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On the Symmetric Division deg Index of Graph

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Abstract. The Symmetric division deg index [SDD] is one of the 148 discrete Adriatic indices [22] is good predictor of total surface area for polychlorobiphenyls. The Symmetric division deg index of a connected graph G, is defined as $SDD(G) = \sum_{uv\in E(G)} \frac{d_u}{d_v} + \frac{d_v}{d_u}$ where d_v is the degree of a vertex v in G. In this paper, we provide a lower and upper bounds of Symmetric division deg index of connected graphs. Also, established the Nordhaus - Gaddum-type relations for Symmetric division deg index of a connected graphs, unicyclic and bicyclic graph.

Keywords: Graph operations Symmetric division deg index; Maximum degree; Pendent vertices; Unicyclic graphs; Bicyclic graphs.

1. Introduction

Molecular descriptors, being numerical functions of molecular structure, play a fundamental role in mathematical chemistry [1]. They are used in Quantitative structure property relations and Quantitative structure activity relations (QSAR and QSPR) studies to relates biological or chemical properties of molecules to specific molecular descriptors [6]. In 1992, N. Trinajastic describe in his book chemical graph theory is the topology, branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena. i.e, Topological indices, being numerical functions of the underlying molecular graph, represent an important type of molecular descriptors [21].

The smart polymers are macromolecules that display a dramatic change in respect to small changes in the environment. In 2012, some applications related topological indices for Dox-loaded micelle comprising block co-polymer with chemically conjuated Dox (smart polymers) are found in [17], and comparative study of topological indices and molecular weight of some carbohydrates (Chetin and Cellulose) are in [19]. Recently, in [9], C.K. Gupta and et al. constructed a calyey graph for multiplicative group of upper-triangular 2*2 matrices over *zmodn*. Also, established some topological indices of that graph and the relations on graph operations on matrix group.

Inspired by the most successful indices of the form, such as second Zagreb index [8], ABC index [7], Randic index [16], Harmonic index [20], and others, there was defined a whole family of Adriatic indices in [23]. Also posed a series of open problems respect to mathematical properties of discrete adriatic indices.

In recent times [22], D. Vukicevic revealed the set of 148 discrete Adriatic indices. They were analyzed on the testing sets provided by the International Academy of Mathematical Chemistry and it had been shown that they have good predictive properties in many cases. There was a vast research regarding various properties of this topological index (see [12, 13, 17, 24]).

In 2014, M. Azari [3] is using Narumi Katayama index $NK(G)$ of a simple graph G is equal to the product of the degrees of the vertices of G. They found sharp lower bounds of Narumi Katayama index for several classes of graph operations.

In a new article [23], D. Vukicevic analyzed maximal value of max-min index for different graphs with maximal degree and minimal values of index for graphs with minimal degree. He posed the open questions in his conclusions. Stimulate from that, here we ardent one of the index specifically, Symmetric division deg index [SDD]. This emphasizes the development of lower and upper bounds for graphs. This acquires some results that are partial answer to the open queries.

Symmetric division deg index is one of the discrete adriatic indices that is good predictor of total surface area for polychlorobiphenyls.

We recall some definitions which are essential in our study. Let G be a simple graph, the vertex-set and edge-set of which are represented by $V(G)$ and $E(G)$ respectively. Notations used in this work are standard and mainly from [10].

Definition 1.1. *The Hyper-zagreb index* [18] *is defined as*

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

Definition 1.2. *The Symmetric division deg index of a connected graph G, (SDD) is defined as*

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

where d_u and d_v are the degrees of respective vertices of u and v in G.

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

$$\sum_{uv \in E(G)} f(h(u), h(v)).$$

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

This paper starts with preliminaries, then coming up with lower and upper bounds of Symmetric division deg index in section 3. Section 4 consists of results related to Nordhaus - Gaddum-type. Final two sections dealt with Symmetric division deg index of unicyclic and bi-cyclic graphs.

2. Preliminary Results

In this section, we discussed some useful Lemmas which are essential for the forthcoming section results.

Let $\alpha(x, y) = \frac{x^2+y^2}{xy}$ where x, y are positive integers, where, $\alpha : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$. Then Symmetric division deg index $SDD(G)$ representation interms of α as

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

Lemma 2.1. *Let x and y are positive integers. Then*

(i) $\alpha(x, y) = 2$ *whenever $x = y$.*

(ii) *For fixed* $y \geq 2$,

  (a) $\alpha(x, y)$ *is decreasing for* $x < y$.

  (b) $\alpha(x, y)$ *is increasing for* $x > y$.

(iii) $\alpha(x, 1)$ *is increasing for* $x \geq 1$.

Proof. (i) By direct computation, $\alpha(x, x) = \frac{x^2+x^2}{x^2} = 2$ when $x = y$.

(ii) Consider, $\alpha(x, y) = \frac{x^2+y^2}{xy}$, for fixed $y \geq 2$.

$$\frac{\partial\alpha(x, y)}{\partial x} = \frac{x^2 - y^2}{yx^2} = \frac{(x + y)(x - y)}{yx^2}.$$

Therefore, $\frac{\partial\alpha(x,y)}{\partial x} > 0$ for $x > y$ and $\frac{\partial\alpha(x,y)}{\partial x} < 0$ for $x < y$.

Hence, for fixed $y \geq 2$, we have (a) and (b).

(iii) Trivially, $\alpha(x, 1) = \frac{x^2+1}{x}$ is increases for $x \geq 1$. ∎

Lemma 2.2. *Let* $f(x, y) = \alpha(x+1, y) - \alpha(x, y)$ *where* x *and* y *are positive integer, then*

(i) $f(x, y)$ *is increasing for* $x > y$.

(ii) $f(x, y)$ *is decreasing for* $x < y$.

Proof. From the Lemma 2.1 (2), $\alpha(x, y)$ is increasing for $x > y$, therefore $f(x, y)$ is increasing for $x > y$. Similarly, the $\alpha(x, y)$ is increasing for $x > y$ and $f(x, y)$ is decreasing for $x < y$. ∎

Lemma 2.3. *Let* $g_n(x) = x\alpha(1, x + n + 1) - (x - 1)\alpha(1, x + n)$ *for* $x > 0$, $n > 1$. *Then* $g_n(x)$ *increases for* x.

Proof. We prove by induction process.

Case 1. For $n = 1$, let $l(x) = x\alpha(1, x + 2) = \frac{x(1+(x+2)^2)}{x+2}$. Consider, $g_1(x) = l(x) - l(x - 1)$. Then,

$$l'(x) = \frac{2x^3 + 10x^2 + 16x + 10}{(x + 2)^2} > 0$$

and

$$l''(x) = \frac{2x^4 + 10x^2 + 16x + 10}{(x + 1)^4} > 0$$

By Lagrange's mean value theorem, $g_1'(x) = l'(x) - l'(x - 1) = l''(c) > 0$ for some $x - 1 \leq c \leq x$. Thus $g_1(x)$ is increasing for x.

Case 2. For $n = 2$, let $h(x) = x\alpha(1, x + 3) = \frac{x^3+6x^2+10x}{x+3}$.

