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Study of Bounds and Extremal Graphs of Symmetric Division Degree Index for Bicyclic Graphs with Perfect Matching

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ABSTRACT

In this article, we complement the study of Pan and Li by computing the first five minimum values of the symmetric division degree (*SDD*) index attained by bicyclic graphs that have a perfect matching. One of our main contributions is identifying the graphs that attain the bounds. Further, we compute the upper bound of the *SDD* index for bicyclic graphs with a maximum degree of four, which admits a perfect matching and prove the bound is also tight by identifying the graphs that attain it.

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1. INTRODUCTION

In 2010, Vukičević and Gašperov [9] constructed a broad class of molecular descriptors consisting of 148 discrete Adriatic descriptors to improve the QSPR/QSAR (Quantitative structure-property/activity relationship). They found that only the *SDD* index has the best correlation ability for predicting the total surface area of polychlorobiphenyls (PCB). Recently, Furtula, Das, and Gutman [5] analyzed the *SDD* index for the data of octane

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isomers and compared it with other popular *VDB* indices, such as Zagreb indices, geometric-arithmetic index, atom-bond connectivity index, and inverse sum index. They concluded that the *SDD* index has the right to be considered a viable and applicable molecular descriptor. Recently, the authors of [13, 11] have given bounds for the *SDD* index using the edge/vertex-degree-based indices, including Zagreb indices. We refer to some recent articles for more details on the *SDD* index [1, 3, 4, 6, 7, 8, 12, 14–16].

In CGT, cycles exist in aromatic compounds which contain the Kekule structure. The corresponding graph representation involves the study of perfect matching as it plays an essential role in analyzing the resonance energy and stability of hydrocarbons. Such an application also propels our interest in studying the *SDD* index's behavior for the bicyclic graphs having a perfect matching. In this direction, we complement the study of [16] and present the first five lower bounds of the *SDD* index for all bicyclic graphs with perfect matching and the graphs that attain the bounds. Further, we also compute an upper bound of the *SDD* index for bicyclic graphs with a maximum degree of four, which admits a perfect matching.

The organization of the paper is as follows. Section 2 describes the required notions and results from the literature. Section 3.1 presents the first five lower bounds of the *SDD* index for all bicyclic graphs with perfect matching. Finally, in Section 3.2, we compute the upper bound of bicyclic graphs that admit a perfect matching and have a maximum degree of at most four.

2. PRELIMINARIES

Throughout this paper, we consider only nontrivial connected simple graphs. A graph is denoted by $G = G(V, E)$, where V and E represent the vertex and edge sets of the graph, respectively. Let $N_G(x) = \{y \in G: xy \in E\}$ denote the neighbors of a vertex $x \in V$, and $d_G(x)$ denotes the degree of a vertex $x \in V$, then $|N_G(x)| = d_G(x)$. Let Δ denote the maximum degree of the vertices in G. A vertex of degree one is called a *pendant vertex*, and a path $< v_1 v_2 \dots v_{k-1} v_k >$ is called a *pendant path* if $d_G(v_1) = 1$, $d_G(v_i) = 2$, for $i = 2,3, \dots, k-1$ and $d_G(v_k) \geq 3$. A graph G is called a bicyclic graph if it has exactly two cycles. If G is a bicyclic graph on $n(\geq 3)$ vertices and m edges, then $m = n + 1$. A matching M of a graph G is a subset of edge set E such that no two edges are adjacent in G. If $|M| = |V|/2$, then matching M is called a perfect matching. Other definitions and notations are taken from the Book [10].

Symmetric division degree index $SDD(G)$ is defined as

$$SDD(G) = \sum_{uv \in E(G)} \left\{\frac{d_G^2(u) + d_G^2(v)}{d_G(u) d_G(v)}\right\}, \quad (1)$$

where $d_G(u)$ and $d_G(v)$ denote the degree of the end vertices of an edge $uv \in E(G)$ in the graph G.

Suppose the degree of the vertex $x \in V(G)$ is i and the vertex $y \in V(G)$ is j, then the edge $e = xy$ is referred to as an (i, j)-edge, and the total number of (i, j)-edges are denoted by e_{ij}. Let

$$S_{(i,j)} = \frac{i^2+j^2}{ij}, \tag{2}$$

then, from Equation (1), the *SDD* index for a graph G is written as

$$SDD(G) = \sum_{i \leq j} e_{ij}\, S_{(i,j)}. \tag{3}$$

Lemma 2.1. [16] If G has K pendants paths, then $SDD(G) \geq \frac{2}{3}K + 2|E(G)|$.

Lemma 2.2. [2] If G is a connected graph, then $\min\{S_{(1,x)}\} \geq \max\{S_{(u,v)}\}$, where $u, v, x \in \{2,3,4\}$ and equality holds only for $x = 2, u = 2$ and $v = 4$.

Lemma 2.3. $S_{(1,x)} = \frac{x^2+1}{x}, x \geq 2$, is a monotonic increasing function.

Proof. Let $f(x) = \frac{x^2+1}{x}$ then $f'(x) = 1 - \frac{1}{x^2} > 0$, since $x \geq 2$. Hence $S_{(1,x)} = \frac{x^2+1}{x}$ is an increasing function. ∎

Remark 2.1. Note that the minimum value of $S_{(x,y)} = \frac{x^2+y^2}{xy} \geq 2$, and equality holds if and only if $x = y$.

3. Bounds of *SDD* Index for Bicyclic Graphs with A Perfect Matching

Recall that widely in chemical graph theory, the computation of topological indices is on hydrogen-suppressed chemical structures and that the PCB compounds as a molecular graph are bicyclic. Additionally, the existence of perfect matchings in molecular graphs tells us about the aromaticity of the compound. In the rest of this article, we give bounds of *SDD* index for bicyclic graphs with a perfect matching.

Before proving the results, we define some required notations and definitions.

Let β_{2n} denote the set of all bicyclic graphs which have a *perfect matching* on $2n$ vertices. Next, we define three of its subsets which also form a partition of β_{2n}.

1. Let $\beta_{2n}^1 \subset \beta_{2n}$ denote the set of bicyclic graphs on $2n$ vertices such that if $G \in \beta_{2n}^1$, then the two cycles in G are joined by a path, as shown in Figure 1(a).
2. Let $\beta_{2n}^2 \subset \beta_{2n}$ denote the set of bicyclic graphs on $2n$ vertices such that if $G \in \beta_{2n}^2$ then the two cycles in G are joined by a common vertex, see Figure 1(b).

