Symmetric division deg index of tricyclic and tetracyclic graphs

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Abstract— The symmetric division deg index (SDD) is one of the 148 discrete Adriatic indices analyzed by Vukčević and Gašperov on the benchmark datasets of the International Academy of Mathematical Chemistry. SDD is a significant predictor of total surface area for polychlorobiphenyls. In this article, we characterize the SDD index for the class of all n-vertex tricyclic and tetracyclic graphs.

Index Terms — Symmetric division deg index, cyclomatic number, tricyclic graph, tetracyclic graph, pendant vertices, maximum degree and minimum degree.

1 INTRODUCTION

Let \( \sum \) denotes the class of all graphs, then a function \( T: \sum \rightarrow \mathbb{R}^+ \) is known as topological index if for every graph \( H \) isomorphic to \( G \), \( T(G) = T(H) \).

Different topological indices are found to be useful in isomer discrimination, Quantitative structure-activity relationship (QSAR), Quantitative structure-property relationship (QSPR), pharmaceutical drug design, etc. in chemistry, biochemistry, medicine and nanotechnology [6-17].

If \( G \) has order \( n \) and size \( m \) containing \( k \) components, then \( c = m - n + k \) is called the cyclomatic number of \( G \) then \( G \) is called unicyclic, bicyclic, tricyclic and tetracyclic, respectively.

In [1-4] some of the present authors computed the first and second maximum values of the Symmetric division deg index in the class of all \( n \)-vertex unicyclic and bicyclic graphs. Also computed first, second and third maximum values of atom-bond connectivity index in the class of all \( n \)-vertex tricyclic and tetracyclic graphs.

This paper is motivated from the works of C. K. Gupta, V. Lokesha et. al [3] we established the first and second maximum values of SDD index in all class of all \( n \)-vertex tricyclic(TrG) graphs [2]. The SDD index is defined as

\[
\text{SDD}(G) = \sum_{u \in E(G)} \frac{\max(d_u, d_v)}{\min(d_u, d_v)} + \frac{\min(d_u, d_v)}{\max(d_u, d_v)}
\]

Many topological indices are bond-additive [5], they can be presented as a sum of edge contributions and have the following term:

\[
\sum_{u \in E(G)} f[h(u), h(v)]
\]

Where \( (x, t) \geq 1 \in \mathbb{Z}^+ \) and consider the function,

\[
f(a, x) = \phi(x, a) - \phi(x, a - 1), a \geq 2.
\]

Lemma 1: Let \( G = TrG_{n,p} \) be the tricyclic graph of order \( n \) and size \( m \) with exactly \( p \) pendant vertices then

\[
\text{SDD}(G) \leq \frac{p(\epsilon_2 - 1)(\epsilon_2^2 - \epsilon_2) + n(\epsilon_1^2 + \epsilon_2^2)}{\epsilon_1 \epsilon_2}
\]

where \( \epsilon_1 \) and \( \epsilon_2 \) are maximum and minimum degree.

Proof: Since \( G \) is a tricyclic graph with size \( m = n + 2 \),

\[
4 \leq \epsilon_1 \leq p + 3. \text{ Thus}
\]

\[
\text{SDD}(G) = p \left( \frac{(p + 3)^2 + 1}{p + 3} \right) + (m - p) \left( \frac{(p + 3)^2 + 9}{3(p + 3)} \right)
\]

\[
\leq p \left( \frac{p^2 + 6p + 10}{p + 3} \right) + (n - p) \left( \frac{p^2 + 6p + 18}{3(p + 3)} \right)
\]

\[
\leq \frac{p(\epsilon_2 - 1)(\epsilon_2^2 - \epsilon_2) + n(\epsilon_1^2 + \epsilon_2^2)}{\epsilon_1 \epsilon_2}.
\]

Hence the proof.

