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On the Inverse Symmetric Division Deg Index of Unicyclic Graphs

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Abstract: The symmetric division deg (SDD) index is among the 148 discrete Adriatic indices that were developed about a decade ago. Motivated by the success of the SDD index, Ghorbani et al. in a recent paper proposed the inverse version of this index and called it the inverse symmetric division deg (ISDD) index. In the aforementioned paper, the graphs possessing the maximum and minimum ISDD index over the set of all tree graphs having the given order were found. The present paper addresses the problem of finding the graphs having the largest and smallest ISDD index from the set of all connected unicyclic graphs having the specified order.

Keywords: topological index; symmetric division deg index; inverse symmetric division deg index; unicyclic graph; chemical graph theory

MSC: 05C07; 05C90



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1. Introduction

This paper is only concerned with connected and finite graphs. The graph theoretical terms that are utilized in this paper may be found in [1,2]. A function I defined on the set of all graphs is said to be a topological index if the equation $I(G) = I(H)$ holds for every pair of isomorphic graphs G and H .

The authors of [3] investigated a novel class of topological indices, the “discrete Adriatic indices”, which consist of 148 indices, for enhancing quantitative structure–property relationships/quantitative structure–activity relationships investigations, and discovered that just a handful of them were beneficial. The symmetric division deg (SDD) index is one of such handful indices; for a graph G , the SDD index is defined as

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

where $E(G)$ and $V(G)$ represent the edge set and vertex set, respectively, of the graph G ; uv represents the edge between the vertices u, v ; and d_w represents the degree of the vertex $w \in V(G)$. In the class of all existing topological indices, the SDD index has the highest correlating potential for predicting the total surface area of polychlorobiphenyls [3]. In the paper [4], the authors did a rigorous study of the SDD index and determined that this index was feasible and practical, whose performance beat that of several more popular topological indices. Details about some extremal results involving the SDD index can be found in the articles [5–7]. The readers interested in sharp bounds on the index under consideration can consult [8–10].

Motivated by the success of the SDD index, Ghorbani et al. [11] proposed the inverse version of the SDD index and called it the inverse symmetric division deg (ISDD) index. For a graph G , its ISDD index can be calculated by using the following formula:

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

The graphs possessing the maximum and minimum ISDD index over the set of all trees having the given number of vertices were determined in [11]. It is natural to consider the following related extremal problem concerning the ISDD index of unicyclic graphs. (A connected graph having exactly one cycle is referred to as a unicyclic graph; a connected graph is unicyclic if and only if its order and size are the same, see [12].)

Problem 1. Determine the graphs possessing the maximum and minimum ISDD index from the set of all unicyclic graphs having the given number of vertices.

The primary goal of this paper is to give results towards the solution of Problem 1.

2. Results

We start this section by stating the following existing result, which is due to Ghorbani et al. [11].

Lemma 1 (see [11]). *If G is a graph with m edges and with at least three vertices, then*

$$ISDD(G) \leq \frac{m}{2}.$$

Moreover, a necessary and sufficient for G being a regular graph is that the equation

$$ISDD(G) = \frac{m}{2}$$

holds.

Since all the graphs discussed in this study are connected, the bound (established by Ghorbani et al. [11]) as stated in Lemma 1 gives a solution to the part of Problem 1 that is related to the maximum value of the ISDD index.

Corollary 1. *For $n \geq 4$, the cycle graph C_n uniquely possesses the maximum ISDD index in the set of all unicyclic graphs having a given number of vertices n .*

Next, we move towards a solution to the part of Problem 1 that is related to the minimum value of the ISDD index. For this purpose, we require the following elementary lemma.

Lemma 2. *The function Φ given by*

$$\Phi(x, y) = \frac{xy}{x^2 + y^2},$$

with $x \geq y \geq 1$, is strictly decreasing in x and strictly increasing in y .

A vertex v in a graph such that v has the degree one is called a pendent vertex. An edge that has a pendent neighbor is known as a pendent edge. If uv is an edge, then u and v are called end-vertices of uv . The next lemma gives a lower bound on the ISDD index for general graphs.

Lemma 3. *If G is a graph of order at least three with m edges, p pendent edges, and maximum degree Δ , then*

$$ISDD(G) \geq \frac{p \Delta}{\Delta^2 + 1} + \frac{2\Delta(m - p)}{\Delta^2 + 4}$$

where the equality sign holds if and only if the end-vertices of every nonpendent edge have degrees two and Δ , and every pendent edge is incident with a vertex of degree Δ (for example, see Figure 1).

