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Tricyclic graphs with the minimum symmetric division deg index

Chang Liu[1], Yingui Pan[1,2,*], Jianping Li[1]

[1]*College of Liberal Arts and Sciences, National University of Defense Technology, Changsha, Hunan, 410073, P. R. China*
[1]*Sanya Station, China Xi'an Statellite Control Center, Sanya, Hainan, 572427, P. R. China*

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Abstract

The symmetric division deg (SDD) index of a simple graph G is defined as $SDD(G) = \sum_{uv\in E(G)}(\frac{d_u}{d_v} + \frac{d_v}{d_u})$, where $E(G)$ is the edge set of G and d_u denotes the degree of the vertex u in G. In this paper, we determine the n-vertex tricyclic graphs with the first and the second minimum SDD indices, where $n \geq 6$.

Keywords: symmetric division deg index; tricyclic graphs.

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1. Introduction

Topological indices play an important role in mathematical chemistry especially in the QSPR/QSAR investigations [3, 5, 9, 12, 15, 16]. In the last decade, various topological indices were introduced and used to characterize the physical-chemical properties of molecules [15]. For example, Vukičević and Gašperov [19] proposed 148 discrete Adriatic indices and evaluated their predictive properties using the benchmark dataset provided by the International Academy of Mathematical Chemistry [11]. However, just 20 indices among these Adriatic indices were selected as significant predictors of physical-chemical properties of molecules. A simple connected graph G with n vertices and m edges is called a tricyclic graph if $m = n + 2$. All graphs considered in this paper are simple and connected.

The symmetric division deg index, which was selected in [19] as a significant predictor of total surface area of polychlorobiphenyls and for which the extremal graphs obtained with the help of MathChem [18] have a particularly simple and elegant structure, is defined as

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

where d_u is the degree of the vertex u and $E(G)$ is the edge set of the graph G.

Recently, many researches were devoted to the study of the SDD index. Furtula *et al.* [6] found that SDD index deserves to be considered as a viable and applicable topological index, whose quality exceeds that of some popular topological indices. Vasilyev [17] obtained lower and upper bounds of the SDD index for some classes of graphs and determined the corresponding extremal graphs. Das *et al.* [4] also gave some bounds for the SDD index of graphs. Gupta *et al.* [7] established the Nordhaus-Gaddum-type relations for the SDD index of connected graphs, unicyclic graphs and bicyclic graphs. Gupta *et al.* [8] studied the SDD index under some graph operations including the lexicographic product and corona product. Ali *et al.* [1] established a lower bound on the SDD index of any molecular graph of order n and size m and gave a further result about the minimum symmetric division deg index of trees. Palacios [13] gave some new upper bounds for the SDD index of graphs. Trees, unicyclic graphs and bicyclic graphs that minimize the SDD index were investigated in [14, 20].

Motivated by the result obtained in [2], we aim to determine the n-vertex tricyclic graphs with the first and the second minimum SDD indices, where $n \geq 6$.

2. Preliminaries

Let $m_{i,j}$ be the number of edges connecting a vertex of degree i and a vertex of degree j. For a simple graph G with n vertices and m edges, the symmetric division deg index of G can be rewritten as

$$SDD(G) = \sum_{1\leq i\leq j\leq n-1} \frac{i^2 + j^2}{ij} m_{i,j} = \sum_{1\leq i\leq j\leq n-1} \left[2 + \frac{(i-j)^2}{ij}\right] m_{i,j} = 2m + \sum_{1\leq i\leq j\leq n-1} \frac{(i-j)^2}{ij} m_{i,j}.$$

*Corresponding author (panygui@163.com)

