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Maximum Symmetric Division Deg Index of Cactus Graphs With a Fixed Number of Cycles and Order

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Abstract: The symmetric division deg (SDD) index of a graph G is the addition of the numbers $(d_v d_u)^{-1}[(d_v)^2 + (d_u)^2]$ over all the edges uv of G, where d_v and d_u represent degrees of the vertices v and u, respectively. A connected graph in which every edge lies on at most one cycle is usually referred to as a cactus graph. (Every tree as well as every unicyclic graph is a cactus graph; the converse is not generally true.) The primary goal of the present paper is to characterize the unique graph possessing the maximum value of the SDD index over the class of all cactus graphs with a fixed order and number of cycles.

Keywords: topological indices, symmetric division deg index, cactus graph.

1 Introduction

Throughout this paper, only connected and finite graphs are considered. Those terms and notions of graph theory that are utilized in the present paper without giving their definition, may be found in the books [2,6].

A connected graph in which every edge lies on at most one cycle is usually referred to as a cactus graph. The trees and unicyclic graphs form subclasses of the class of all cactus graphs; where a unicyclic graph is a connected graph of the same order and size. Husimi trees were the name given to cactus graphs by Harary and Uhlenbeck [7] in remembrance of Husimi's earlier research in this direction (for example, see [8]). Actually, Harary and Uhlenbeck reserves the term "cactus graphs" for those graphs in which every cycle is a triangle, however it is nowadays a common practice to allow cycles of any length in cactus graphs.

A topological index TI is a function defined on the set of all graphs under the constraint that the equation $TI(H_1) = TI(H_2)$ holds if the graphs H_1 and H_2 are isomorphic. The symmetric division deg (SDD) index is a topological index introduced in the paper [13] for improving the QSAR/QSPR studies. For a graph G, its SDD index is defined as

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

where d_v and d_u indicate the degrees of the vertices v and u, respectively, and $E(G)$ represents the set of edges of G. Because of the chemical applications (see for example [13,4]) of the SDD index, it has gained a considerable attention from researchers, which resulted in many publications. Most of these publications involve mathematical investigation of the SDD index. For instance, we mention some of them. The extremal graph-theoretical problems involving the SDD index were studied in the papers [1,11]. The article [3,5] gives several different sharp bounds for the index under consideration. Some additional mathematical results on the SDD index can be found in [9,10].

The primary goal of the present paper is to characterize the unique graph possessing the maximum value of the SDD index over the class of all cactus graphs with a fixed order and number of cycles. The obtained result actually extends two results, reported in [12,14] independently, concerning the maximum value of the SDD index of trees and unicyclic graphs with a given order (because the trees and unicyclic graphs form subclasses of the class of all cactus graphs).

2 Main Result

For proving the main result, some lemmas are required first. Let us start with the following elementary result.

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Lemma 1. *Let x and n_1 be fixed real numbers satisfying $x > n_1 \geq 1$. Define*

$$f(y) = \frac{x^2+y^2}{xy} - \frac{(x-n_1)^2+y^2}{(x-n_1)y}.$$

The function f is strictly decreasing for $y \geq 2$.

Proof. Note that the derivative function

$$f'(y) = -\frac{n_1(x(x-n_1)+y^2)}{x(x-n_1)y^2}$$

is negative-valued under given constraints.

The next two results were reported in [12,14] independently.

Lemma 2(see [14,12]). *If G is a non-trivial tree with n vertices then*

$$SDD(G) \leq (n-1)^2+1,$$

where the equality sign holds if and only if G is the star graph S_n.

Lemma 3(see [14,12]). *If G is a (connected) unicyclic graph with n vertices then*

$$SDD(G) \leq \frac{n^2+3}{n-1} + (n-3)\left(\frac{(n-1)^2+1}{n-1}\right),$$

where the equality sign holds if and only if G is the graph formed by inserting an additional edge in the star graph S_n.

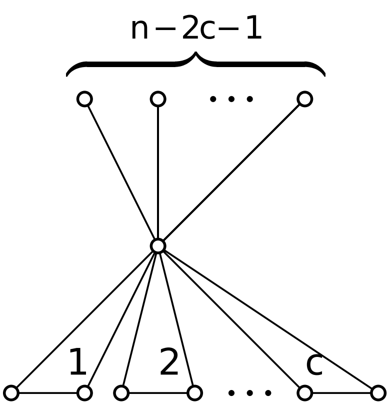

Fig. 1: The cactus graph $S^+_{n,c}$.