3. Let $\beta_{2n}^3 \subset \beta_{2n}$ denote the set of bicyclic graphs such that for $G \in \beta_{2n}^3$, the two cycles of G have a common path, as shown in Figure 1(c).

A representative for each of the graph classes defined above is shown in Figure 1.

(a) $G \in \beta_{2n}^1$ (b) $G \in \beta_{2n}^2$ (c) $G \in \beta_{2n}^3$

Figure 1: Bicyclic graph.

Note that any graph $G \in \beta_{2n}$ belongs to precisely one of the three subsets β_{2n}^1, β_{2n}^2, or β_{2n}^3, and hence $\beta_{2n} = \beta_{2n}^1 \cup \beta_{2n}^2 \cup \beta_{2n}^3$.

3.1. LOWER BOUNDS OF SDD INDEX FOR BICYCLIC GRAPHS WITH A PERFECT MATCHING

In this section, we compute the first five minimum values of the *SDD* index for all the bicyclic graphs that admit a perfect matching. To this end, we identify those graphs that possess the smallest *SDD* index value in each of the subclass β_{2n}^1, β_{2n}^2, and β_{2n}^3.

3.1.1. $\boldsymbol{\beta_{2n}^1}$

Before proving the required bounds of β_{2n}^1, we define some special classes of bicyclic graphs in β_{2n}^1, which play a primary role in our proof.

Let $F_1^1(2n) \subset \beta_{2n}^1$, $n \geq 3$ be a collection such that for any $G \in F_1^1(2n)$, the edge-degree partition of G is given by $E_1^1(G) = \{e_{22} = 2n-4,\ e_{23} = 4,\ e_{33} = 1\}$.

For $n \geq 4$ and $i = 2, 3$, let $F_i^1(2n) \subset \beta_{2n}^1$ represent those graphs G with edge-degree partitions $E_2^1(G) = \{e_{22} = 2n-5,\ e_{23} = 6\}$ and $E_3^1(G) = \{e_{12} = 1, e_{22} = 2n-7,\ e_{23} = 5,\ e_{33} = 2\}$, respectively.

For $n \geq 5$ and $i = 4, 5, 6$, let $F_i^1(2n) \subset \beta_{2n}^1$ be defined by the edge-degree partitions $E_4^1(G) = \{e_{12} = 2, e_{22} = 2n-9,\ e_{23} = 4,\ e_{33} = 4\}$, $E_5^1(G) = \{e_{12} = 1, e_{22} = 2n-8,\ e_{23} = 7,\ e_{33} = 1\}$, and $E_6^1(G) = \{e_{12} = 1, e_{22} = 2n-9,\ e_{23} = 9\}$ respectively.

Let $F_7^1(2n) \subset \beta_{2n}^1$, $n \geq 4$ be defined such that for any $G \in F_7^1(2n)$, the edge-degree partition of G is given by $E_7^1(G) = \{e_{13} = 1, e_{22} = 2n-6,\ e_{23} = 4,\ e_{33} = 2\}$.

Finally, let us define $F_8^1(2n) \subset \beta_{2n}^1$ for $n \geq 6$ to be the collections of the bicyclic graphs G, whose edge-degree partition is given by $E_8^1(G) = \{e_{12} = 2, e_{22} = 2n - 10,\ e_{23} = 6,\ e_{33} = 3\}$.

A representative for each graph class defined above is shown in Figures 2(a) to 2(h).

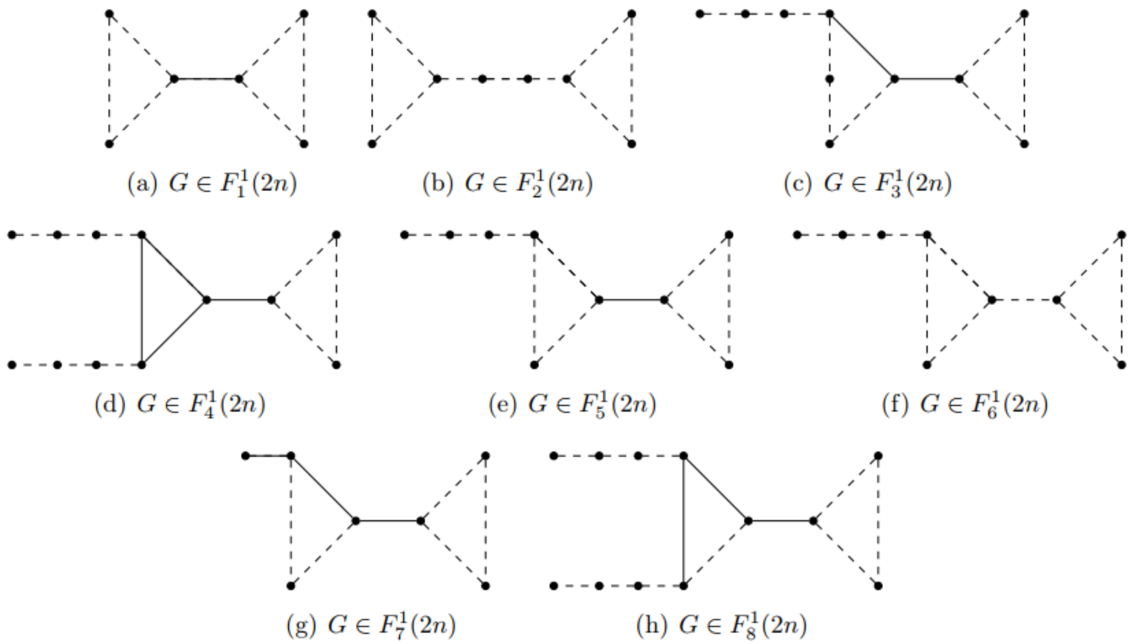


Figure 2: Representation of graphs corresponding to edge-degree partition $E_i^1(G)$, $i = 1, 2, \ldots, 8$ of bicyclic graphs $F_i^1(2n)$, $i = 1, 2, \ldots, 8$ respectively.

THEOREM 3.1. Let $G \in \beta_{2n}$.

