Upper and lower bounds of symmetric division deg index

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ABSTRACT. Symmetric division deg index is one of the 148 discrete Adriatic indices that showed good predictive properties on the testing sets provided by International Academy of Mathematical Chemistry.

Symmetric division deg index is defined by

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

where d_i is the degree of vertex i in graph G. In this paper we provide lower and upper bounds of symmetric division deg index in some classes of graphs and determine the corresponding extremal graphs.

Keywords: Symmetric division deg index, Adriatic index.

1. INTRODUCTION

Molecular descriptors, being numerical functions of molecular structure, play a fundamental role in mathematical chemistry [1]. They are used in QSAR and QSPR studies to relate biological or chemical properties of molecules to specific molecular descriptors [2, 3]. Topological indices, being numerical functions of the underlying molecular graph, represent an important type of molecular descriptors.

Many topological indices are *bond-additive*, i.e. they can be presented as a sum of edge contributions and have the following form:

$$\sum_{uv\in E} f\,(g(u), g(v))$$

where $g(u)$ are usually degrees or the sum of distances from u to all other vertices of G.

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Inspired by the most successful indices of this form, such as Randić index [4], second Zagreb index [5], ABC index [6], and others, there was defined a whole family of Adriatic indices [7, 8]. An especially interesting subclass of these descriptors consists of 148 *discrete Adriatic indices*. They were analyzed on the testing sets provided by the International Academy of Mathematical Chemistry [9], and it had been shown that they have good predictive properties in many cases.

Symmetric division deg (SDD) index was selected as a significant predictor of total surface area of polychlorobiphenyls (PCB). Moreover, its extremal graphs obtained with the help of MathChem [10] have particularly simple and elegant structure.

In the following sections we determine extremal values and extremal graphs of the SDD index in several classes of graphs (with given number of vertices): the class of all connected graphs, the class of all trees, the class of all unicyclic graphs, the class of all graphs with given minimum degree, and the class of all chemical graphs, that are the graphs with maximum degree at most four. We also determine maximum values of the SDD index in the class of all graphs with given maximum degree.

Let us rewrite the definition of SDD index in the following way.

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

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

Let us denote by $\alpha(d_u, d_v)$ the individual contribution of an edge uv to SDD index.

$$\alpha(d_u, d_v) = \frac{d_u}{d_v} + \frac{d_v}{d_u} = \frac{d_u^2 + d_v^2}{d_u d_v}. \quad (1)$$

The definition of SDD index using α become more compact:

$$SDD(G) = \sum_{uv \in E(G)} \alpha\,(d_u, d_v). \quad (2)$$

2. MINIMUM VALUES OF SDD INDEX

We first establish a lower bound on the SDD index with respect to the number of edges. The next theorem is the direct result of the fact, that the individual contribution $\alpha(d_u, d_v) = \frac{d_u}{d_v} + \frac{d_v}{d_u} \geq 2$.

Theorem 1. Let G be a simple connected graph with m edges. Then $SDD(G) \geq 2m$.

Note that the equality holds if and only if $d_u = d_v$ for all $uv \in E(G)$, or alternatively, G is regular. The lower bound described in Theorem 1 can be achieved in the class of unicyclic graphs. In this case the corresponding extremal graph is the cycle

C_n. The next theorem provides a lower bound on the SDD index in the class of all connected graphs with respect to the number of vertices.

Theorem 2. Let G be a simple connected graph with $n \geq 3$ vertices. Then

$$SDD(G) \geq 2n - 1.$$

The equality holds if and only if G is isomorphic to path P_n with n vertices.

Proof. Let us distinguish two cases:

Case 1: G is a tree.

Every tree has at least two pendant vertices. Each edge incident with that vertices contributes at least $\alpha(1,2) = 2.5$. Each other edge contributes at least 2. Hence, $SDD(G) \geq 2(n-3) + 2 \cdot 2.5 = 2n - 1$. Moreover, the equality implies that G has exactly two pendant vertices, that is possible only if $G \cong P_n$.

It can be easily checked that $SDD(P_n) = 2n - 1$.

Case 2: G is not a tree.

G has at least n edges each of which contributes at least 2, hence

$$SDD(G) \geq 2n > 2n - 1.$$

□

The same lower bound holds for trees and chemical graphs since P_n belongs to these two graph classes.