Consider, $g_2(x) = h(x) - h(x-1)$. Then,

$$h'(x) = \frac{2x^3 + 15x^2 + 36x + 30}{(x+3)^2} > 0$$

and

$$h''(x) = \frac{2x^4 + 24x^3 + 108x^2 + 210x + 144}{(x+3)^4} > 0.$$

By Lagrange's mean value theorem, $g_2'(x) = h'(x) - h'(x-1) = h''(c) > 0$ for some $x - 1 \leq c \leq x$. Thus $g_2(x)$ is increasing for x.

Observing the cases (1) and (2) we arrive the conclusion that, for similar arguments the result is true for n. Hence, $g_n(x)$ is increasing for x. ■

3. Lower and Upper Bounds on Symmetric Division deg Index

This section deals with relations via bounds of Hyper zagreb indices and Symmetric division deg indices. First we concentrate with lower bounds for Symmetric division deg indices.

We would like to quote the following well-known folklore results.

Lemma 3.1. [23] *Let G be a simple connected graph with n vertices that does not have isolated vertices. Then*

$$\sum_{uv \in E(G)} \Big(\frac{1}{d_u} + \frac{1}{d_u}\Big) = n.$$

Lemma 3.2. [15, Ozeki's Inequality] *Let $(a_1, a_2, ..., a_n)$ and $(b_1, b_2, ..., b_n)$ be two positive $n-$ tuples such that there exist a positive numbers M_1, m_1, M_2, m_2 satisfying;* $0 < m_1 \leq a_i \leq M_1$, $0 < m_2 \leq b_i \leq M_2$, $1 \leq i \leq n$. *Then*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \sum_{i=1}^{n} (a_i b_i)^2 \leq \frac{1}{4} n^2 (M_1 M_2 - m_1 m_2).$$

Theorem 3.3. *Let G be a simple connected graph with order n, size m, p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1. Then*

$$SDD(G) \geq p\Big(\frac{{\delta_1}^2 + 1}{\delta_1}\Big) + 2(m-p). \tag{1}$$

For the regular and star graph equality hold.

Proof. We recall the Theorem 1 of [4]. Utilizing in the process of the result.

Consider,

$$\begin{aligned}
SDD(G) &= \sum_{uv\in E(G)} \Big(\frac{d_u}{d_v}+\frac{d_v}{d_u}\Big)\\
&= \sum_{uv\in E(G),d_u=1} \Big(\frac{d_v}{1}+\frac{1}{d_v}\Big) + \sum_{uv\in E(G),d_u,d_v\neq 1} \Big(\frac{d_u}{d_v}+\frac{d_v}{d_u}\Big)\\
&\geq \sum_{uv\in E(G),d_u=1} \Big(\frac{\delta_1}{1}+\frac{1}{\delta_1}\Big) + \sum_{uv\in E(G),d_u,d_v\neq 1} 2\\
&= p\Big(\frac{{\delta_1}^2+1}{\delta_1}\Big) + 2(m-p).
\end{aligned}$$

■

Theorem 3.4. *Let G be a simple connected graph with order n, size m, p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1. Then*

$$\begin{aligned}
SDD(G) \geq & p\Big(\frac{{\delta_1}^2+1}{\delta_1}\Big)\\
& + \sqrt{\frac{(n-p(\Delta+\frac{1}{\Delta}))^2(HM(G)-p(1+\Delta)^2)}{(m-p)} - 4(m-p)^2\Big(\frac{\Delta}{\delta_1}-\frac{\delta_1}{\Delta}\Big)^2}\\
& - 2(m-p)
\end{aligned}$$

Where $HM(G)$ is Hyper-Zagreb index. For the regular and star graph equality hold.

Proof. Consider,

$$\begin{aligned}
SDD(G) &= \sum_{uv\in E(G)} \Big(\frac{d_u}{d_v}+\frac{d_v}{d_u}\Big)\\
&= \sum_{uv\in E(G),d_u=1} \Big(\frac{d_v}{1}+\frac{1}{d_v}\Big) + \sum_{uv\in E(G),d_u,d_v\neq 1} \Big(\frac{d_u}{d_v}+\frac{d_v}{d_u}\Big) \qquad (2)
\end{aligned}$$

For $d_v \neq 1$ and $\delta_1 \leq d_v \leq \Delta$, we have

$$\sum_{uv\in E(G),d_u=1} \Big(\frac{d_v}{1}+\frac{1}{d_v}\Big) \geq \sum_{uv\in E(G),d_u=1} \Big(\frac{\delta_1}{1}+\frac{1}{\delta_1}\Big) = p\Big(\frac{{\delta_1}^2+1}{\delta_1}\Big) \qquad (3)$$

Since p is the number of pendent vertices in G, we have $m-p$ number of non-pendent edges in G.

Therefore,

$$
\begin{aligned}
&\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{d_u}{d_v}+\frac{d_v}{d_u}\Big)\\
=&\sum_{uv\in E(G),d_u,d_v\neq 1}\Big[\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)(d_u+d_v)-2\Big]\\
=&\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)(d_u+d_v)-2(m-p)
\end{aligned}\tag{4}
$$

By Ozeki inequality, we have

$$
\begin{aligned}
&\Big[\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)(d_u+d_v)\Big]^2\\
\geq&\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)^2\times\sum_{uv\in E(G),d_u,d_v\neq 1}(d_u+d_v)^2\\
&-\frac{1}{4}(m-p)^2\Big(\frac{4\Delta}{\delta_1}-\frac{4\delta_1}{\Delta}\Big)^2\\
=&\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)^2\times\Big(HM(G)-\sum_{uv\in E(G),d_u=1}(1+d_v)^2\Big)\\
&-4(m-p)^2\Big(\frac{\Delta}{\delta_1}-\frac{\delta_1}{\Delta}\Big)^2\\
\geq&\frac{1}{m-p}\Big[n-p(\Delta+\frac{1}{\Delta})\Big]^2\times\Big[HM(G)-p(1+\Delta)^2\Big]\\
&-4(m-p)^2\Big(\frac{\Delta}{\delta_1}-\frac{\delta_1}{\Delta}\Big)^2
\end{aligned}\tag{5}
$$

Since by Cauchy-Schwarz inequality

$$
\Big(\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)\Big)^2\leq(m-p)\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)^2
$$

Hence

$$
\begin{aligned}
&\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)^2\\
\geq&\frac{1}{m-p}\Big[\sum_{uv\in E(G)}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)-\Big(\sum_{uv\in E(G),d_u=1}\Big(d_v+\frac{1}{d_v}\Big)\Big]^2\\
\geq&\frac{1}{m-p}\Big[n-p\Big(\Delta+\frac{1}{\Delta}\Big)\Big]^2
\end{aligned}
$$

Utilizing the equations (3)- (5) in equation (2), we obtain

$$\begin{aligned} SDD(G) \geq & p\Big(\frac{{\delta_1}^2+1}{\delta_1}\Big) \\ & + \sqrt{\frac{(n-p(\Delta+\frac{1}{\Delta}))^2(HM(G)-p(1+\Delta)^2)}{(m-p)} - 4(m-p)^2\Big(\frac{\Delta}{\delta_1}-\frac{\delta_1}{\Delta}\Big)^2} \\ & - 2(m-p). \end{aligned}$$

■

Corollary 3.5. *Let G be a simple connected graph with order n, size m, maximum degree Δ and minimum degree δ. Then*

$$SDD(G) \geq \sqrt{\frac{n^2HM(G)}{m} - 4m^2\Big(\frac{\Delta}{\delta}-\frac{\delta}{\Delta}\Big)^2} - 2m$$

Proof. Put $p = 0$ in Theorem 3.4, we get required result. ■

Corollary 3.6. *Let T be a tree of order n, p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1. Then*

$$\begin{aligned} SDD(G) \geq & p\Big(\frac{{\delta_1}^2+1}{\delta_1}\Big) \\ & + \sqrt{\frac{(n-p(\Delta+\frac{1}{\Delta}))^2(HM(G)-p(1+\Delta)^2)}{(n-1-p)} - 4(n-1-p)^2\Big(\frac{\Delta}{\delta_1}-\frac{\delta_1}{\Delta}\Big)^2} \\ & - 2(n-1-p) \end{aligned}$$

In star graph equality hold.