1. If $G \in \beta_{2n}^1$, then $SDD(G) = 4n + \frac{8}{3}$. Equality holds if and only if $G \in F_1^1(2n)$, $n \geq 3$.
2. If $G \in \beta_{2n}^1 \backslash \{F_1^1(2n)\}$, then $SDD(G) \geq 4n + 3$. Equality holds if and only if $G \in F_2^1(2n)$, $n \geq 4$.
3. If $G \in \beta_{2n}^1 \backslash \{F_1^1(2n), F_2^1(2n)\}$, then $SDD(G) = 4n + \frac{10}{3}$. Equality holds if and only if $G \in F_3^1(2n)$, $n \geq 4$.
4. If $G \in \beta_{2n}^1 \backslash \{F_1^1(2n), F_2^1(2n), F_3^1(2n)\}$, then $SDD(G) = 4n + \frac{11}{3}$. Equality holds if and only if $G \in F_4^1(2n), or\ G \in F_5^1(2n)$, $n \geq 5$.
5. If $G \in \beta_{2n}^1 \backslash \{F_1^1(2n), F_2^1(2n), F_3^1(2n), F_4^1(2n), F_5^1(2n)\}$, then $SDD(G) \geq 4(n+1)$. Equality holds if and only if $G \in F_6^1(2n)$, $n \geq 5$ or $G \in F_7^1(2n)$, $n \geq 4$ or $G \in F_8^1(2n)$, $n \geq 6$.

Proof. We prove this lemma by taking conditions on the number of pendant paths K in the bicyclic graph $G \in \beta_{2n}^1$.

CASE (1) If $K = 0$, then $\Delta = 3$ and $G \in F_1^1(2n)$ with $n \geq 3$ or $G \in F_2^1(2n)$ with $n \geq 4$. Note that by direct computation, $SDD(G) = 4n + \frac{8}{3}$ if $G \in F_1^1(2n)$, and $SDD(G) = 4n + 3$, if $G \in F_2^1(2n)$.

CASE (2) If $K = 1$, then $3 \leq \Delta \leq 4$, and we need to consider the following two subcases: (2.1) when the length of the pendant path is one and (2.2) when the length of the pendant path is at least two.

SUBCASE (2.1) If the length of the pendant path is one, then by taking the condition on maximum degree Δ, we have:

I. If $\Delta = 3$, then G has exactly three vertices w_1, w_2, w_3 of degree three. Now, again analyzing the vertices w_1, w_2, w_3, since $G \in \beta_{2n}^1$, we see that G can have at most two adjacent pairs among them.
   (a) Suppose G has two pairs of adjacent vertices among w_1, w_2, w_3, then $G \in F_7^1(2n)$ with $n \geq 4$ and $SDD(G) = 4(n + 1)$.
   (b) Suppose that at most one pair of vertices are adjacent among w_1, w_2, w_3, then G has at least six edges that connect the vertices having degrees two and three. Since the contribution of an edge *uv* is at least 2, we get
$$SDD(G) \geq 6S_{(2,3)} + S_{(1,3)} + 4(n - 3) = 4n + \frac{13}{3} > 4(n + 1).$$

II. If $\Delta = 4$, then G has at least two edges connecting the vertices of degree two and Δ. Then
$$SDD(G) \geq 2S_{(2,4)} + S_{(1,4)} + 4(n - 1) = 4n + \frac{21}{4} > 4(n + 1).$$

SUBCASE (2.2) If the length of the pendant path is at least two, then we again make conditions on the maximum degree Δ.

(I) Let $\Delta = 3$, then G has exactly three vertices w_1, w_2, w_3 of degree three. Again we observe that G can have at most two pairs of adjacent vertices among w_1, w_2, w_3, since $G \in \beta_{2n}^1$.
   (a) Suppose two pairs of vertices among w_1, w_2, w_3, are adjacent, then $G \in F_3^1(2n)$ with $n \geq 4$ and $SDD(G) = 4n + \frac{10}{3}$.
   (b) Suppose one pair of the vertices among w_1, w_2, w_3, are adjacent, then $G \in F_5^1(2n)$ with $n \geq 5$ and $SDD(G) = 4n + \frac{11}{3}$.
   (c) Suppose that no pair of vertices w_1, w_2, w_3, are adjacent, then $G \in F_6^1(2n)$ with $n \geq 5$ and $SDD(G) = 4(n + 1)$.

(II) Let $\Delta = 4$, then G has at least three edges connecting the vertices of degree two and Δ. In this subcase, we have $SDD(G) \geq 3S_{(2,4)} + S_{(1,2)} + 2S_{(2,3)} + 2(2n-5) = 4n + \frac{13}{3} > 4(n+1)$.

CASE (3) If $K = 2$, then $3 \leq \Delta \leq 5$. Now, we need to consider two subcases.

SUBCASE (3.1) If G has at least one pendant path of length one, then from Lemma 2.3, we have

$$SDD(G) \geq S_{(1,3)} + S_{(1,2)} + 2S_{(2,3)} + 2(2n-3) = 4n + \frac{25}{6} > 4(n+1).$$

SUBCASE (3.2) If both the pendant paths have lengths at least two, then

(I) If $\Delta = 3$, then G has four vertices w_1, w_2, w_3, w_4 of degree three. Now, we analyze the position of these vertices w_1, w_2, w_3, w_4 in G. Since $G \in \beta_{2n}^1$, cycles are joined by a path, so among the vertices w_1, w_2, w_3, w_4, at most four pair of vertices are adjacent.

(a) Suppose G has four pairs of adjacent vertices among $w_1, w_2, w_3,$ and w_4, then G will have exactly four edges that connect the vertices of degrees two and three. Hence $G \in F_4^1(2n)$ with $n \geq 5$ and $SDD(G) = 4n + \frac{11}{3}$.

(b) Suppose G has three pairs of adjacent vertices from $w_1, w_2, w_3,$ and w_4, then G will have exactly six edges that connect the vertices of degrees two and three. In that case, $G \in F_8^1(2n)$ with $n \geq 6$ and $SDD(G) = 4(n+1)$.

(c) Suppose that G has at most two pairs of adjacent vertices among w_1, w_2, w_3, w_4, then G has at least eight edges that connect the vertices of degrees two and three. Then, $SDD(G) \geq 8S_{(2,3)} + 2S_{(1,2)} + 2(2n-9) = 4n + \frac{13}{3} > 4(n+1)$

(II) If $\Delta \geq 4$, then G has at least two edges that connect the vertices of degrees two and Δ. Then, $SDD(G) \geq 2S_{(1,2)} + 2S_{(2,\Delta)} + 2S_{(2,3)} + 2(2n-5) \geq 2S_{(1,2)} + 2S_{(2,4)} + 2S_{(2,3)} + 2(2n-5) = 4n + \frac{13}{3} > 4(n+1)$.

CASE (4) If $K = 3$, then $3 \leq \Delta \leq 6$, and we need to consider the following two subcases: (4.1) when at least one pendant path has length one, and (4.2) all three pendant paths have length at least two.