The cactus graph $S^+_{n,c}$ depicted in Figure 1 has c cycles (each having length 3) and $n-2c-1$ pendent edges. Note that $S^+_{n,0}$ is the star graph S_n and $S^+_{n,1}$ is the graph attaining the equality sign in the inequality given in Lemma 3. Elementary computations yield

$$SDD\left(S^+_{n,c}\right) = 2c\left(\frac{(n-1)^2+4}{2(n-1)}\right) + (n-2c-1)\left(\frac{(n-1)^2+1}{n-1}\right) + 2c$$

which can be rewritten as

$$SDD\left(S^+_{n,c}\right) = c\left(\frac{n^2+3}{n-1}\right) + (n-2c-1)\left(\frac{(n-1)^2+1}{n-1}\right).$$

In what follows, we take

$$\Theta(n,c) = c\left(\frac{n^2+3}{n-1}\right) + (n-2c-1)\left(\frac{(n-1)^2+1}{n-1}\right).$$

Now, with the above preparation, the main result of this paper can be proved.

Theorem 1. *If G is a non-trivial cactus graph with n vertices and c cycles then*

$$SDD(G) \leq \Theta(n,c) = c\left(\frac{n^2+3}{n-1}\right) + (n-2c-1)\left(\frac{(n-1)^2+1}{n-1}\right),$$

where the equation $SDD(G) = \Theta(n,c)$ holds if and only if $G = S^+_{n,c}$.

Proof. Note that $n+c$ is a natural number greater than or equal to 2. The result is proved by using the mathematical induction on $n+c$. By Lemmas 2 and 3, the result holds for $c=0$ and $c=1$, respectively. Also, when $c \geq 2$ and $n=5$, the result trivially holds because there is a unique cactus graph $S^+_{5,2}$ in this case. Thus, the induction starts. In what follows, suppose that G is a cactus graph with n vertices and c cycles such that $c \geq 2$ and $n \geq 6$. The proof will be completed by subdividing it into two cases: (i) the minimum degree of G is 1 (ii) the minimum degree of G is greater than 1

Case 1. The minimum degree of G is 1.
Let $v_0u \in E(G)$ be an edge such that the vertex v_0 has degree 1 and that the set of vertices adjacent with u is

$$N_G(u) = \{v_0, v_1, v_2, \ldots, v_{x-1}\}.$$

Since $c \geq 2$, at least vertex in the set $N_G(u)$ has degree at least 2. Suppose that the number of vertices in the set $N_G(u)$ having degree 1 is n_1. Then $n_1 \leq n-5$ because $c \geq 2$. Without loss of generality, it is assumed that

$$d_{v_i}\begin{cases} = 1 & \text{when } 0 \leq i \leq n_1-1, \\ \geq 2 & \text{when } n_1 \leq i \leq x-1. \end{cases}$$

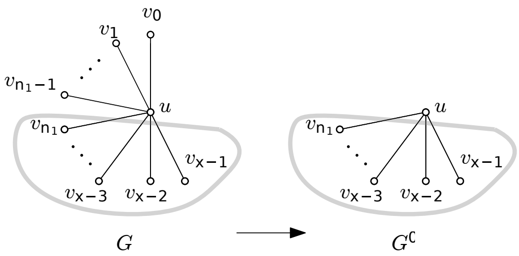

Fig. 2: The transformation used in the Case 1 of the proof of Theorem 1.

Denote by G' the graph generated from G by dropping the vertices $v_0, v_1, v_2, \ldots, v_{n_1-1}$ and their incident edges; see Figure 2. Observe that the graph G' has $n-n_1$ vertices and c cycles and thence the result holds for G' by inductive hypothesis. On the other hand, one has

$$SDD(G) = SDD(G') + n_1\left(\frac{x^2+1}{x}\right) + \sum_{i=n_1}^{x-1}\left(\frac{x^2+(d_{v_i})^2}{xd_{v_i}} - \frac{(x-n_1)^2+(d_{v_i})^2}{(x-n_1)d_{v_i}}\right),$$