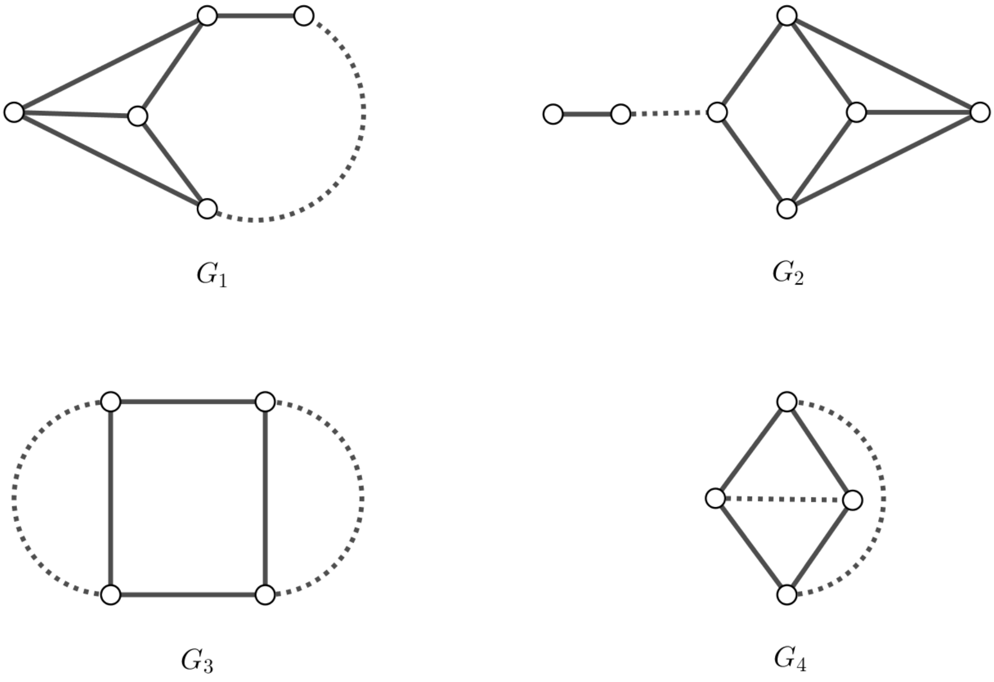

Figure 1: The tricyclic graphs G_1, G_2, G_3 and G_4.

Thus, we get the following lemma.

Lemma 2.1. [1] *If G is a simple graph with m edges, then*

$$SDD(G) = 2m + \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u d_v}.$$

Let $f(G) = \sum_{uv \in E(G)} \frac{(d_u-d_v)^2}{d_u d_v}$. Then $SDD(G) = 2m + f(G)$. In order to determine the graphs with the minimum SDD index among all connected tricyclic graphs with m edges, we just need to find the tricyclic graphs with the minimum value of $f(G)$.

Let $\mathcal{G}_n$ denote the set of all connected tricyclic graphs of order n. Let $\mathcal{G}_n^1 = \{G | G \in \mathcal{G}_n \text{ and } m_{3,3} = 5, m_{2,3} = 2,\ m_{2,2} = n-5\}$, $\mathcal{G}_n^2 = \{G | G \in \mathcal{G}_n \text{ and } m_{1,2} = m_{2,3} = 1,\ m_{3,3} = 7,\ m_{2,2} = n-7\}$, and $\mathcal{G}_n^3 = \{G | G \in \mathcal{G}_n \text{ and } m_{3,3} = 4,\ m_{2,3} = 4,\ m_{2,2} = n-6\}$. In fact, it is easy to verify that $\mathcal{G}_n^1 = \{G_1\}$, $\mathcal{G}_n^2 = \{G_2\}$ and $\mathcal{G}_n^3 = \{G_3, G_4\}$, see Figure 1.

In Table 1, we list the equivalence classes of $\mathcal{G}_n$ with $n_1 = 0$ (i.e., each equivalence class pertaining to a particular degree sequence) that are interesting for consideration.

Table 1: Degree distributions of connected tricyclic graphs with $n_1 = 0$.

Classes	n_6	n_5	n_4	n_3	n_2	n_1	$n_i (i \geq 7)$
D_1	1	0	0	0	$n-1$	0	0
D_2	0	1	0	1	$n-2$	0	0
D_3	0	0	2	0	$n-2$	0	0
D_4	0	0	1	2	$n-3$	0	0
D_5	0	0	0	4	$n-4$	0	0

3. Main result

In this section, we will determine the n-vertex tricyclic graphs with the first and second minimum SDD indices.

Lemma 3.1. *[10] There is a tricyclic graph G of order n with $n_1(G) = 0$ if and only if the graph G belongs to the five classes of graphs shown in Table 1.*

Lemma 3.2. *For the tricyclic graphs as shown in Figure 1, we have*

$$SDD(G_1) = 2n + \frac{13}{3} \quad \textit{and} \quad SDD(G_2) = SDD(G_3) = SDD(G_4) = 2n + \frac{14}{3}.$$

Theorem 3.1. *Let $G \in \mathcal{G}_n \setminus (\mathcal{G}_n^1 \cup \mathcal{G}_n^2 \cup \mathcal{G}_n^3)$ for $n \geq 6$, then*

$$SDD(G) > 2n + \frac{14}{3} > 2n + \frac{13}{3}.$$

Proof. If G is a tricyclic graph without pendant vertices, then by Lemma 3.1, we can get the following results shown in Table 2.

Table 2: The connected tricyclic graphs with $n_1 = 0$ and their *SDD* indices.

Classes	$m_{2,3}$	$m_{2,4}$	$m_{2,5}$	$m_{2,6}$	$m_{3,3}$	$m_{3,4}$	$m_{3,5}$	$m_{4,4}$	$m_{2,2}$	*SDD*
D_1	0	0	0	6	0	0	0	0	$n-4$	$2n+12$
D_2	2	0	4	0	0	0	1	0	$n-5$	$2n+\frac{41}{5}$
D_2	3	0	5	0	0	0	0	0	$n-6$	$2n+9$
D_3	0	6	0	0	0	0	0	1	$n-5$	$2n+7$
D_3	0	8	0	0	0	0	0	0	$n-6$	$2n+8$
D_4	4	4	0	0	1	0	0	0	$n-7$	$2n+\frac{20}{3}$
D_4	6	4	0	0	0	0	0	0	$n-8$	$2n+7$
D_4	5	3	0	0	0	1	0	0	$n-7$	$2n+\frac{77}{12}$
D_4	3	3	0	0	1	1	0	0	$n-6$	$2n+\frac{73}{12}$
D_4	4	2	0	0	0	2	0	0	$n-6$	$2n+\frac{35}{6}$
D_4	2	2	0	0	1	2	0	0	$n-5$	$2n+\frac{11}{2}$
D_5	12	0	0	0	0	0	0	0	$n-10$	$2n+6$
D_5	10	0	0	0	1	0	0	0	$n-9$	$2n+\frac{17}{3}$
D_5	8	0	0	0	2	0	0	0	$n-8$	$2n+\frac{16}{3}$
D_5	6	0	0	0	3	0	0	0	$n-7$	$2n+5$
D_5	4	0	0	0	4	0	0	0	$n-6$	$2n+\frac{14}{3}$
D_5	2	0	0	0	5	0	0	0	$n-5$	$2n+\frac{13}{3}$