Proof. We know that tree with order n having size $m = n-1$. The result follows from Theorem 3.4. ■

Now we establish some results relate to an upper bound on Symmetric division deg index.

Theorem 3.7. *Let G be a simple connected graph with order n, size m, maximum degree Δ and minimum degree δ. Then*

$$SDD(G) \leq m\Big(\frac{\Delta^2+\delta^2}{\Delta\delta}\Big) \tag{6}$$

For the regular and star graph equality hold.

Proof. Consider,

$$\begin{aligned}
SDD(G) &= \sum_{uv\in E(G)} \Big(\frac{Max(d_u,d_v)}{Min(d_u,d_v)} + \frac{Min(d_u,d_v)}{Max(d_u,d_v)}\Big)\\
&\le \sum_{uv\in E(G)} \Big(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\Big)\\
&= m\Big(\frac{\Delta^2+\delta^2}{\Delta\delta}\Big)
\end{aligned}$$

Case 1. For G is a star graph. Equality hold only if $d_u = \Delta$ and $d_v = \delta = 1$ for any edge $uv \in E(G)$.

Case 2. For G is a regular graph. Equality hold only if $d_u = d_v$ for any edge $uv \in E(G)$. ■

Theorem 3.8. *Let G be a simple connected graph with order n, size m, p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1. Then*

$$SDD(G) \le p\Big(\frac{\Delta^2+1}{\Delta}\Big) + (m-p)\Big(\frac{\Delta^2+{\delta_1}^2}{\Delta\delta_1}\Big)$$

Equality hold only if graph is regular and star.

Proof. Consider,

$$\begin{aligned}
SDD(G) &= \sum_{uv\in E(G)} \Big(\frac{d_u}{d_v} + \frac{d_v}{d_u}\Big)\\
&= \sum_{uv\in E(G), d_u=1} \Big(\frac{d_v}{1} + \frac{1}{d_v}\Big) + \sum_{uv\in E(G), d_u,d_v\neq 1} \Big(\frac{d_u}{d_v} + \frac{d_v}{d_u}\Big)\\
&\le \sum_{uv\in E(G), d_u=1} \Big(\frac{\Delta}{1} + \frac{1}{\Delta}\Big) + \sum_{uv\in E(G), d_u,d_v\neq 1} \Big(\frac{\Delta}{\delta_1} + \frac{\delta_1}{\Delta}\Big)\\
&= p\Big(\frac{\Delta^2+1}{\Delta}\Big) + (m-p)\Big(\frac{\Delta^2+{\delta_1}^2}{\Delta\delta_1}\Big)
\end{aligned}$$

Equality trivially holds for regular and star graph. ■

Theorem 3.9. *Let G be a simple connected graph with order n, size m, p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1. Then*

$$SDD(G) \le p\Big(\frac{\Delta^2+1}{\Delta}\Big) + \frac{1}{{\delta_1}^2}[HM(G) - p(1+\delta_1)^2] - 2(m-p)$$

Where $HM(G)$ is Hyper-Zagreb index. Equality hold only if graph is regular or star.

Proof. For $d_v \neq 1$ and $\delta_1 \leq d_v \leq \Delta$, we have

$$\sum_{uv\in E(G),d_u=1}\Big(\frac{d_v}{1}+\frac{1}{d_v}\Big) \leq \sum_{uv\in E(G),d_u=1}\Big(\frac{\Delta}{1}+\frac{1}{\Delta}\Big) = p\Big(\frac{\Delta^2+1}{\Delta}\Big) \tag{7}$$

Since p is the number of pendent vertices in G, then $m-p$ number of non-pendent edges in G.

By Cauchy-Schwarz inequality,

$$\begin{aligned}
&\Big[\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)(d_u+d_v)\Big]^2\\
&\leq \sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)^2 \times \sum_{uv\in E(G),d_u,d_v\neq 1}(d_u+d_v)^2\\
&= \sum_{uv\in E(G),d_u,d_v\neq 1}\frac{(d_u+d_v)^2}{(d_ud_v)^2} \times \Big[HM(G) - \sum_{uv\in E(G),d_u=1}(1+d_v)^2\Big]\\
&\leq \frac{1}{{\delta_1}^4}\Big[HM(G) - \sum_{uv\in E(G),d_u=1}(1+d_v)^2\Big] \times \Big[HM(G) - \sum_{uv\in E(G),d_u=1}(1+d_v)^2\Big]\\
&\leq \frac{1}{{\delta_1}^4}\Big[HM(G) - p(1+\delta_1)^2\Big]^2
\end{aligned}$$

Finally,

$$\sum_{uv\in E(G),d_u,d_v\neq 1}\Big(\frac{1}{d_u}+\frac{1}{d_v}\Big)(d_u+d_v) \leq \frac{1}{{\delta_1}^2}\Big[HM(G) - p(1+\delta_1)^2\Big] \tag{8}$$

utilizing equations (4), (7) and (8) in equation (2), we obtain

$$SDD(G) \leq p\Big(\frac{\Delta^2+1}{\Delta}\Big) + \frac{1}{{\delta_1}^2}[HM(G) - p(1+\delta_1)^2] - 2(m-p)$$

∎

Corollary 3.10. *Let G be a simple connected graph with order n, size m, maximum degree Δ and minimum degree δ. Then*

$$SDD(G) \leq \frac{1}{\delta^2}[HM(G)] - 2m$$

Proof. Put $p = 0$ in Theorem 2.1, we get required results. ∎

Corollary 3.11. *Let T be a tree of order n, p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1. Then*

$$SDD(G) \leq p\Big(\frac{\Delta^2+1}{\Delta}\Big) + \frac{1}{{\delta_1}^2}[HM(G) - p(1+\delta_1)^2] - 2(n-1-p)$$

Equality hold only if graph is star.

Proof. The number of edges in a tree having n vertices is $m = n - 1$, result follows from Theorem 2.1. ■

4. Nòrdhaus-Gaddum-Type Results for Symmetric Division deg Index

In 1956, E.A. Nordhaus and J.W. Gaddum [14] gave tight bounds on the product and sum of the chromatic numbers of a graph and its complement. Since then, such type of results have been derived for several other graph invariants, see the recent survey [2]. Nordhauss-Gaddum type results for ABC index are established by Das and et al [5]. Inspired from this, we found the relations for symmetric division deg index.