Lemma 2: The tricyclic graph \( TrG_{n,p} \) where \( n \in \mathbb{Z}^+ \),

\[
0 \leq p \leq n - 4 \text{ holds that}
\]

\[
\text{SDD}(TrG_{n,p}) > \text{SDD}(TrG_{n,p-1}) > \text{SDD}(TrG_{n,p-2}) > \text{SDD}(TrG_{n,p-3}) > \ldots \ldots > \text{SDD}(TrG_{n,0}).
\]

Proof: Consider the function,

\[
a(p) = p \left( \frac{(p + 3)^2 + 1}{p + 3} \right) + (n - p) \left( \frac{(p + 3)^2 + 9}{3(p + 3)} \right)
\]

Therefore,

\[
a'(p) = p \left( \frac{2p - p^2 + 8}{(p + 3)^2} \right) + (n - p) \left( \frac{2p - p^2}{9(p + 3)^2} \right)
\]
In this section, we determine \( H \) and \( \alpha(p) \) is increasing function for \( 0 \leq p \leq n - 4 \) and
\[
\alpha(1) = \frac{17}{4} + (n - 1) \frac{25}{12} > \alpha(0) = 2n
\]
Thus we have
\[
\begin{align*}
SDD(TrG_n) & > SDD(TrG_{n-1}) > SDD(TrG_{n-2}) > \\
SDD(TrG_{n-3}) & > \ldots \ldots > SDD(TrG_{n,0})
\end{align*}
\]

2 MAXIMUM VALUES OF SDD INDEX WITH FOUR NON-PENDANT VERTICES

Let \( n \)-vertex tricyclic graphs, \( n \geq 4 \) with four non-pendant vertices will be determined. We assume that \( K_{4,p} \), \( p_1, p_2, p_3, p_4 \) is a tricyclic graph obtained from the complete graph \( K_4 \) by attaching \( p \) vertices to \( v_j \) where \( v_1, v_2, v_3, \ldots, v_p \) be the vertices of \( G \) are consecutively labeled, and \( p_i \geq 0 \) for \( i = 1, 2, \ldots, r \) and \( p_1 \geq p_2 \geq \ldots \geq p_r \). Since \( \sum_{i=1}^{r} p_i = n - r \).

Theorem 2.1: Let \( G = K_{4,p}(p_1 - 1, p_2 - 2, p_3, p_4) \) where
\( p_1 \geq p_2 \geq 2 \) and \( G' = K_{4,p}(p_1, p_2 - 1, p_3, p_4) \) then
\[
SDD(G) < SDD(G').
\]
Proof: Consider
\[
\begin{align*}
SDD(G) - SDD(G') & = [p_1 \phi(1, p_1, 3) - (p_1 - 1) \phi(1, p_1 + 2)] + \\
& [(p_2 - 2) \phi(1, p_2 + 1) - (p_2 - 1) \phi(1, p_2 + 2)] + \\
& [\phi(p_1 + 1, 3, p_2 + 3) - \phi(1, p_2 + 2)] + \\
& [\phi(p_1 + 3, p_2 + 2) - \phi(1, p_2 + 2)] + \\
& [\phi(p_1 + 3, p_2 + 2) - \phi(p_1 + 1, 3, p_2 + 3)] + \\
& [\phi(p_1 + 3, 2) - \phi(p_1 + 2, 2)] \\
& = \alpha(p_1) - \alpha(p_2) + f(p_4 + 2, p_1 + 1) - f(p_4 + 2, p_2 + 1 + 1) + \\
& (p_1 + 2)^2 + (p_2 + 2)^2 - (p_1 + 3)(p_2 + 1) > 0
\end{align*}
\]
Since by lemma 1 and lemma 2 of [3] \( \alpha(p_1) > \alpha(p_2 - 1) \), therefore \( p_1 > p_2 - 1 \). Similarly, \( f(p_3 + 2, p_1 + 1) > f(p_4 + 2, p_2 + 2) \) and \( f(p_3 + 2, p_1 + 3) > f(p_3 + 2, p_2 + 2) \) and also \( \phi(p_1 + 3, 2) > \phi(p_1 + 2, 2) \).

Hence this completes the proof.

3 MAXIMUM VALUES OF SDD INDEX WITH FIVE NON-PENDANT VERTICES

In this section, we determine \( n \)-vertex tricyclic graphs with five non-pendant vertices.