The following theorem describes minimum value of the SDD index for graphs with given minimum vertex degree.

Theorem 3. Let G be a graph with n vertices and minimum vertex degree δ. Then $SDD(G) \geq n\delta$. The equality holds if and only if G is δ-regular graph.

Proof. First, let us recall the well-known fact [8], that for any graph G without isolated vertices

$$\sum_{uv \in E(G)} \left(\frac{1}{d_u} + \frac{1}{d_v} \right) = n. \quad (3)$$

Then, let us consider the individual contribution of an edge uv to SDD index (1)

$$\begin{aligned}
\alpha(d_u, d_v) &= \frac{d_u}{d_v} + \frac{d_v}{d_u} = \left(\frac{1}{d_u} + \frac{1}{d_v}\right)(d_u + d_v) - 2 \\
&= d_u\left(\frac{1}{d_u} + \frac{1}{d_v}\right) + d_v\left(\frac{1}{d_u} + \frac{1}{d_v}\right) - 2 \\
&= min\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) + max\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) - 2 \\
&= min\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) + \frac{max\{d_u, d_v\}}{d_u} + \frac{max\{d_u, d_v\}}{d_v} - 2 \\
&= min\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) + \frac{max\{d_u, d_v\}}{min\{d_u, d_v\}} + 1 - 2 \\
&\geq min\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) \geq \delta\left(\frac{1}{d_u} + \frac{1}{d_v}\right).
\end{aligned}$$

The equality holds if and only if $d_u = d_v = \delta$. Hence using (2) and (3),

$$SDD(G) = \sum_{uv \in E(G)} \alpha\,(d_u, d_v) \geq \sum_{uv \in E(G)} \delta\left(\frac{1}{d_u} + \frac{1}{d_v}\right) = n\delta,$$

with equality if and only if the degrees of all the vertices are equal to the minimum degree δ, or alternatively G is δ-regular. □

3. Maximum Values of SDD Index

Our first result on the maximum value of the SDD index is an upper bound with regards to the maximum degree Δ.

Theorem 4. Let G be a simple connected graph with $n \geq 2$ vertices and maximum degree Δ. Then $SDD(G) \leq n\Delta$. The equality holds if and only if G is Δ-regular graph.

Proof. The theorem can be proved in exactly same the way as the previous one. Let us consider the individual contribution of an edge uv to SDD index and use the equation (3).

$$\begin{aligned}
\alpha(d_u, d_v) &= d_u\left(\frac{1}{d_u} + \frac{1}{d_v}\right) + d_v\left(\frac{1}{d_u} + \frac{1}{d_v}\right) - 2 \\
&= max\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) + min\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) - 2 \\
&= max\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) + \frac{min\{d_u, d_v\}}{d_u} + \frac{min\{d_u, d_v\}}{d_v} - 2 \\
&= max\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) + \frac{min\{d_u, d_v\}}{max\{d_u, d_v\}} + 1 - 2 \\
&\leq max\{d_u, d_v\}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) \leq \Delta\left(\frac{1}{d_u} + \frac{1}{d_v}\right).
\end{aligned}$$

The equality holds if and only if $d_u = d_v = \Delta$. Hence using (2) and (3),

$$SDD(G) = \sum_{uv\in E(G)} \alpha\,(d_u, d_v) \leq \sum_{uv\in E(G)} \Delta\left(\frac{1}{d_u} + \frac{1}{d_v}\right) = n\Delta,$$

with equality if and only if the degree of the all vertices is equal to the maximum degree, or alternatively G is Δ-regular. □

Now we can provide an upper bound on the SDD index in the class of all connected graphs and in the class of chemical graphs.

Corollary 1. Let G be a simple connected graph with $n \geq 2$ vertices. Then

$$SDD(G) \leq n(n-1).$$

The equality holds if and only if G is the complete graph K_n.

Proof. It is clear, that $\Delta \leq n-1$. From Theorem 4, it follows that:

$$SDD(G) \leq n\Delta \leq n(n-1).$$

The equality holds if and only if G is $(n-1)$–regular graph. The only such graph is the complete graph K_n. □

Corollary 2. Let G be a chemical graph with $n \geq 2$ vertices. Then $SDD(G) \leq 4n$. The equality holds if and only if G is 4-regular.