Theorem 4.1. *Let G be a simple connected graph on n vertices with a connected complement $\overline{G}$. Then*

$$SDD(G) + SDD(\overline{G}) \leq \binom{n}{2}\Big(\frac{k^2+1}{k}\Big)$$

where $k = max\{\frac{\Delta}{\delta}, \frac{\overline{\Delta}}{\overline{\delta}}\}$; Δ, δ, $\overline{\Delta}$ and $\overline{\delta}$ are the maximum vertex degree and minimum vertex degree of G and $\overline{G}$ respectively. Moreover, the equality holds if and only if G is isomorphic to a regular graph.

Proof. Let G be a simple connected graph on n vertices and $k \geq \frac{\Delta}{\delta} \geq 1$ and $1 - \frac{\delta}{k\Delta} \geq 0$. Then,

$$\Big(k - \frac{\Delta}{\delta}\Big)\Big(1 - \frac{\delta}{k\Delta}\Big) \geq 0$$

Implies,

$$\Big(\frac{k^2+1}{k}\Big) \geq \Big(\frac{\delta^2+\Delta^2}{\Delta\delta}\Big) \tag{9}$$

The $\overline{G}$ is complement of G, $k \geq \frac{\overline{\Delta}}{\overline{\delta}} \geq 1$ and $1 - \frac{\overline{\delta}}{k\overline{\Delta}} \geq 0$.

Similarly,

$$\Big(\frac{k^2+1}{k}\Big) \geq \Big(\frac{\overline{\delta}^2+\overline{\Delta}^2}{\overline{\Delta}\overline{\delta}}\Big) \tag{10}$$

We have $m + \overline{m} = \binom{n}{2}$, $\overline{\Delta} = n - 1 - \delta$ and $\overline{\delta} = n - 1 - \Delta$ where $\overline{m}$, $\overline{\Delta}$ and $\overline{\delta}$ are the number of edges, maximum vertex degree and minimum vertex degree of $\overline{G}$

respectively. Applying Theorem 3.7 for G and $\overline{G}$ then,

$$\begin{aligned}
SDD(G)+SDD(\overline{G}) &\leq m\Big(\frac{\Delta^2+\delta^2}{\Delta\delta}\Big)+\overline{m}\Big(\frac{\overline{\Delta}^2+\overline{\delta}^2}{\overline{\Delta}\overline{\delta}}\Big)\\
&\leq m\Big(\frac{k^2+1}{k}\Big)+\overline{m}\Big(\frac{k^2+1}{k}\Big) \quad \text{(Using Eqs. 9 and 10)}\\
&=(m+\overline{m})\Big(\frac{k^2+1}{k}\Big)\\
&=\binom{n}{2}\Big(\frac{k^2+1}{k}\Big).
\end{aligned}$$

Moreover, the equality holds if and only if G is isomorphic to a regular graph. ■

Theorem 4.2. *Let G be a simple connected graph of order n such that its complement $\overline{G}$ is connected. Let Δ, δ_1, p and $\overline{\Delta}$, $\overline{\delta_1}$, $\overline{p}$ denotes the maximum vertex degree, minimum non-pendent vertex degree and pendent vertices of G and $\overline{G}$ respectively.*

If $\alpha = min\{\delta_1, \overline{\delta_1}\}$ Then

$$SDD(G)+SDD(\overline{G}) \geq 2\binom{n}{2}-2(p+\overline{p})+(p+\overline{p})\Big(\frac{\alpha^2+1}{\alpha}\Big)$$

Equality holds only if G is $k-$ regular graph with $2k+1$ vertices.

Proof. Let m and $\overline{m}$ are the number of edges in G and $\overline{G}$ respectively. We know $m+\overline{m}=\binom{n}{2}$.

Applying Theorem 3.3 for G and $\overline{G}$. Then

$$\begin{aligned}
SDD(G)+SDD(\overline{G}) &\geq p\Big(\frac{{\delta_1}^2+1}{\delta_1}\Big)+2(m-p)+\overline{p}\Big(\frac{\overline{\delta_1}^2+1}{\overline{\delta_1}}\Big)+2(\overline{m}-\overline{p})\\
&=2(m+\overline{m})-2(p+\overline{p})+p\Big(\frac{{\delta_1}^2+1}{\delta_1}\Big)+\overline{p}\Big(\frac{\overline{\delta_1}^2+1}{\overline{\delta_1}}\Big) \quad (11)
\end{aligned}$$

$\alpha = min\{\delta_1, \overline{\delta_1}\}$ i.e, $\delta_1, \overline{\delta_1} \geq \alpha \geq 2$ and also, $\Big(\frac{{\delta_1}^2+1}{\delta_1}\Big)$ is monotonic increasing, from equation (11) it follows that,

$$\begin{aligned}
SDD(G)+SDD(\overline{G}) &\geq 2\binom{n}{2}-2(p+\overline{p})+p\Big(\frac{\alpha^2+1}{\alpha}\Big)+\overline{p}\Big(\frac{\alpha^2+1}{\alpha_1}\Big)\\
&=2\binom{n}{2}-2(p+\overline{p})+(p+\overline{p})\Big(\frac{\alpha^2+1}{\alpha}\Big)
\end{aligned}$$

If G is $k-$ regular graph with $2k+1$ vertices, it can be easily seen that equality holds. ■

5. Symmetric Division deg Index of Unicyclic Graph

Unicyclic graphs are often considered in the field of mathematical chemistry. Zhang F and et al [25] discussed the unicylic graphs for augmented zagreb index motivated from that works, In this section, we determine the unicyclic graph of order n with the maximum and the second maximum SDD indices for $n \geq 5$.

Let U_n be the set of $n-$ vertex unicyclic graph. Let $U_{n,p}$ be the set of unicyclic graph with n vertices and p pendent vertices.

Let $C_{n,p}$ be the unicyclic graph formed by attaching p pendent vertices to a vertex of the cycle C_{n-p}, where $0 \leq p \leq n-3$.

Corollary 5.1. *Let $G \in U_{n,p}$, where $0 \leq p \leq n-3$. Then*

$$SDD(G) \leq p\Big(\frac{p^2+4p+5}{p+2}\Big) + (n-p)\Big(\frac{p^2+4p+8}{2(p+2)}\Big)$$

Equality hold only if graph $G \cong C_{n,p}$.