Theorem 3.1: Let \( G \in TrG_{5,p}(p_1, p_2, p_3, p_4, p_5) \)
\( i \) If \( p_2 \geq 2 \) then \( SDD(TrG_{5,p}(p_1 + 1, p_2 - 1, p_3, p_4, p_5) > SDD(G) \)
\( ii \) If \( p_4 \geq 2 \) then \( SDD(TrG_{5,p}(p_1, p_2, p_3 + 1, p_4 - 1, p_5) > SDD(G) \)
\( iii \) If \( p_5 \geq 2 \) then \( SDD(TrG_{5,p}(p_1, p_2, p_3 + 1, p_4, p_5 - 1) > SDD(G) \)

Proof: (i) Assume that \( G' = Q_{4,p}(p_1 + 1, p_2 - 1, p_3, p_4, p_5) \) where \( p_5 \geq 2 \) then
\[
SDD(G') - SDD(G) = [p_2 \phi(1, p_1 + 3) - (p_1 - 1) \phi(1, p_1 + 2)] + \\
[(p_2 - 2) \phi(1, p_2 + 1) - (p_2 - 1) \phi(1, p_2 + 2)] + \\
\phi(p_1 + 1, 3 p_2 + 3) - \phi(1, p_2 + 2) + \\
\phi(p_1 + 3, p_2 + 2) - \phi(1, p_2 + 2) + \\
\phi(p_1 + 3, p_2 + 2) - \phi(p_1 + 1, 3 p_2 + 3) + \\
\phi(p_1 + 3, 2) - \phi(p_1 + 2, 2) + \\
\phi_\alpha(p_1) - \phi(p_2) + f(p_4 + 2, p_1 + 1) - f(p_4 + 2, p_2 + 1) + \\
(p_1 + 2)^2 + (p_2 + 2)^2 - (p_1 + 3)(p_2 + 1) > 0
\]

Hence the result.

Similar arguments are followed for the case (iii) to obtain the result.

4 MAXIMUM VALUES OF SDD INDEX OF TETRACYCLIC GRAPHS

Let \( TG(n) \) and \( TG(n, p) \), \( 0 \leq p \leq n - 5 \) denote the set of all \( n \)-vertex tetracyclic graphs \([4]\). In this section we determined the maximum values of \( SDD \) index of \( n \)-vertex tetracyclic graphs.

Considering the complete graph \( K_4 \) and construct a graph \( M_4 \) by adding a vertex \( v_5 \) and connecting it to the adjacent vertices of \( K_4 \). Since we have
\[
d(v_5) = d(v_4) = 4, d(v_3) = d(v_2) = 3 \text{ and } d(v_1) = 2.
\]

Let us suppose that \( F_{n,p}(p_1, p_2, p_3, p_4, p_5) \) is a graph obtained from \( M_4 \) by attaching \( \sum_{i=1}^{r} p_i = n - r \) vertices.
Theorem 4.1: Let $G = F_{5,p}(p_1, p_2, p_3, p_4, p_5)$ then
(i) $SDD(G) < SDD(F_{5,p}(p_1 + 1, p_2 - 1, p_3, p_4, p_5))$ when $p_2 \geq 2$
(ii) $SDD(G) < SDD(F_{5,p}(p_1, p_2, p_3 + 1, p_4 - 1, p_5))$ when $p_2 \geq 2$.

Theorem 4.2: If $G = F_{6,p}(p_1, p_2, p_3, p_4, p_5, p_6)$ then we have
(i) If $p_2 \geq 2$ then $SDD(G) < SDD(F_{6,p}(p_1 + 1, p_2 - 1, p_3, p_4, p_5, p_6))$
(ii) If $p_3 \geq 2$ then $SDD(G) < SDD(F_{6,p}(p_1, p_2, p_3 + 1, p_4 - 1, p_5, p_6))$
(iii) If $p_5 \geq 2$ then $SDD(G) < SDD(F_{6,p}(p_1, p_2, p_3, p_4 + 1, p_5 - 1, p_6))$
(iv) If $p_6 \geq 2$ then $SDD(G) < SDD(F_{6,p}(p_1, p_2, p_3, p_4, p_5, p_6 - 1))$

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