)=7=n\delta+2+\frac{2}{\delta+1},\quad SDD(S_4)=10>7=n\delta+2+\frac{2}{\delta+1}$$

$$SDD(S_4')=\frac{29}{3}>7=n\delta+2+\frac{2}{\delta+1},\ SDD(K_4')=\frac{32}{3}=n\delta+2+\frac{2}{\delta+1}.$$

Thus the result (2) holds as $P_4\in\Gamma^2_{4,1}$ and $K_4'\in\Gamma^2_{4,2}$. Otherwise, $n\geq 5$. Since G is non-regular, then there exists an edge $v_iv_j\in E(G)$ such that

$$\frac{d_i}{d_j}+\frac{d_j}{d_i}>2\ \text{ and hence }\ SDD(G)>2\,(n-1)\geq n+3=n\delta+2+\frac{2}{\delta+1}$$

as G is connected and $\delta=1$. Thus, the result (2) strictly holds.

Next we assume that $\delta\geq 2$. We consider two cases:

Case 2.1. $\Delta=\delta+1$. For $k=1$, we have $d_1=\Delta=\delta+1$, $d_2=d_3=\cdots=d_n=\delta$, that is, $2m=n\delta+1$, a contradiction as $n\delta+1$ is odd. So we now assume that $k\geq 2$. We have

$$2m=k(\delta+1)+(n-k)\,\delta=n\,\delta+k\geq n\,\delta+2.$$

If $2m\geq n\,\delta+4$, then from (4), we obtain

$$SDD(G)\geq n\delta+4+\frac{1}{(\Delta-1)\,\Delta}>n\delta+2+\frac{2}{\delta+1}.$$

Again the result (2) strictly holds. Otherwise, $2m=n\,\delta+2$ as $n\,\delta+3$ is odd. Then we must have $d_1=\Delta=\delta+1=d_2$ and $d_3=d_4=\cdots=d_n=\delta$. For $v_1v_2\in E(G)$, we have $G\in\Gamma^2_{n,\delta}$ with

$$SDD(G)=n\delta+2+\frac{2}{\delta+1}$$

and hence the equality holds in (2).

For $v_1v_2 \notin E(G)$, we obtain

$$SDD(G) = \sum_{\substack{v_iv_j\in E(G),\\ d_i=d_j}} \left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right) + \sum_{\substack{v_iv_j\in E(G),\\ d_i>d_j}} \left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)$$

$$= 2(m-2\delta-2) + \left(\frac{\delta+1}{\delta}+\frac{\delta}{\delta+1}\right)(2\delta+2)$$

$$= 2m+\frac{2}{\delta} = n\delta+2+\frac{2}{\delta} > n\delta+2+\frac{2}{\delta+1}.$$

Again the result (2) strictly holds.

Case 2.2. $\Delta \geq \delta+2$. If $2m \geq n\,\delta+4$, then from (4), we obtain

$$SDD(G) \geq n\delta+4+\frac{1}{(\Delta-1)\,\Delta} > n\delta+2+\frac{2}{\delta+1}.$$

Again the inequality (2) strictly holds. Otherwise, $2m = n\,\delta+2$ as $n\,\delta+3$ is odd and $\Delta \geq \delta+2$. Then $k=1$, $d_1=\Delta=\delta+2$ and $d_2=d_3=\cdots=d_n=\delta$. Thus we obtain

$$SDD(G) = 2(m-\delta-2)+\left(\frac{\delta+2}{\delta}+\frac{\delta}{\delta+2}\right)(\delta+2) = n\delta+2+\frac{4}{\delta} > n\delta+2+\frac{2}{\delta+1}.$$

Again the inequality (2) strictly holds. This completes the proof of the theorem. ■

***Acknowledgment*:** K. C. Das is supported by National Research Foundation funded by the Korean government (Grant No. 2021R1F1A1050646).

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