Proof. The claim immediately follows from Theorem 4 assuming $\Delta = 4$. □

Let $KD_{n,\delta}$ be the graph obtained from the complete graph K_{n-1} by adding to it a new vertex, adjacent to exactly δ vertices in K_{n-1}. Another corollary of Theorem 4 is the following:

Corollary 3. If G is a graph with n vertices and minimum vertex degree δ, then $SDD(G) \leq SDD\big(KD_{n,\delta}\big)$ with equality if and only if G is isomorphic to $KD_{n,\delta}$.

Proof. Let u be the vertex in G having degree δ. As the part of G, induced by vertices different from u, can be made into the complete graph K_{n-1} by adding edges between all pairs of nonadjacent vertices, we immediately obtain that $SDD(G) \leq SDD(KD_{n,\delta})$ by Corollary 1 with equality if and only if no edges were added to G, *i.e.*, if and only if $G \cong KD_{n,\delta}$. □

Another important class of graphs is the class of trees. The next theorem shows that the star S_n has maximum value of the SDD index among all trees.

Theorem 5. Let T be a tree with $n \geq 2$ vertices. Then $SDD(T) \leq (n-1)^2 + 1$. The equality holds if and only if T is isomorphic to star S_n with n vertices.

Proof. In order to prove the upper bound it is sufficient to note that the contribution of each edge is at most $\alpha(1, n-1) = \frac{1}{n-1} + n - 1$. The only such graph is the star S_n. By summing up the contributions of all the edges we get

$$SDD(S_n) = \sum_{uv \in E(G)} \alpha\,(1, n-1) = (n-1)\left(\frac{1}{n-1} + n - 1\right) = (n-1)^2 + 1.$$

□

Unicyclic graphs are often considered in the field of mathematical chemistry. Let S_n^+ be the graph obtained from the star S_n by adding an edge that connects two pendant vertices.

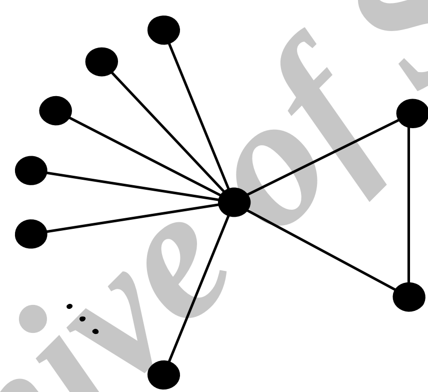

Figure 1. Graph S_n^+ whose value of the SDD index is maximal in the class of unicyclic graphs.

Theorem 6. Let G be a unicyclic connected graph with $n \geq 3$ vertices. Then

$$SDD(G) \leq \frac{n+1}{n-1} + (n-1)(n-2) + 2.$$

The equality holds if and only if G isomorphic to the graph S_n^+.

Proof. Let us distinguish two cases:

Case 1: G has a vertex of degree $n-1$.

It can be checked that S_n^+ is the only such graph with n vertices and that

$$SDD(S_n^+) = \frac{n+1}{n-1} + (n-1)(n-2) + 2.$$

Case 2: G does not have a vertex of degree $n-1$ and it has a cycle of length at least 3. Note that it is only possible when $n \geq 4$.

In this case the contribution of each edge in the cycle is at most $\alpha(2, n-2)$ and the contribution of each other edge is at most $\alpha(1, n-2)$, so it is sufficient to prove that:

$$3 \cdot \alpha(2, n-2) + (n-3) \cdot \alpha(1, n-2) < SDD(S_n^+).$$

Let us consider the function $f(n)$ defined as follows:

$$f(n) = 3 \cdot \alpha(2, n-2) + (n-3) \cdot \alpha(1, n-2) - SDD(S_n^+) = \frac{(n+3)(n^2-4n+2)}{2(n^2-3n+2)}.$$

The roots of equation $f(n) = 0$ are $n \in \{-3; 2-\sqrt{2}; 2+\sqrt{2}\}$. It is easy to check that $f(n) < 0$ for $n \geq 4$. □

4. Conclusion

The paper presents initial results on SDD index, one of the 148 discrete Adriatic indices, providing upper and lower bounds for certain classes of graphs.

It is clear that SDD index is in a sense a (local) measure of irregularity. It could be profitable to learn more on its behavior with respect to edge deletion and addition and various "transplantation" type transformations.

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