SUBCASE (4.1) If G has at least one pendant path of length one, then from Remark 2.1 and Lemma 2.3, we have

$$SDD(G) \geq S_{(1,3)} + 2S_{(1,2)} + 4(n-1) = 4n + \frac{13}{3} > 4(n+1).$$

SUBCASE (4.2) If all the three pendant paths in G have lengths at least two, then we have the following cases based on the maximum degree Δ.

(i) If $\Delta = 3$, then G has five vertices w_1, w_2, w_3, w_4, w_5 of degree three. Since $G \in \beta_{2n}^1$, is a bicyclic graph in which cycles are joined by a path, G has at most five pairs of adjacent vertices among w_1, w_2, w_3, w_4, w_5. Then G has at least five edges that connect the vertices of degrees two and three. Since G has three pendant paths, then

$$SDD(G) \geq 3S_{(1,2)} + 5S_{(2,3)} + 2(2n-7) = 4n + \frac{13}{3} > 4(n+1).$$

(ii) If $\Delta \geq 4$, then G has at least one edge which connects the vertices of degrees two and Δ, then

$$\begin{aligned} SDD(G) &\geq 3S_{(1,2)} + S_{(2,\Delta)} + 2S_{(2,3)} + 2(2n-5) \\ &\geq 3S_{(1,2)} + S_{(2,4)} + 2S_{(2,3)} + 2(2n-5) \\ &= 4n + \frac{13}{3} > 4(n+1). \end{aligned}$$

CASE (5) If $K \geq 4$, then from Lemma 2.1

$$SDD(G) = \frac{2}{3}K + 2|E(G)| \geq \frac{2}{3} \times 4 + 2(2n+1) > 4(n+1).$$

Hence the result. ∎

3.1.2 $\boldsymbol{\beta_{2n}^2}$

Before proving the required bounds of β_{2n}^2, first, we identify a bicyclic graph in β_{2n}^2 which is required for our proof. Let $J_{2n}^2 \subset \beta_{2n}^2$ be a collection of bicyclic graphs on $2n$ vertices, such that if $G \in J_{2n}^2$, then G has an edge-degree partition $E(G) = \{e_{24} = 4,\ e_{22} = 2n-3\}$, $n \geq 3$, see Figure 1(b).

Theorem 3.2. If $G \in \beta_{2n}^2$, then $SDD(G) \geq 4(n+1)$. Equality holds if and only if $G \in J_{2n}^2$, $n \geq 3$.

Proof. The proof follows by case analysis similar to Theorem 3.1. For brevity, we omit the proof here. ∎

3.1.3 $\boldsymbol{\beta_{2n}^3}$

Before proving the required bounds of β_{2n}^3, first, we identify and define some special classes of bicyclic graphs in β_{2n}^3, which are required for our proof.

Let $H_1^3(2n) \subset \beta_{2n}^3$, $n \geq 2$; $H_2^3(2n)$, $H_3^3(2n) \subset \beta_{2n}^3$, $n \geq 3$; $H_4^3(2n) \subset \beta_{2n}^3$, $n \geq 2$; $H_5^3(2n)$, $H_6^3(2n) \subset \beta_{2n}^3$, $n \geq 4$; $H_7^3(2n) \subset \beta_{2n}^3$, $n \geq 3$; $H_8^3(2n) \subset \beta_{2n}^3$, $n \geq 4$; $H_9^3(2n) \subset \beta_{2n}^3$, $n \geq 5$; $H_{10}^3(2n) \subset \beta_{2n}^3$, $n \geq 3$; $H_{11}^3(2n) \subset \beta_{2n}^3$, $n \geq 5$, and $H_{12}^3(2n) \subset \beta_{2n}^3$, $n \geq 6$ be the collection of bicyclic graphs which has a perfect matching such that if $G \in H_i^3(2n),\ i = 1,2,\dots,12$, then it has the following edge-degree partitions.

$$E_1^3(G) = \{e_{22} = 2n-4,\ e_{23} = 4,\ e_{33} = 1\};$$
$$E_2^3(G) = \{e_{22} = 2n-5,\ e_{23} = 6\};$$
$$E_3^3(G) = \{e_{12} = 1, e_{22} = 2n-6,\ e_{23} = 3,\ e_{33} = 3\};$$
$$E_4^3(G) = \{e_{12} = 2, e_{22} = 2n-9,\ e_{23} = 4,\ e_{33} = 4\};$$
$$E_5^3(G) = \{e_{12} = 2, e_{22} = 2n-8,\ e_{23} = 2,\ e_{33} = 5\};$$
$$E_6^3(G) = \{e_{12} = 1, e_{22} = 2n-7,\ e_{23} = 5,\ e_{33} = 2\};$$
$$E_7^3(G) = \{e_{13} = 1, e_{22} = 2n-5,\ e_{23} = 2,\ e_{33} = 3\};$$
$$E_8^3(G) = \{e_{12} = 1, e_{22} = 2n-8,\ e_{23} = 7,\ e_{33} = 1\};$$
$$E_9^3(G) = \{e_{12} = 1, e_{22} = 2n-9,\ e_{23} = 9\};$$
$$E_{10}^3(G) = \{e_{13} = 1, e_{22} = 2n-6,\ e_{23} = 4,\ e_{33} = 2\};$$
$$E_{11}^3(G) = \{e_{12} = 2, e_{22} = 2n-10,\ e_{23} = 6,\ e_{33} = 3\};$$
$$E_{12}^3(G) = \{e_{12} = 3, e_{22} = 2n-11,\ e_{23} = 3,\ e_{33} = 6\},$$

respectively, see Figure 3 for a graph representing each of these classes.