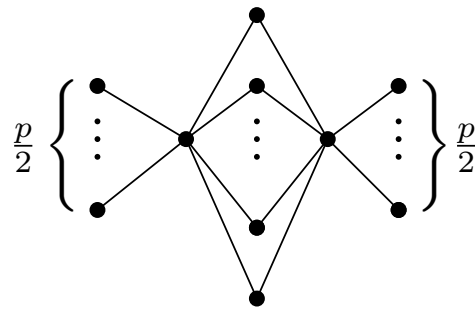


Figure 1. A graph attaining the bound mentioned in Lemma 3.

Proof. If $d_u \geq d_v \geq 2$ then by Lemma 2, one has

$$\frac{d_u d_v}{(d_u)^2 + (d_v)^2} \geq \frac{\Delta d_v}{\Delta^2 + (d_v)^2} \geq \frac{2\Delta}{\Delta^2 + (2)^2}.$$

Note that

$$\frac{d_u d_v}{(d_u)^2 + (d_v)^2} = \frac{2\Delta}{\Delta^2 + (2)^2}$$

if and only if $d_u = \Delta$ and $d_v = 2$. Thus, if u_1, u_2, \dots, u_p , are the vertices adjacent to pendent vertices of G then one has

$$\begin{aligned} ISDD(G) &= \sum_{i=1}^p \frac{d_{u_i}}{(d_{u_i})^2 + 1} + \sum_{uv \in E(G); d_u \geq d_v \geq 2} \frac{d_u d_v}{(d_u)^2 + (d_v)^2} \\ &\geq \sum_{i=1}^p \frac{\Delta}{\Delta^2 + 1} + \sum_{uv \in E(G); d_u \geq d_v \geq 2} \frac{2\Delta}{\Delta^2 + 4} \\ &= \frac{p \Delta}{\Delta^2 + 1} + \frac{2\Delta(m - p)}{\Delta^2 + 4}. \end{aligned}$$

□

Since a connected graph is unicyclic if and only if its order and size are the same, the following result is a particular case of Lemma 3.

Corollary 2. If G is a unicyclic graph with n vertices, p pendent vertices, and maximum degree Δ , then

$$ISDD(G) \geq \frac{p \Delta}{\Delta^2 + 1} + \frac{2\Delta(n - p)}{\Delta^2 + 4}$$

with equality if and only if G is the unicyclic graph attaining the equality in Lemma 3.

Since the function f defined by

$$f(x, \Delta) = \frac{2\Delta(n - x)}{\Delta^2 + 4} + \frac{\Delta x}{\Delta^2 + 1}$$

is strictly decreasing in x for $0 \leq x \leq n - 3$ and $2 \leq \Delta \leq n - 1$, one has

$$f(x, \Delta) \geq f(n - 3, \Delta).$$

Now, if we take $g(y) = f(n - 3, y)$, then

$$g'(y) = -\frac{h(n)}{(y^2 + 1)^2(y^2 + 4)^2}, \tag{1}$$

where $h(z) = zy^6 + 7zy^4 + 8zy^2 - 16z - 9y^6 - 9y^4 + 18y^2 + 72$. The function h is strictly increasing because

$$h'(z) = (y - 1)(y + 1)(y^2 + 4)^2 > 0$$

for $2 \leq y \leq n - 1$, and thence

$$h(n) \geq h(9) = 18(3y^4 + 5y^2 - 4) > 0$$

for $n \geq 9$ and $2 \leq y \leq n - 1$. Consequently, Equation (1) yields

$$g(y) \geq g(n - 1)$$

for $n \geq 9$ and $2 \leq y \leq n - 1$. Therefore, by Corollary 2, if G is a unicyclic graph with $n \geq 9$ vertices, then

$$ISDD(G) \geq \frac{(n - 3)(n - 1)}{(n - 1)^2 + 1} + \frac{6(n - 1)}{(n - 1)^2 + 4}. \tag{2}$$

Although the lower bound (2) on the $ISDD$ index of a unicyclic graph G depends only on the order of G , it does not give the solution to the minimal part of Problem 1.

The set of all vertices adjacent to a vertex v of a graph G is denoted by $N_G(v)$ (or simply by $N(v)$ if there is no confusion about the graph under consideration). The members of the set $N(v)$ are called neighbors of v . Next, we define a graph transformation, which is crucial for the rest of this paper.