Proof. Since G is an unicyclic graph with size $m = n$, $3 \leq \Delta \leq p+2$. By Theorem 3.8

$$\begin{aligned} SDD(G) &\leq p\Big(\frac{\Delta^2+1}{\Delta}\Big) + (m-p)\Big(\frac{\Delta^2+{\delta_1}^2}{\Delta\delta_1}\Big) \\ &\leq p\Big(\frac{(p+2)^2+1}{(p+2)}\Big) + (n-p)\Big(\frac{(p+2)^2+2^2}{2(p+2)}\Big) \\ &= p\Big(\frac{p^2+4p+5}{p+2}\Big) + (n-p)\Big(\frac{p^2+4p+8}{2(p+2)}\Big). \end{aligned}$$

■

Lemma 5.2. *For every positive integer n, with $0 \leq p \leq n-3$, graph $C_{n,p}$ holds that*

$$SDD(C_{n,0}) < SDD(C_{n,1}) < ... < SDD(C_{n,n-4}) < SDD(C_{n,n-3}).$$

Proof. Consider the function

$$g(p) = p\Big(\frac{p^2+4p+5}{p+2}\Big) + (n-p)\Big(\frac{p^2+4p+8}{2(p+2)}\Big).$$

Then

$$g'(p) = p\Big(\frac{p^2+4p+5}{(p+2)^2}\Big) + (n-p)\Big(\frac{2p^2+8p}{4(p+2)^2}\Big) + \Big(\frac{p^2+4p+2}{2(p+2)}\Big) > 0 \ \ as \ \ p \geq 1.$$

Thus $g(p)$ is increasing function for $0 \leq p \leq n-3$ and $g(1) = \frac{10}{3} + (n-1)\frac{13}{6} > g(0) = 2n$. Thus we have

$$SDD(C_{n,0}) < SDD(C_{n,1}) < ... < SDD(C_{n,n-4}) < SDD(C_{n,n-3}).$$

■

Theorem 5.3. *Among all graphs in U_n with $n \geq 3$, $C_{n,n-3}$ is the unique graph with the maximum SDD index, which is equal to*

$$\frac{1}{2(n-1)}(2n^3 - 7n^2 + 10n + 3).$$

Proof. By Corollary 5.1, $C_{n,p}$ with $0 \leq p \leq n-3$ is the unique graph with the maximum SDD index

$$g(p) = p\Big(\frac{p^2+4p+5}{p+2}\Big) + (n-p)\Big(\frac{p^2+4p+8}{2(p+2)}\Big)$$

and by Lemma 5.2, $C_{n,n-3}$ is the unique graph with the maximal SDD index in U_n. It is clear that

$$\begin{aligned} SDD(C_{n,n-3}) =&(n-3)\Big(\frac{(n-3)^2+4(n-3)+5}{(n-3)+2}\Big) \\ &+ (n-(n-3))\Big(\frac{(n-3)^2+4(n-3)+8}{2((n-3)+2)}\Big) \\ =&\frac{1}{2(n-1)}(2n^3-7n^2+10n+3). \end{aligned}$$

■

Let $v_1, v_2, ..., v_r$ be the vertices of C_r are consecutively labelled.

Let $Q_n(p_1, p_2, ..., p_r)$ be the unicyclic graph formed by attaching p_i vertices to v_i where $p_i \geq 0$ for $i = 1, ..., r$ and $p_1 \geq p_2 \geq ... \geq p_r$ and $\sum_{i=1}^{r} p_i = n - r$.

Lemma 5.4. *Let $G \cong Q_n(p_1, p_2, p_3)$ with $p_1 \geq p_2 \geq 1$ and $G' \cong Q_n(p_1+1, p_2-1, p_3)$. Then*

$$SDD(G') > SDD(G).$$

Proof. Consider,

$$\begin{aligned} &SDD(G') - SDD(G) \\ =&(p_1+1)\alpha(1, p_1+3) + (p_2-1)\alpha(1, p_2+1) \\ &+ \alpha(p_1+3, p_2+1) + \alpha(p_2+1, p_3+2) + \alpha(p_3+2, p_1+3) \\ &- [p_1\alpha(1, p_1+2) + p_2\alpha(1, p_2+2)] \\ &- [\alpha(p_1+2, p_2+2) + \alpha(p_2+2, p_3+2) + \alpha(p_3+2, p_1+2)] \\ =&(p_1+1)\alpha(1, p_1+3) - p_1\alpha(1, p_1+2) - [p_2\alpha(1, p_2+2) \\ &- (p_2-1)\alpha(1, p_2+1)] + \alpha(p_3+2, p_1+3) - \alpha(p_3+2, p_1+2) \\ &- [\alpha(p_2+2, p_3+2) - \alpha(p_2+1, p_3+2)] \\ &+ \alpha(p_1+3, p_2+1) - \alpha(p_1+2, p_2+2) \\ =&g_1(p_1+1) - g_1(p_2) + f(p_1+2, p_3+2) - f(p_2+1, p_3+2) \\ &+ \alpha(p_1+3, p_2+1) - \alpha(p_1+2, p_2+2) \\ >&0 \end{aligned}$$

Because, By Lemma 2.3, $g_1(p_1+1) > g_1(p_2)$ since $(p_1+1) > p_2$. By Lemma 2.2, $f(p_1+2, p_3+2) > f(p_2+1, p_3+2)$, since $p_1+2 > p_2+1 > p_3+2$ and

$$\begin{aligned}&\alpha(p_1+3, p_2+1) - \alpha(p_1+2, p_2+2)\\=&\Big(\frac{(p_1+3)^2+(p_2+1)^2}{(p_1+3)(p_2+1)} - \frac{(p_1+2)^2+(p_2+2)^2}{(p_1+2)(p_2+2)}\Big) > 0 \ \ for\ p_1 > p_2\end{aligned}$$

Hence $SDD(G') > SDD(G)$. ■

Theorem 5.5. *Among all graphs in U_n with $n \geq 4$,*

(i) *For $n = 4$ or $n \geq 12$, $C_{n,n-4}$ is the unique graph with the second maximal SDD index, which is equal to*

$$(n-4)\Big(\frac{n^2-4n+5}{n-2}\Big) + \Big(\frac{n^2-4n+8}{n-2}\Big) + 4.$$

(ii) *For $5 \leq n \leq 11$, $Q_n(n-4,1,0)$ is the unique graph with the second maximal SDD index, which is equal to*

$$(n-4)\Big(\frac{n^2-4n+5}{n-2}\Big) + \Big(\frac{n^2-4n+8}{2(n-2)}\Big) + \Big(\frac{n^2-4n+13}{3(n-2)}\Big) + \frac{33}{6}.$$

Proof. By Lemma 5.2, the second maximal SDD index of graph in U_n with $n \geq 4$ is achieved by the graph in $U_{n,n-3} \setminus \{C_{n,n-3}\}$ and $C_{n,n-4}$.

Case 1. If $n = 4$ is trivial.

Here, C_4 is the unique graph with the second maximal SDD index, which is equal to 8.

Case 2. If $n \geq 5$.

By Lemma 5.4, if $p_2 \geq p_3 \geq 1$, we can observe that $Q_n(n-4,1,0)$ is the unique graph with the maximum SDD index among all of the graph in $U_{n,n-3}\setminus\{C_{n,n-3}\}$.