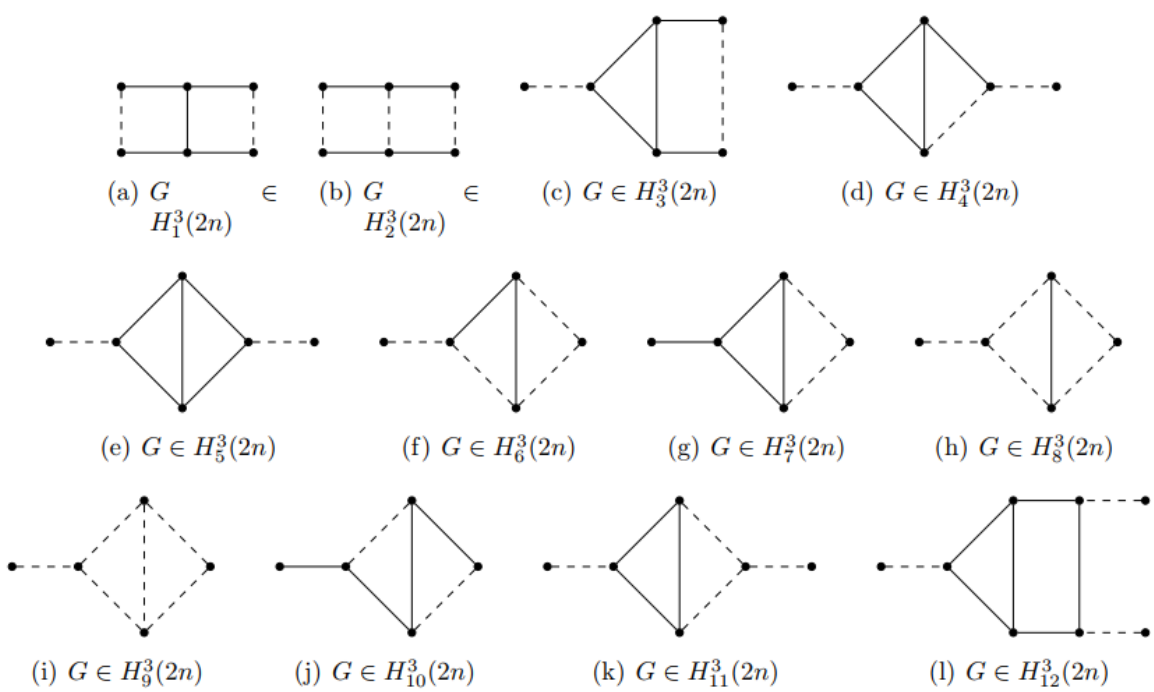


Figure 3: Representation of graphs corresponding to edge-degree partition $E_i^3(G)$, of bicyclic graphs in $H_i^3(2n),\ i = 1,2,\dots,12$, respectively.

THEOREM 3.3.

1. If $G \in \beta_{2n}^3$, then $SDD(G) \geq 4n + \frac{8}{3}$. Equality holds if and only if $G \in H_1^3(2n)$, $n \geq 4$.
2. If $G \in \beta_{2n}^3 \backslash \{H_1^3(2n)\}$, then $SDD(G) \geq 4n + 3$. Equality holds if and only if $G \in H_2^3(2n)$ or $G \in H_3^3(2n), n \geq 3$ or $G \in H_4^3(2n), n \geq 5$.
3. If $G \in \beta_{2n}^3 \backslash \{H_i^3(2n)\}$, i =1,2,3,4, then $SDD(G) \geq 4n + \frac{10}{3}$. Equality holds if and only if $G \in H_5^3(2n)$ or $G \in H_6^3(2n), n \geq 4$.
4. If $G \in \beta_{2n}^3 \backslash \{H_i^3(2n)\}$, i =1,...,6, then $SDD(G) \geq 4n + \frac{11}{3}$. Equality holds if and only if $G \in H_7^3(2n), n \geq 3$ or $G \in H_8^3(2n), n \geq 4$.
5. If $G \in \beta_{2n}^3 \backslash \{H_i^3(2n)\}$, i =1,...,8, then $SDD(G) \geq 4(n + 1)$. Equality holds if and only if $G \in H_{10}^3(2n), n \geq 4$ or $G \in H_9^3(2n)$ or $G \in H_{11}^3(2n)$, $n \geq 5$ or $G \in H_{12}^3(2n)$, $n \geq 6$.

Proof. The proof is obtained by making cases on the number and length of the pendant paths, similar to Theorem 3.1. For brevity, we omit the proof here. ∎

Now, combining the above three theorems, we are ready with the first five minimum values for the *SDD* index of all bicyclic graphs, which have a *perfect matching*.

Theorem 3.4. Let $G \in \beta_{2n}$ be a bicyclic graph that has a perfect matching.

1. The minimum value of $SDD(G)$ is $4n + \frac{8}{3}$, and equality holds if and only if $G \in F_1^1(2n), n \geq 3$ or $G \in H_1^3(2n)$, $n \geq 4$.
2. The second-minimum value for $SDD(G)$ is $4n + 3$, and equality holds if and only if $G \in H_2^3(2n)$ or $G \in H_3^3(2n)$, $n \geq 3$ or $G \in F_2^1(2n)$ *or* $G \in H_4^3(2n)$, $n \geq 4$.
3. The third-minimum value of $SDD(G)$ is $4n + \frac{10}{3}$, and equality holds if and only if $G \in F_3^1(2n)$ or $G \in H_5^3(2n)$ or $G \in H_6^3(2n)$, $n \geq 4$.
4. The fourth-minimum value of $SDD(G)$ is $4n + \frac{11}{3}$, and equality holds if and only if $G \in H_7^3(2n)$, for $n \geq 3$ or $H_8^3(2n)$, for $n \geq 4$ or $G \in F_4^1(2n)$ or $G \in F_5^1(2n)$, $n \geq 5$.
5. The fifth-minimum value of $SDD(G)$ is $4(n + 1)$, and equality holds if and only if $G \in J_{2n}^2$, $n \geq 3$ or $F_7^1(2n)$ or $G \in H_{10}^3(2n)$, $n \geq 4$ or $G \in F_6^1(2n)$ or $G \in H_9^3(2n)$ or $G \in H_{11}^3(2n)$, $n \geq 5$ or $G \in F_8^1(2n)$ or $G \in H_{12}^3(2n)$, $n \geq 6$.

Proof. The theorem follows directly from Theorems 3.1, 3.2, and 3.3. ∎

3.2. Upper Bounds of SDD Index for Bicyclic Graphs with a Perfect Matching and Maximum Degree at Most 4

In this section, we compute the upper bounds of the *SDD* index for bicyclic graphs, which has maximum degree four and that admits a *perfect matching*. Before proving the results, we identify and define some interesting classes of graphs that play a crucial role in the computation of upper bounds.

Let $D_i^1(2n) \subset \beta_{2n}^1$, $D_i^3(2n) \subset \beta_{2n}^3$, $i = 1, 2, 3$ be the set of bicyclic graphs such that, if $G \in D_1^3(2n)$, $n \geq 6$ or $G \in D_1^1(2n)$, $n \geq 10$, then depending on n being even or odd, we have two sets of edge-degree partition of G. When n is even, then the edge-degree partition is given by

$$E(G) = \{e_{12} = \frac{n-2}{2}, e_{14} = \frac{n+2}{2}, e_{24} = \frac{n-2}{2}, e_{44} = \frac{n+4}{2}\},$$

See Figure 4(a) and Figure 4(c). When n is odd, the edge-degree partition is

$$E(G) = \{e_{12} = \frac{n-3}{2}, e_{13} = 1, e_{14} = \frac{n+1}{2}, e_{24} = \frac{n-3}{2}, e_{34} = 2, e_{44} = \frac{n+1}{2}\},$$

see Figure 4(b) and Figure 4(d).