Transformation 1. Let G be a graph of order n and maximum degree of at most $n - 2$. Let $vw \in E(G)$ be an edge such that

- (i). $d_v \geq d_z$ for every $z \in N(v) \cup N(w)$ and
- (ii). The vertex w has at least one neighbor (different from v) that is not adjacent to v .

Take $N(w) \setminus N(v) := \{v, w_1, \dots, w_k\}$. Let G' be the graph deduced from G by inserting the edges vw_1, vw_2, \dots, vw_k and dropping the edges ww_1, ww_2, \dots, ww_k .

Lemma 4. If G is a unicyclic graph of order n and girth greater than three, then there exists at least one unicyclic graph G' of order n and girth three such that

$$ISDD(G) > ISDD(G')$$

Proof. We note that the graph G has the maximum degree less than $n - 1$. Let $v \in V(G)$ be a vertex having the maximum degree. Choose $vw \in E(G)$ such that w has at least one neighbor that is not adjacent to v . Since the girth of G is greater than three, it holds that $N(w) \cap N(v) = \emptyset$ and thus $N(w) \setminus N(v) = N(w)$. Take

$$N(w) = \{v, w_1, \dots, w_k\}.$$

Let G' be the graph deduced from G by applying Transformation 1. Note that whether the edge vw lies on the cycle or not (see Figures 2 and 3), in either case we have

$$\begin{aligned}
 ISDD(G') - ISDD(G) &= \sum_{\substack{x \in N(v) \setminus N(w), \\ x \neq w}} (\Phi(d_v + k, d_x) - \Phi(d_v, d_x)) \\
 &+ \sum_{i=1}^k (\Phi(d_v + k, d_{w_i}) - \Phi(d_w, d_{w_i})) \\
 &+ \Phi(d_v + k, d_w - k) - \Phi(d_v, d_w). \tag{3}
 \end{aligned}$$

where the function Φ is defined in Lemma 2 and $d_v - k \in \{1, 2\}$, and all the degrees of vertices are being considered in G . Note that the inequalities $d_v \geq d_x$ and $d_v \geq d_{w_i}$ hold for all $x \in N_G(v) \setminus (N_G(w) \cup \{w\})$ and $i \in \{1, 2, \dots, k\}$. Furthermore, if $d_w - k = 1$ then

$$\Phi(d_v + k, d_w - k) - \Phi(d_v, d_w) = -\frac{k(d_v + k + 1)^2(d_v - 1)}{((d_v + k)^2 + 1)((d_v)^2 + (k + 1)^2)} < 0$$

and if $d_w - k = 2$ then

$$\Phi(d_v + k, d_w - k) - \Phi(d_v, d_w) = -\frac{k(d_v + k + 2)^2(d_v - 2)}{((d_v + k)^2 + 4)((d_v)^2 + (k + 2)^2)} < 0,$$

and hence, by using Lemma 2, we get

$$ISDD(G') < ISDD(G).$$

If the girth of G' is three then we obtain the desired conclusion. If G' has a girth greater than three, then by repeating the above process (after applying Transformation 1 finite number of times), we get a unicyclic graph G'' of order n and girth three such that

$$ISDD(G'') < ISDD(G).$$

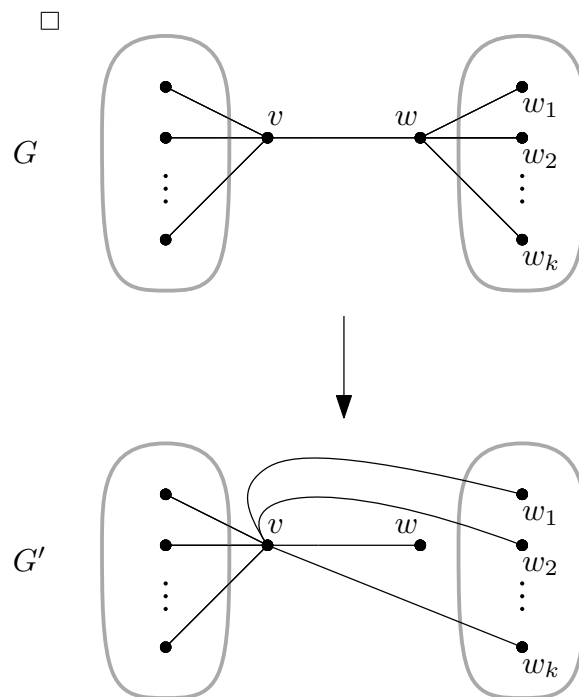


Figure 2. Transformation 1 used in the proof of Lemma 4, when the edge vw does not lie on a cycle.