which gives (by Lemma 1 because $d_{v_i} \geq 2$ for $n_1 \leq i \leq x-1$):

$$SDD(G) \leq SDD(G') + n_1\left(\frac{x^2+1}{x}\right) + \sum_{i=n_1}^{x-1}\left(\frac{x^2+(2)^2}{2x} - \frac{(x-n_1)^2+(2)^2}{2(x-n_1)}\right) \quad (1)$$

with equality if and only if $d_{v_i} = 2$ for every $i \in \{n_1, n_1+1, \ldots, x-1\}$. By using inductive hypothesis in (1), one gets

$$SDD(G) \leq \Theta(n-n_1, c) + \frac{n_1(3x^2 - n_1x - 2)}{2x} \quad (2)$$

with equality if and only if $d_{v_i} = 2$ for every $i \in \{n_1, n_1+1, \ldots, x-1\}$ and $G' = S^+_{n-n_1,c}$. Inequality (2) further implies that

$$SDD(G) \leq \Theta(n-n_1, c) + \frac{n_1\left(3(n-1)^2 - n_1(n-1) - 2\right)}{2(n-1)} \quad (3)$$

with equality if and only if $d_{v_i} = 2$ for every $i \in \{n_1, n_1+1, \ldots, x-1\}$, $G' = S^+_{n-n_1,c}$, and $x = n-1$. Since $4 \leq 2c \leq n-n_1-1$ (as $c \geq 2$), it holds that

$$\Theta(n-n_1, c) + \frac{n_1\left(3(n-1)^2 - n_1(n-1) - 2\right)}{2(n-1)} - \Theta(n,c)$$

$$= -\frac{n_1(n-n_1-2c-1)[n(n-n_1-2)+n_1+3]}{(2(n-1)(n-n_1-1))} \leq 0$$

where the equation

$$-\frac{n_1(n-n_1-2c-1)[n(n-n_1-2)+n_1+3]}{(2(n-1)(n-n_1-1))} = 0$$

holds if and only if $n-n_1-1 = 2c$, and hence from (3) it follows that

$$SDD(G) - \Theta(n,c) \leq -\frac{n_1(n-n_1-2c-1)[n(n-n_1-2)+n_1+3]}{(2(n-1)(n-n_1-1))} \leq 0$$

where the equation $SDD(G) - \Theta(n,c) = 0$ holds if and only if $d_{v_i} = 2$ for every $i \in \{n_1, n_1+1, \ldots, x-1\}$, $G' = S^+_{n-n_1,c}$, $x = n-1$, and $n-n_1-1 = 2c$. In other words, the equation $SDD(G) - \Theta(n,c) = 0$ holds if and only if $G = S^+_{n,c}$.

Case 2. The minimum degree of G is greater than 1.
In this case, there exist vertices $u, v, w \in V(G)$ on a cycle of G provided that $uv, uw \in E(G)$ and $d_v = 2 = d_u$. Take $d_w = x$. Certainly, it holds that $x \geq 3$. This case is subdivided into two subcases.

Case 2.1. The vertices w and v are not adjacent.

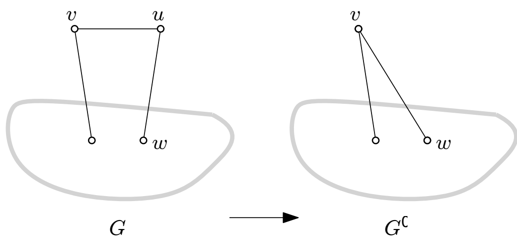

Fig. 3: The transformation used in Case 2.1 of the proof of Theorem 1.

Let G' be the graph deduced from G by dropping the vertex u and then inserting the edge wv; see Figure 3. Observe that the graph G' has $n-1$ vertices and c cycles. Now, by using the assumptions $c \leq \frac{n-1}{2}$, $n \geq 6$, and the inductive hypothesis, one has

$$\begin{aligned}SDD(G)-\Theta(n,c) &= SDD(G')+2-\Theta(n,c)\\ &\le \Theta(n-1,c)+2-\Theta(n,c)\\ &= 2c\left(\frac{1}{n-2}-\frac{1}{n-1}\right)-2n+c+5\\ &\le 2\left(\frac{n-1}{2}\right)\left(\frac{1}{n-2}-\frac{1}{n-1}\right)-2n\\ &+\frac{n-1}{2}+5\\ &= -\frac{3n(n-5)+16}{2(n-2)}\\ &< 0.\end{aligned}$$