It is easily seen that

$$\begin{aligned}&SDD(C_{n,n-4}) - SDD(Q_n(n-4,1,0))\\=&(n-4)\alpha(1,n-2) + 2\alpha(n-2,2) + 2\alpha(2,2)\\&-[(n-4)\alpha(1,n-2) + \alpha(n-2,2) + \alpha(2,3) + \alpha(3,n-2) + \alpha(1,3)]\\=&\frac{n^2-4n-2}{6(n-2)} - \frac{3}{2} = \frac{n(n-13)+16}{6(n-2)}\end{aligned}$$

By simple calculation

$$SDD(C_{n,n-4}) - SDD(Q_n(n-4,1,0)) < 0 \ \ for\ \ 5 \leq n \leq 11.$$

i.e

$$SDD(C_{n,n-4}) < SDD(Q_n(n-4,1,0)) \ \ for\ \ 5 \leq n \leq 11.$$

and

$$SDD(C_{n,n-4}) - SDD(Q_n(n-4,1,0)) > 0 \;\; for \;\; n \geq 12.$$

i.e

$$SDD(C_{n,n-4}) > SDD(Q_n(n-4,1,0)) \;\; for \;\; n \geq 12.$$

Also

$$\begin{aligned} SDD(C_{n,n-4}) &= (n-4)\alpha(1,n-2) + 2\alpha(n-2,2) + 2\alpha(2,2) \\ &= (n-4)\Big(\frac{n^2-4n+5}{n-2}\Big) + \Big(\frac{n^2-4n+8}{n-2}\Big) + 4 \;\; for \;\; n \geq 12. \end{aligned}$$

$$\begin{aligned} &SDD(Q_n(n-4,1,0)) \\ =&(n-4)\alpha(1,n-2) + \alpha(n-2,2) + 2\alpha(2,3) + \alpha(3,n-2) + \alpha(1,3) \\ =&(n-4)\Big(\frac{n^2-4n+5}{n-2}\Big) + \Big(\frac{n^2-4n+8}{2(n-2)}\Big) \\ &+ \Big(\frac{n^2-4n+13}{3(n-2)}\Big) + \frac{33}{6} \;\; for \;\; 5 \leq n \leq 11. \end{aligned}$$

■

Lemma 5.6. *Let* $G \cong Q_n(p_1,p_2,p_3,p_4)$ *with* $p_3 \geq 2$. *Then*

$$SDD(Q_n(p_1+1,p_2,p_3-1,p_4)) > SDD(G).$$

If $p_1 \geq p_2 \geq p_4 \geq 2$, *then*

$$SDD(Q_n(p_1,p_2+1,p_3,p_4-1)) > SDD(G).$$

Proof. From the Lemmas 2.2 and 2.3, we have

$$\begin{aligned} &SDD(Q_n(p_1+1,p_2,p_3-1,p_4)) - SDD(G) \\ =&(p_1+1)\alpha(1,p_1+3) + (p_3-1)\alpha(1,p_3+1) + \alpha(p_1+3,p_2+2) \\ &+ \alpha(p_2+2,p_3+1) + \alpha(p_3+1,p_4+2) + \alpha(p_1+3,p_4+2) \\ &- [p_1\alpha(1,p_1+2) + p_3\alpha(1,p_3+2) + \alpha(p_1+2,p_2+2)] \\ &- [\alpha(p_2+2,p_3+2) + \alpha(p_3+2,p_4+2) + \alpha(p_1+2,p_4+2)] \\ =&(p_1+1)\alpha(1,p_1+3) - p_1\alpha(1,p_1+2) - [p_3\alpha(1,p_3+2) \\ &- (p_3-1)\alpha(1,p_3+1)] + \alpha(p_1+3,p_2+2) - \alpha(p_1+2,p_2+2) \\ &- [\alpha(p_2+2,p_3+2) - \alpha(p_2+2,p_3+1)] + \alpha(p_3+1,p_4+2) \\ &- \alpha(p_3+2,p_4+2) - [\alpha(p_1+2,p_4+2) - \alpha(p_1+3,p_4+2)] \\ =&g_1(p_1+1) - g_1(p_3) + f(p_1+2,p_2+2) - f(p_3+1,p_2+2) \\ &+ f(p_1+2,p_4+2) - f(p_3+2,p_4+2) \\ >&0 \end{aligned}$$

Hence $SDD(Q_n(p_1, p_2+1, p_3, p_4-1)) > SDD(G)$. similar arguments we obtain the following;

If $p_1 \geq p_2 \geq p_4 \geq 2$, then $SDD(Q_n(p_1, p_2+1, p_3, p_4-1)) > SDD(G)$. ■

Lemma 5.7. *Let $G \cong Q_n(p_1, p_2, 1, 1)$ with $p_1 \geq p_2 \geq 2$. Then*

$$SDD(Q_n(p_1+1, p_2-1, 1, 1)) > SDD(G).$$

Proof. Consider from the Lemmas 2.2, 2.3 and 5.6, we have

$$\begin{aligned}
&SDD(Q_n(p_1+1, p_2-1, 1, 1)) - SDD(G) \\
=&(p_1+1)\alpha(1, p_1+3) + (p_2-1)\alpha(1, p_2+1) + \alpha(p_1+3, p_2+1) \\
&+ \alpha(p_1+3, 3) + \alpha(p_2+1, 3) - [p_1\alpha(1, p_1+2) + p_2\alpha(1, p_2+2) \\
&+ \alpha(p_1+2, p_2+2) + \alpha(p_1+2, 3) + \alpha(p_2+2, 3)] \\
=&g_1(p_1+1) - g_1(p_2) + f(p_1+2, 3) - f(p_2+1, 3) + \alpha(p_1+3, p_2+1) \\
&- \alpha(p_1+2, p_2+2) \\
>&0
\end{aligned}$$

Hence $SDD(Q_n(p_1+1, p_2-1, 1, 1)) > SDD(G)$. ■

6. Symmetric Division deg Index of Bicyclic Graph

In [11], Y. Hu discussed the bicyclic graph on harmonic index. Motivated from this, in this section we determine the bicyclic graph of order n with the maximum and the second maximum SDD indices for $n \geq 5$.

Let $B_{n,p}$ be the set of bicyclic graph with n vertices and p pendent vertices for $0 \leq p \leq n-4$.

Let $S_{n,p}^{r,t}$ be the $n-$ vertex bicyclic graph by identifying one vertex of two cycles C_r and C_t and attaching $p = n+1-r-t$ pendent vertices to the common vertex, where $t \geq r \geq 3$ and $0 \leq p \leq n-5$.

Corollary 6.1. *Let G be a bicyclic graph with $n \geq 5$ vertices and p pendent vertices, where $0 \leq p \leq n-5$. Then*

$$SDD(G) \leq p\Big(\frac{p^2+8p+14}{2(p+4)}\Big) + (n+1)\Big(\frac{p^2+8p+20}{2(p+4)}\Big).$$

Equality hold only if graph $G \cong S_{n,p}^{r,t}$.

Proof. Since G is an bicyclic graph with size $m = n+1$ and $3 \leq \Delta \leq p+4 \leq n-1$.