If $G \in D_2^3(2n)$, $n \geq 4$ or $G \in D_2^1(2n)$, $n \geq 6$, then the edge-degree partition of G is

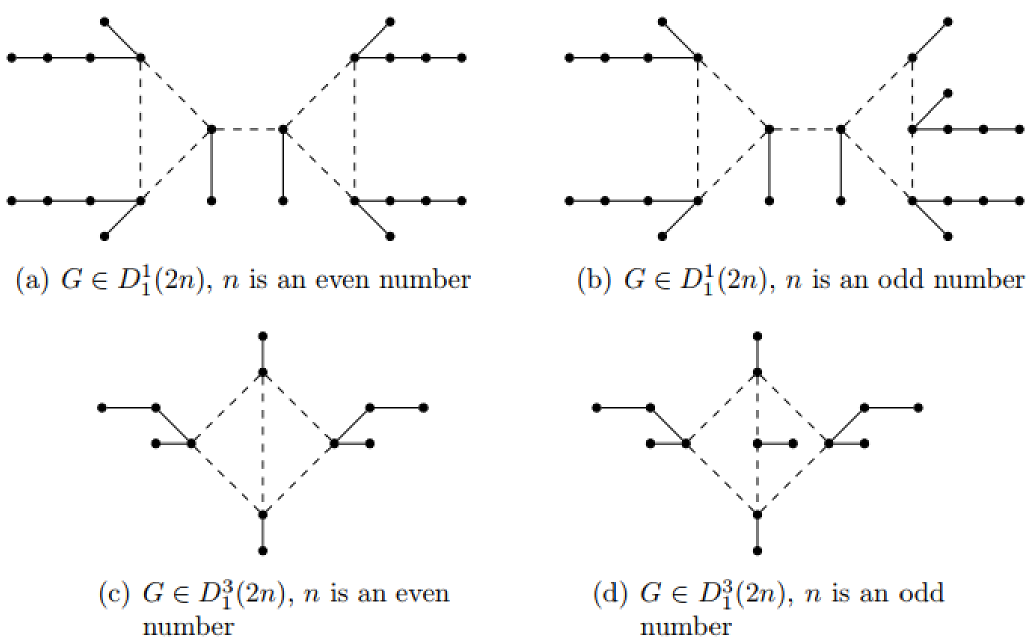
$$E(G) = \{e_{13} = n-2, e_{14} = 2, e_{33} = n-4, e_{34} = 4, e_{44} = 1\},$$

see Figure 5(a) and Figure 5(c).

For $G \in D_3^3(2n)$, $n \geq 5$ or $G \in D_3^1(2n)$, $n \geq 7$, then the edge-degree partition of bicyclic graph G is

$$E(G) = \{e_{13} = n-2, e_{14} = 2, e_{33} = n-5, e_{34} = 6\},$$

see Figure 5(b) and Figure 5(d).



(a) $G \in D_1^1(2n)$, n is an even number

(b) $G \in D_1^1(2n)$, n is an odd number

(c) $G \in D_1^3(2n)$, n is an even number

(d) $G \in D_1^3(2n)$, n is an odd number

Figure 4: Representation of bicyclic graphs which attains maximum *SDD* index.

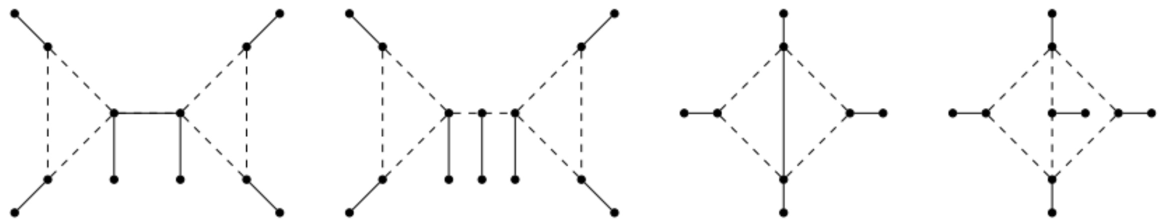


Figure 5: Representation of graphs corresponding to the edge-degree partition $E(G)$ of bicyclic graphs $D_2^1(2n), D_3^1(2n), D_2^3(2n), D_3^3(2n)$, respectively.

Theorem 3.5. Let $G \in \beta_{2n}$ for $n \geq 6$, and G has a maximum degree at most four, then

$$SDD(G) \leq \begin{cases} \frac{1}{8}(45n+25) & n \text{ is odd}, \\ \frac{1}{8}(45n+26) & n \text{ is even}. \end{cases}$$

Equality holds if and only if $G \in D_1^3(2n),\ n \geq 6$ or $G \in D_1^1(2n),\ n \geq 9$.

Proof. Let

$$\Psi(n) = \begin{cases} \frac{1}{8}(45n+25) & n \text{ is odd}, \\ \frac{1}{8}(45n+26) & n \text{ is even}. \end{cases} \tag{4}$$

We prove this theorem by considering two cases depending on the number of pendant vertices in $G \in \beta_{2n}$: (1) G has exactly n pendant vertices and (2) G has at most $n-1$ pendant vertices.

CASE (1) When G has n pendant vertices, then each non-pendant vertex of G is adjacent to a vertex of degree one, and that, in this case, either $G \in \beta_{2n}^1$ or $G \in \beta_{2n}^3$ and $G \notin \beta_{2n}^2$ as the graphs under study have a maximum degree of at most four.

We consider two subcases: (1.1) If $G \in \beta_{2n}^1$ or (1.2) If $G \in \beta_{2n}^3$.

SUBCASE (1.1) Suppose $G \in \beta_{2n}^1$. We prove this case by the method of induction.

I. When $n = 6$, then $G \cong \rho_1$ (as shown in Figure 6(a)) and $SDD(\rho_1) = 36.16 < \Psi(6)$.

II. When $n = 7$, then $G \cong \rho_2$ (as shown in Figure 6(b)) or $G \cong \rho_3$ (Figure 6(c)) or $G \cong \rho_4$ (Figure 6(d)) and $SDD(\rho_2) = 41.66 < \Psi(7) = 42.5$, $SDD(\rho_3) = 41.5 < \Psi(7)$ and $SDD(\rho_4) = 42.08 < \Psi(7)$.