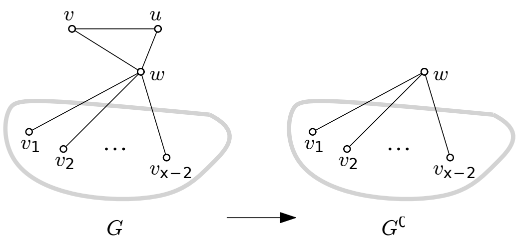

Fig. 4: The transformation used in Case 2.2 of the proof of Theorem 1.

Case 2.2. The vertices w and v are adjacent.
Denote by G' the graph generated from G by dropping the vertices v,u, and their incident edges; see Figure 4. Observe that the graph G' has $n-2$ vertices and c cycles and thence the desired result holds for G' by the inductive hypothesis. Take $N_G(w)=\{u,v,v_1,v_2,\ldots,v_{x-2}\}$. Here, one has

$$\begin{aligned}SDD(G) &= SDD(G')+2+\frac{x^2+4}{x}\\ &+\sum_{i=1}^{x-2}\left(\frac{x^2+(d_{v_i})^2}{xd_{v_i}}-\frac{(x-2)^2+(d_{v_i})^2}{(x-2)d_{v_i}}\right)\end{aligned}$$

which gives (by Lemma 1 because $d_{v_i}\ge 2$ for $1\le i\le x-2$):

$$\begin{aligned}SDD(G) &\le SDD(G')+2+\frac{x^2+4}{x}\\ &+\sum_{i=1}^{x-2}\left(\frac{x^2+(2)^2}{2x}-\frac{(x-2)^2+(2)^2}{2(x-2)}\right) \qquad (4)\end{aligned}$$

with equality if and only if $d_{v_i}=2$ for every $i\in\{1,2,\ldots,x-2\}$. By using the inductive hypothesis in (4), one gets

$$\begin{aligned}SDD(G)-\Theta(n,c) &\le \Theta(n-2,c-1)+2x-\Theta(n,c)\\ &\le \Theta(n-2,c-1)+2(n-1)-\Theta(n,c) \qquad (5)\end{aligned}$$

where the equation $SDD(G)=\Theta(n-2,c-1)+2(n-1)$ holds if and only if $d_{v_i}=2$ for every $i\in\{1,2,\ldots,x-2\}$, $G'=S^+_{n-2,c-1}$, and $x=n-1$. On the other hand, one has

$$\begin{aligned}&\Theta(n-2,c-1)+2(n-1)-\Theta(n,c)\\ &= -\frac{(n-2c-1)\big(n(n-4)+5\big)}{(n-3)(n-1)}\le 0\end{aligned}$$

because $n-2c-1\ge 0$ and $n\ge 6$, where the equation

$$-\frac{(n-2c-1)\big(n(n-4)+5\big)}{(n-3)(n-1)}=0$$

holds if and only if $n=2c-1$; therefore, (5) implies that

$$SDD(G)-\Theta(n,c)\le -\frac{(n-2c-1)\big(n(n-4)+5\big)}{(n-3)(n-1)}\le 0,$$

where the equation $SDD(G)-\Theta(n,c)=0$ holds if and only if $d_{v_i}=2$ for every $i\in\{1,2,\ldots,x-2\}$, $G'=S^+_{n-2,c-1}$, $x=n-1$, and $n=2c-1$. In other words, the equation $SDD(G)-\Theta(n,c)=0$ holds if and only if $G=S^+_{n,c}$.

3 Concluding Remarks

The main result of this paper is Theorem 1, which states that the graph obtained from the n-vertex star graph S_n by adding t independent edges is the unique graph possessing the maximum value of the symmetric division deg index over the class of all cactus graphs with a fixed order n and given number of cycles t. Finding graph(s) possessing the minimum value of the symmetric division deg index over the aforementioned class of cactus graphs is a natural extension of the present study. Also, it seems to be interesting to see if these problems can be solved for the recently introduced inverse version of the symmetric division deg index [5].

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This research has been not funded.

5 Data Availability Statement

Data about this study may be requested from the authors.

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