By Theorem 3.8,

$$\begin{aligned}SDD(G) &\leq p\Big(\frac{\Delta^2+1}{\Delta}\Big)+(m-p)\Big(\frac{\Delta^2+{\delta_1}^2}{\Delta\delta_1}\Big)\\ &\leq p\Big(\frac{(p+4)^2+1}{(p+4)}\Big)+(n+1-p)\Big(\frac{(p+4)^2+2^2}{2(p+4)}\Big)\\ &= p\Big(\frac{p^2+8p+14}{2(p+4)}\Big)+(n+1)\Big(\frac{p^2+8p+20}{2(p+4)}\Big).\end{aligned}$$

■

Lemma 6.2. *For the graph in $S_{n,p}$ with $0 \leq p \leq n-5$ and $n \geq 5$, it holds that*

$$SDD(S_{n,0}) < SDD(S_{n,1}) < ... < SDD(S_{n,n-6}) < SDD(S_{n,n-5}).$$

Proof. Consider the function

$$l(p) = p\Big(\frac{p^2+8p+14}{2(p+4)}\Big)+(n+1)\Big(\frac{p^2+8p+20}{2(p+4)}\Big)$$

Then

$$l'(p) = p\Big(\frac{2p^2+16p+36}{4(p+4)^2}\Big)+(n+1)\Big(\frac{2p^2+16p+24}{4(p+4)^2}\Big)+\Big(\frac{p^2+8p+14}{2(p+4)}\Big)>0$$

as $p \geq 1$. Thus $l(p)$ is increasing function for $0 \leq p \leq n-5$ and

$$l(1) = \frac{23}{10}+(n+1)\frac{29}{10} > l(0) = (n+1)\frac{20}{8}$$

Then we have $SDD(S_{n,0}) < SDD(S_{n,1}) < ... < SDD(S_{n,n-6}) < SDD(S_{n,n-5})$.

■

Let C_4^* be the bicyclic graph obtained by adding an edge to the cycle C_4. Label the vertices of C_4^* by v_1, v_2, v_3, v_4 with $d_{v_1} = d_{v_2} = 3$, $d_{v_3} = d_{v_4} = 2$. Let $C_n^*(p_1, p_2, p_3, p_4)$ be the graph formed from C_4^* by attaching p_i pendent vertices to v_i, where $p_i \geq 0$ for $i = 1, 2, 3, 4$, $p_1 \geq p_2$, $p_3 \geq p_4$ and $\sum_{i=1}^4 p_i = n-4$.

Theorem 6.3. *Let $G \in B_{n,n-4}$ with $n \geq 5$. Then*

$$SDD(G) \leq (n-4)\Big(\frac{n^2-2n+2}{n-1}\Big)+\Big(\frac{n^2-2n+10}{3(n-1)}\Big)+\Big(\frac{n^2-2n+5}{(n-1)}\Big)+\frac{13}{3}.$$

with equality if and only if $G \cong C_n^*(n-4, 0, 0, 0)$.

Proof. Let $G \in B_{n,n-4}$ with $n \geq 5$. Then G is of the form $C_n^*(p_1, p_2, p_3, p_4)$ with $p_1 \geq p_2$, $p_3 \geq p_4$ and $\sum_{i=1}^4 p_i = n-4$.

Suppose that $G_1 = C_n^*(p_1, p_2, p_3, p_4)$ is a graph in $B_{n,n-4}$ with maximum SDD index.

Claim 1: Let $G = C_n^*(p_1, p_2, p_3, p_4)$. If $p_2 \geq 1$ and $G' = C_n^*(p_1+1, p_2-1, p_3, p_4)$ then $SDD(G') > SDD(G)$.

Using Lemmas 2.2 and 2.3, we get

$$\begin{aligned}
&SDD(G') - SDD(G)\\
=&(p_1+1)\alpha(1, p_1+4) + (p_2-1)\alpha(1, p_2+2) + \alpha(p_1+4, p_2+2)\\
&+ \alpha(p_1+4, p_3+2) + \alpha(p_1+4, p_4+2) + \alpha(p_2+2, p_3+2)\\
&+ \alpha(p_2+2, p_4+2) - [p_1\alpha(1, p_1+3) + p_2\alpha(1, p_2+3)]\\
&- [\alpha(p_1+3, p_2+3) + \alpha(p_1+3, p_3+2) + \alpha(p_1+3, p_4+2)]\\
&- [\alpha(p_2+3, p_3+2) + \alpha(p_2+3, p_4+2)]\\
=&(p_1+1)\alpha(1, p_1+4) - p_1\alpha(1, p_1+3) - [p_2\alpha(1, p_2+3)\\
&- (p_2-1)\alpha(1, p_2+2)] + \alpha(p_1+4, p_3+2) - \alpha(p_1+3, p_3+2)\\
&- [\alpha(p_2+3, p_3+2) - \alpha(p_2+2, p_3+2)] + \alpha(p_1+4, p_4+2)\\
&- \alpha(p_1+3, p_4+2) - [\alpha(p_2+3, p_4+2) - \alpha(p_2+2, p_4+2)]\\
&+ \alpha(p_1+4, p_2+2) - \alpha(p_1+3, p_2+3)\\
=&g_2(p_1+1) - g_2(p_2) + f(p_1+3, p_3+2) - f(p_2+2, p_3+2)\\
&+ f(p_1+3, p_4+2) - f(p_2+2, p_4+2) + \alpha(p_1+4, p_2+2)\\
&- \alpha(p_1+3, p_2+3)\\
>&0
\end{aligned}$$

Because, By Lemma 2.3, $g_2(p_1+1) > g_2(p_2)$ since $(p_1+1) > p_2$ By Lemma 2.2, $f(p_1+3, p_3+2) > f(p_2+2, p_3+2)$, since $p_1+3 > p_2+2 > p_3+2$ By Lemma 2.2, $f(p_1+3, p_4+2) > f(p_2+2, p_4+2)$, since $p_1+3 > p_2+2 > p_4+2$ and

$$\begin{aligned}
&\alpha(p_1+4, p_2+2) - \alpha(p_1+3, p_2+3)\\
=&\Big(\frac{(p_1+4)^2 + (p_2+2)^2}{(p_1+4)(p_2+2)} - \frac{(p_1+3)^2 + (p_2+3)^2}{(p_1+3)(p_2+3)}\Big) > 0 \text{ for } p_1 > p_2
\end{aligned}$$

Hence

$$SDD(G') > SDD(G).$$

Claim 2: If $p_4 \geq 2$ then $SDD(C_n^*(p_1, p_2, p_3+1, p_4-1)) > SDD(C_n^*(p_1, p_2, p_3, p_4))$.

Using Lemmas 2.2 and 2.3, we get

$$\begin{aligned}
&SDD(C_n^*(p_1, p_2, p_3+1, p_4-1)) - SDD(C_n^*(p_1, p_2, p_3, p_4))\\
=&(p_3+1)\alpha(1, p_3+3) + (p_4-1)\alpha(1, p_4+1) + \alpha(p_1+3, p_3+3)\\
&+ \alpha(p_1+3, p_4+1) + \alpha(p_2+3, p_3+3) + \alpha(p_2+3, p_4+1)\\
&- [p_3\alpha(1, p_3+2) + p_4\alpha(1, p_4+2)] - [\alpha(p_1+3, p_3+2)\\
&+ \alpha(p_1+3, p_4+2) + \alpha(p_2+3, p_3+2) + \alpha(p_2+3, p_4+2)]\\
=&(p_3+1)\alpha(1, p_3+3) - p_3\alpha(1, p_3+2) - [p_4\alpha(1, p_4+2)
\end{aligned}$$

$$\begin{aligned}
&- (p_4-1)\alpha(1,p_4+1)] + \alpha(p_3+3,p_1+3) - \alpha(p_3+2,p_1+3)\\
&- [\alpha(p_4+2,p_1+3) - \alpha(p_4+1,p_1+3)] + \alpha(p_3+3,p_2+3)\\
&- \alpha(p_3+2,p_2+3) - [\alpha(p_4+2,p_2+3) - \alpha(p_4+1,p_2+3)]\\
>&0
\end{aligned}$$