III. For $n = 8, 9,$ and 10, G is one of the graphs $\beta_{16}^1, \beta_{18}^1, \beta_{20}^1$, which have edge-degree partitions as given in Table 1, Table 2, and Table 3, respectively.

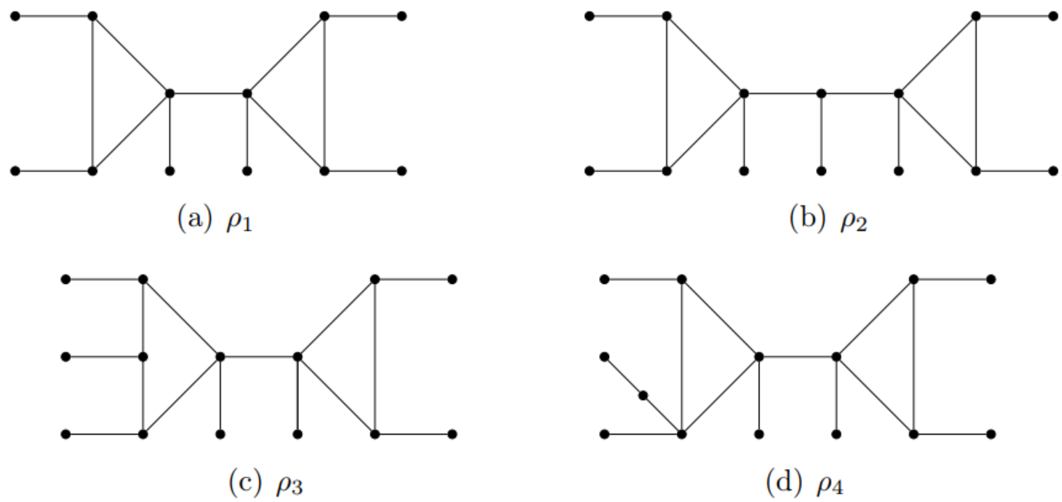


Figure 6: Bicyclic graphs discussed in Subcase 1.1 and have either 12 or 14 vertices.

(a) If $G \in \beta_{16}^{1}$, then from Table 1, $SDD(G) < \Psi(8) = 48.25$.

Table 1: Edge-degree partition for graphs in β_{16}^{1}.

Classes	e_{12}	e_{13}	e_{14}	e_{23}	e_{24}	e_{33}	e_{34}	e_{44}	SDD
I	0	6	2	0	0	3	6	0	47
II	0	6	2	0	0	4	4	1	46.83
III	1	4	3	0	1	1	6	1	47.58
IV	1	4	3	0	1	2	4	2	47.41

(b) If $G \in \beta_{18}^{1}$, then from Table 2, $SDD(G) \leq \Psi(9) = 53.75$ and the equality is attained by graphs in the class (XIII) from Table 2, whose edge-degree partition represents $D_1^1(18)$ that is, equality holds if $G \in D_1^1(18)$.

(c) **Table 2:** Edge-degree partition for graphs in β_{18}^{1}.

Classes	e_{12}	e_{13}	e_{14}	e_{23}	e_{24}	e_{33}	e_{34}	e_{44}	SDD
I	0	7	2	0	0	4	6	0	52.33
II	0	7	2	0	0	5	4	1	52.166
III	1	5	3	0	1	2	6	1	52.91
IV	1	5	3	0	1	3	4	2	52.75
V	1	5	3	0	1	1	8	0	53.08
VI	1	5	3	1	0	2	5	2	52.5
VII	1	5	3	1	0	1	7	1	52.66
VIII	2	3	4	0	2	1	4	3	53.33
IX	2	3	4	0	2	1	5	2	53.41
X	2	3	4	0	2	0	6	2	53.5
XI	2	3	4	0	2	2	2	4	53.166
XII	2	3	4	1	1	0	5	3	53.08
XIII	**3**	**1**	**5**	**0**	**3**	**0**	**2**	**5**	**53.75**

(d) If $G \in \beta_{20}^{1}$, then from Table 3, $SDD(G) \leq \Psi(10) = 59.5$, and equality is attained by graphs in the class (X) from Table 3, whose edge-degree partition represents $D_1^1(20)$, that is, equality holds if $G \in D_1^1(20)$.

Thus the results hold for $6 \leq n \leq 10$.

Table 3: Edge-degree partition for graphs in β_{20}^{1}.

Classes	e_{12}	e_{13}	e_{14}	e_{23}	e_{24}	e_{33}	e_{34}	e_{44}	SDD
I	0	8	2	0	0	5	6	0	57.66
II	0	8	2	0	0	6	4	1	57.5
III	1	6	3	0	1	2	8	0	58.41
IV	2	4	4	0	2	2	4	3	58.66
V	2	4	4	0	2	1	6	2	58.833
VI	1	6	3	0	1	3	6	1	58.25
VII	3	2	5	0	3	1	2	5	59.083
VIII	3	2	5	0	3	0	4	4	59.25
IX	1	6	3	0	1	4	4	2	58.08
X	**4**	**0**	**6**	**0**	**4**	**0**	**0**	**7**	**59.5**
XI	3	2	5	1	2	0	3	5	58.833
XII	2	4	4	2	0	0	6	3	58.166
XIII	1	6	3	1	0	3	5	2	57.833
XIV	2	4	4	1	1	1	5	3	58.41
XV	2	4	4	1	1	2	3	4	58.25
XVI	3	2	5	0	3	0	4	1	53.25
XVII	2	4	4	2	0	1	4	4	58
XVIII	2	4	4	1	1	0	7	2	58.58
XIX	1	6	3	1	0	2	7	1	58
XX	2	4	4	0	2	0	8	1	59
XXI	2	4	4	0	2	3	2	4	58.5
XXII	1	6	3	1	0	1	9	0	58.166

IV. For $n > 10$, we prove the theorem by induction by assuming that the result holds for $G \in \beta_{2m}^{1}$, for $10 < m < n$, where each non-pendant vertex of G has a pendant-neighbor.

Let M be the *perfect matching* of $G \in \beta_{2n}^{1}$ and let each non-pendant vertex of G have a pendant-neighbor. Suppose $x_1, \dots, x_n$ are the pendant vertices adjacent to the vertices $y_1, \dots, y_n$, respectively, where $d_G(y_i) \geq 2,\ 1 \leq i \leq n$. Then $\{x_i y_i : 1 \leq i \leq n\} \in M$.

We complete the proof of this case by considering two subcases.

SUBCASE (1.1)(IV).1: If G has at least one vertex $y \in \{y_1, \dots, y_n\}$ such that $d_G(y) = 2$.