Assume now that G is a tricyclic graph with at least one pendant vertex. If G has at least two pendant vertices, let u_1 and u_2 be two pendant vertices which are adjacent to vertices v_1 and v_2, respectively. For convenience, assume that $d_{v_1} = r_1 \geq d_{v_2} = r_2 \geq 2$.

If $r_1 \geq r_2 \geq 3$, then

$$\begin{aligned} f(G) &= \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u d_v} \\ &\geq \frac{(r_1-1)^2}{r_1} + \frac{(r_2-1)^2}{r_2} \\ &\geq 2 \times \frac{(3-1)^2}{3} = \frac{8}{3}. \end{aligned}$$

Then by Lemma 2.1, we have $SDD(G) = 2m + f(G) \geq 2n + \frac{20}{3}$.

If $r_1 \geq 3$ and $r_2 = 2$, then $m_{1,2} \geq 1$ and there are at least one edge connecting vertex of degree 2 and vertex of degree t, where $t \geq 3$. Note that

$$\frac{(r_1-1)^2}{r_1} \geq \frac{(3-1)^2}{3} \quad \text{and} \quad \frac{(t-2)^2}{2t} \geq \frac{(3-2)^2}{2+3}.$$

Then,

$$\begin{aligned} f(G) &= \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u d_v} \\ &\geq \frac{(2-1)^2}{2} + \frac{(3-1)^2}{3} + \frac{(3-2)^2}{6} = 2. \end{aligned}$$

It follows from Lemma 2.1 that $SDD(G) = 2m + f(G) \geq 2n + 6$.

If $r_1 = r_2 = 2$, then G has at least two edges connecting the vertex of degree 2 and the vertex of degree t, where $t \geq 3$. Then

$$\begin{aligned} f(G) &= \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u d_v} \\ &\geq 2 \times \frac{(2-1)^2}{2} + 2 \times \frac{(3-2)^2}{6} = \frac{4}{3}, \end{aligned}$$

which implies that

$$SDD(G) = 2m + f(G) \geq 2n + \frac{16}{3}.$$

Therefore, for any tricyclic graph G with $n \geq 10$ and at least two pendant vertices, we have $SDD(G) \geq 2n + \frac{16}{3}$.

Assume that G has only one pendant vertex. Let x be the pendant vertex and let y be the neighbor of x. Then $d_y = r \geq 2$. If $r \geq 3$, then

$$\begin{aligned} f(G) &= \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u d_v} \\ &\geq \frac{(r-1)^2}{r} \\ &\geq \frac{(3-1)^2}{3} = \frac{4}{3}. \end{aligned}$$

Then by Lemma 2.1, we have $SDD(G) = 2m + f(G) \geq 2n + \frac{16}{3}$.

If $r = 2$, then G has at least one edge connecting the vertex of degree 2 and the vertex of degree t, where $t \geq 3$. If $t \geq 4$, then

$$\begin{aligned} f(G) &= \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u d_v} \\ &> \frac{(2-1)^2}{2} + \frac{(t-2)^2}{2t} \\ &\geq \frac{(2-1)^2}{2} + \frac{(4-2)^2}{8} = 1, \end{aligned}$$

which implies that $SDD(G) \geq 2n + 5$.

If $t = 3$, then $f(G) > \frac{2}{3}$ because G is not isomorphic to G_2. Thus, by Lemma 2.1,

$$SDD(G) = 2m + f(G) > 2n + \frac{14}{3}.$$

For any graph $G \in \mathcal{G}_n \setminus (\mathcal{G}_n^1 \cup \mathcal{G}_n^2 \cup \mathcal{G}_n^3)$, where $n \geq 6$, from the above arguments and calculations, we have

$$SDD(G) > SDD(G_2) = 2n + \frac{14}{3}$$

if G is a tricyclic graph with $\delta = 1$, and

$$SDD(G) > SDD(G_3) = SDD(G_4) = 2n + \frac{14}{3} > SDD(G_1) = 2n + \frac{13}{3}$$

if G is a tricyclic graph with $\delta \geq 2$. □

4. Conclusion

In this paper, we have determined the minimum and second minimum *SDD* index of tricyclic graphs. We think that it would be very interesting to find the tricyclic graph with the maximum *SDD* index, and we will do it in near future.

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