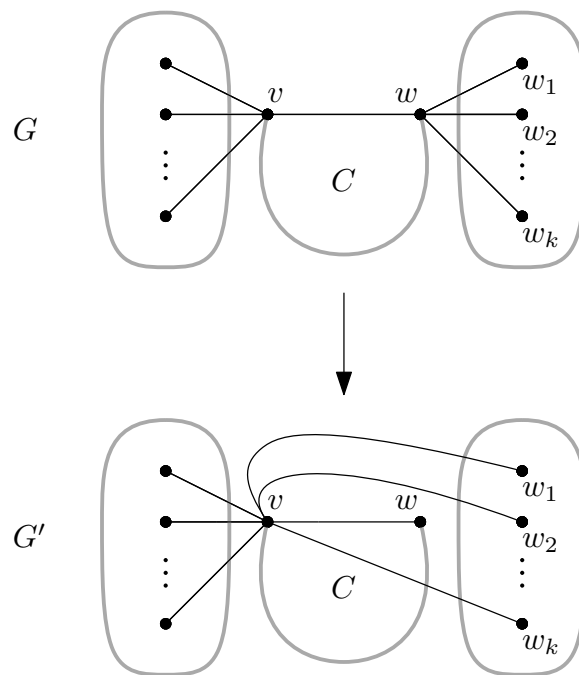


Figure 3. Transformation 1 used in the proof of Lemma 4, when the edge vw lies on the cycle of length greater than 3.

Lemma 5. For $n \geq 4$, if G is a unicyclic graph with the minimum ISDD index in the set of all unicyclic graphs of a given order n and girth three, then every vertex of G with the maximum degree lies on the unique cycle of G .

Proof. Contrarily, assume that $v \in V(G)$ is a vertex with the maximum degree and that it does not lie on the unique cycle of G . Choose $vw \in E(G)$ such that $d_w \geq 2$. Then, $N(w) \cap N(v) = \emptyset$ and hence $N(w) \setminus N(v) = N(w)$. Take $N(w) \setminus \{v\} := \{w_1, w_2, \dots, w_k\}$. Let G' be the graph deduced from G by applying Transformation 1. Then, we get Equation (3), which gives $ISDD(G') < ISDD(G)$ (see the proof of Lemma 4); this contradicts the definition of G . \square

Lemma 6. For $n \geq 4$, let G be a unicyclic graph with the minimum ISDD index in the set of all unicyclic graphs of a fixed order n and girth three. If $v, v_1, v_2 \in V(G)$ lie on the unique cycle of G such that

$$d_v \geq \max\{d_{v_1}, d_{v_2}\},$$

then every member of the set $N(v) \setminus \{v_1, v_2\}$ is a pendent vertex.

Proof. Contrarily, assume that $w \in N(v) \setminus \{v_1, v_2\}$ is a nonpendent vertex of G . By Lemma 5, the vertex v has the maximum degree. Note that $N(w) \cap N(v) = \emptyset$ and hence $N(w) \setminus N(v) = N(w)$. Take $N(w) = \{v, w_1, w_2, \dots, w_k\}$. Let G' be the graph deduced from G by applying Transformation 1. Then, we get Equation (3), which gives $ISDD(G') < ISDD(G)$, which is a contradiction to the definition of G . \square

Theorem 1. For $n \geq 4$, if G is a unicyclic graph with the minimum ISDD index in the set of all unicyclic graphs of a given order n , then G satisfies the following three properties:

- (i). The girth is three.
- (ii). Every vertex of the maximum degree lies on the unique cycle.
- (iii). All the neighbors of every vertex of the maximum degree are pendent.

Proof. Lemmas 4, 5, and 6 lead to the conclusion of the theorem. \square

3. Concluding Remarks

In this paper, we addressed the problem of determining the graphs possessing the maximum and minimum ISDD indexes from the set of all unicyclic graphs of a given number of vertices. For the maximum case, the cycle graph was the unique desired graph. In the case of the minimum, we proved that the desired graph must satisfy the following three properties: (i) the girth is three, (ii) every vertex of the maximum degree lies on the unique cycle, and (iii) all the neighbors of every vertex of the maximum degree are pendent.

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