Hence

$$SDD(C_n^*(p_1,p_2,p_3+1,p_4-1)) > SDD(C_n^*(p_1,p_2,p_3,p_4)).$$

Claim 3: If $p_1, p_3 \geq 2$, then $SDD(C_n^*(p_1+p_3,0,0,0)) > SDD(C_n^*(p_1,0,p_3,0))$.

$$\begin{aligned}
&SDD(C_n^*(p_1+p_3,0,0,0)) - SDD(C_n^*(p_1,0,p_3,0))\\
=&(p_1+p_3)\alpha(1,p_1+p_3+3) + 2\alpha(2,p_1+p_3+3) + \alpha(3,p_1+p_3+3)\\
&+ \alpha(3,2) - [p_1\alpha(1,p_1+3) + p_3\alpha(1,p_3+2)]\\
&- [\alpha(3,p_1+3) + \alpha(3,p_3+2) + \alpha(p_1+3,p_3+2)]\\
=&p_1[\alpha(1,p_1+p_3+3) - \alpha(1,p_1+3)] + p_3[\alpha(1,p_1+p_3+3)\\
&- \alpha(1,p_3+2)] + \alpha(3,p_1+p_3+3) - \alpha(3,p_3+2)\\
&+ 2\alpha(2,p_1+p_3+3) + \alpha(3,2) - \alpha(3,p_3+2) - \alpha(p_1+3,p_3+2)\\
>&0
\end{aligned}$$

Because, By Lemma 2.1, $\alpha(x,y)$ is increasing for $x \geq 1$ $\alpha(1,p_1+p_3+3) - \alpha(1,p_1+3) > 0$, since $p_1+p_3+3 > p_1+3$ $\alpha(1,p_1+p_3+3) - \alpha(1,p_3+2) > 0$, since $p_1+p_3+3 > p_3+2$ By Lemma 2.2, $\alpha(3,p_1+p_3+3) - \alpha(3,p_3+2) > 0$, since $p_1+p_3+3 > p_3+2$ and $2\alpha(2,p_1+p_3+3) + \alpha(3,2) - \alpha(3,p_3+2) - \alpha(p_1+3,p_3+2) > 0$. Hence,

$$SDD(C_n^*(p_1+p_3,0,0,0)) > SDD(C_n^*(p_1,0,p_3,0)).$$

Claim 4: If $p_1, p_3 \geq 2$, then $SDD(C_n^*(0,0,p_1+p_3,0)) > SDD(C_n^*(p_1,0,p_3,0))$.

$$\begin{aligned}
&SDD(C_n^*(0,0,p_1+p_3,0)) - SDD(C_n^*(p_1,0,p_3,0))\\
=&(p_1+p_3)\alpha(1,p_1+p_3+2) + \alpha(3,3) + 2\alpha(3,p_1+p_3+2) + \alpha(3,2)\\
&- [p_1\alpha(1,p_1+3) + p_3\alpha(1,p_3+2) + \alpha(3,p_1+3)] - [\alpha(3,p_3+2)\\
&+ \alpha(p_1+3,p_3+2) + \alpha(2,p_1+3)]\\
=&p_1[\alpha(1,p_1+p_3+2) - \alpha(1,p_1+3)] + p_3[\alpha(1,p_1+p_3+2)\\
&- \alpha(1,p_3+2)] + \alpha(3,p_1+p_3+2) - \alpha(3,p_1+2)\\
&+ \alpha(3,p_1+p_3+2) - \alpha(3,p_3+2) + \alpha(3,3) + \alpha(2,3)\\
&- \alpha(2,p_1+3) - \alpha(p_1+3,p_3+2)\\
>&0
\end{aligned}$$

Hence

$$SDD(C_n^*(0,0,p_1+p_3,0)) > SDD(C_n^*(p_1,0,p_3,0)).$$

From Claims 1 and 2, we can conclude that $G_1 = C_n^*(p_1, 0, p_3, 0)$. From Claims 3 and 4, we can conclude that $G_1 = C_n^*(p_1+p_3, 0, 0, 0)$ or $G_1 = C_n^*(0, 0, p_1+p_3, 0)$ i.e $G_1 = C_n^*(n-4, 0, 0, 0)$ or $G_1 = C_n^*(0, 0, n-4, 0)$ since $\sum_{i=1}^{4} p_i = n-4$.

Claim 5: $SDD(C_n^*(n-4, 0, 0, 0)) > SDD(C_n^*(0, 0, n-4, 0))$.

$$\begin{aligned}
&SDD(C_n^*(n-4,0,0,0)) - SDD(C_n^*(0,0,n-4,0)) \\
=&(n-4)\alpha(1,n-1) + \alpha(3,n-1) + 2\alpha(n-1,2) + \alpha(3,2) \\
&- [(n-4)\alpha(1,n-2) + \alpha(3,3) + 2\alpha(n-2,3) + \alpha(3,2)] \\
=&(n-4)[\alpha(1,n-1) - \alpha(1,n-2)] + [\alpha(n-1,3) - \alpha(n-2,3)] \\
&+ 2\alpha(n-1,2) - \alpha(3,n-2) - \alpha(3,3) \\
>&0
\end{aligned}$$

Hence $SDD(C_n^*(n-4, 0, 0, 0)) > SDD(C_n^*(0, 0, n-4, 0))$. Thus $G_1 = C_n^*(n-4, 0, 0, 0)$ and

$$\begin{aligned}
&SDD(C_n^*(n-4,0,0,0)) \\
=&(n-4)\alpha(1,n-1) + \alpha(3,n-1) + 2\alpha(n-1,2) + 2\alpha(3,2) \\
=&(n-4)\Big(\frac{n^2-2n+2}{n-1}\Big) + \Big(\frac{n^2-2n+10}{3(n-1)}\Big) + \Big(\frac{n^2-2n+5}{(n-1)}\Big) + \frac{13}{3}.
\end{aligned}$$ ■

Corollary 6.4. *Among the graphs in $B_{n,n-4}$ with $n \geq 5$, $C_n^*(0, 0, n-4, 0)$ is the unique graph with the second maximum SDD indices, which are equal to*

$$SDD(C_n^*(0,0,n-4,0)) = (n-4)\Big(\frac{n^2-4n+5}{n-2}\Big) + 2\Big(\frac{n^2-4n+13}{3(n-2)}\Big) + \frac{19}{3}.$$

Proof. Let $G_1 = C_n^*(n_1, n_2, n_3, n_4)$ is a graph in $B_{n,n-4}$ with the second maximum SDD index, which is achieved by the graph in $B_{n,n-4} \setminus C_n^*(n-4, 0, 0, 0)$ with the maximum SDD index.

By the Theorem 6.3, we have $G_1 = C_n^*(0, 0, n-4, 0)$ and

$$\begin{aligned}
&SDD(C_n^*(0,0,n-4,0)) \\
=&(n-4)\alpha(1,n-2) + \alpha(3,3) + 2\alpha(n-2,3) + 2\alpha(3,2) \\
=&(n-4)\Big(\frac{n^2-4n+5}{n-2}\Big) + 2\Big(\frac{n^2-4n+13}{3(n-2)}\Big) + \frac{19}{3}.
\end{aligned}$$ ■

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