Without loss of generality, let $y \coloneqq y_1$. Let x_1 be its neighboring pendant vertex, where $\{x_1y_1\} \in M$. In this subcase, suppose $y_2(\neq x_1)$ is the other neighbor of $y_1 \in G$, then $d_G(y_2) \geq 3$.

(A) Suppose $d_G(y_2) = 3$ with $N_G(y_2) = \{y_1, x_2, y_3\}$, where $d_G(y_3) \geq 3$.

If G has no vertex of degree four, then G will not be a bicyclic graph as each non-pendant vertex of G has a pendant neighbor, so we get a contradiction. Hence, there exists a vertex y_{k+2}, $k \geq 1$ of degree four in G, such that $y_2, \dots, y_{k+1}$ are vertices of degree three in G. Let $\Upsilon_1 = G + \{y_1y_{k+2}\} \setminus \{x_2, y_2, x_3, y_3, \dots, x_{k+1}, y_{k+1}\}$ and $M_1 = M \setminus \{x_2y_2, x_3y_3, \dots, x_{k+1}y_{k+1}\}$. Note that $\Upsilon_1 \in \beta^1_{2(n-k)}$ and M_1 is a *perfect matching* of Υ_1; see Figure 7. By induction hypothesis, we have

$$\begin{aligned} SDD(G) &= SDD(\Upsilon_1) + kS_{(1,3)} + (k-1)S_{(3,3)} + S_{(2,3)} + S_{(3,4)} - S_{(2,4)} \\ &\leq \Psi(n-k) + \frac{1}{12}(64k - 3). \end{aligned}$$

(a) If $n - k$ is even, then from Equation 4, we have

$$\begin{aligned} SDD(G) &\leq \frac{1}{8}\{45(n-k) + 26\} + \frac{1}{12}(64k - 3) \\ &= \Psi(n) - \frac{1}{24}(7k + 6) < \Psi(n) \end{aligned}$$

(b) If $n - k$ is odd, then from Equation 4, we have

$$\begin{aligned} SDD(G) &\leq \frac{1}{8}\{45(n-k) + 25\} + \frac{1}{12}(64k - 3) \\ &= \Psi(n) - \frac{1}{24}(7k + 6) < \Psi(n). \end{aligned}$$

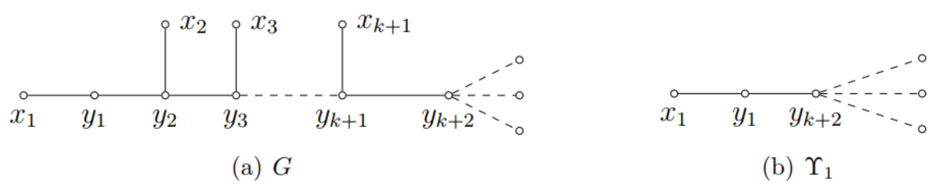


Figure 7: Illustration of induction in Case (A).

(B) When $d_G(y_2) = 4$: and let us denote the neighbors as $N_G(y_2) = \{y_1, x_2, y_3, y_n\}$, where $d_G(x_2) = 1$, $d_G(y_3), d_G(y_n) \geq 2$. Since $n > 10$, either y_3, or y_n has degree greater than or equal to three. Without loss of generality, let $d_G(y_3) \geq 3$. Now, we need to take conditions on $d_G(y_3)$, and $d_G(y_n)$.

(a) Suppose $d_G(y_n) = 2$ and $d_G(y_3) \geq 3$. Let $N_G(y_n) = \{x_n, y_2\}$ and let $\{y_2, x_3, y_4\}$ be the three neighbors of y_3, such that $d_G(y_4) \geq 3$. Note that, if G has no vertex of degree four other than $\{y_2\}$, then G can not be a bicyclic graph. Hence there exist a vertex of degree four in G, say y_{k+2} where $k \geq 1$ is the least. That is, either y_3 is degree 4 or the vertices $y_3, \dots, y_{k+1}$are having degree three.

Let $\gamma_2 := G + \{y_n y_{k+2}\} \backslash \{x_1, y_1, x_2, y_2, \dots, x_{k+1}, y_{k+1}\}$ and let $M_2 = M \backslash \{x_1 y_1, x_2 y_2, \dots, x_{k+1} y_{k+1}\}$. Note that $\gamma_2 \in \beta^1_{2(n-k-1)}$ and M_2 is a *perfect matching* of γ_2; see Figure 8. Hence, by induction hypothesis, we have

I. When $k = 1$, we have

$$SDD(G) = SDD(\gamma_2) + S_{(1,2)} + S_{(2,4)} + S_{(4,1)} + S_{(2,4)} + S_{(4,4)} - S_{(2,4)} \leq \Psi(n-2) + \frac{45}{4} \leq \Psi(n).$$

II. For $k > 1$, we have

$$\begin{aligned} SDD(G) &= SDD(\gamma_2) + S_{(1,2)} + S_{(2,4)} + S_{(1,4)} + S_{(3,4)} \\ &\quad + (k-1)S_{(1,3)} + (k-2)S_{(3,3)} + S_{(2,4)} + S_{(3,4)} - S_{(2,4)} \\ &\leq \Psi(n-k-1) + \frac{1}{12}(64k + 73) \\ &\leq \Psi(n) - \frac{1}{24}(7k - 11), \text{ (From Equation 4)} \\ &< \Psi(n). \end{aligned}$$

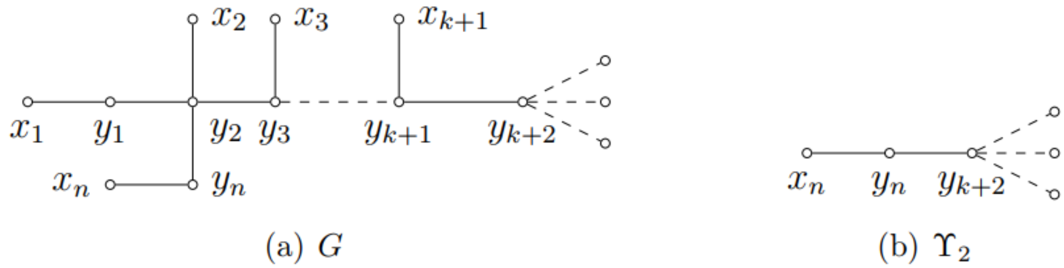


Figure 8: Illustration for the Case (B)(a).

(b) When $d_G(y_n) = d_G(y_3) = 3$. Denote the neighbors of y_n and y_3 by $N_G(y_n) = \{y_{n-1}, x_n, y_2\}$ and $N_G(y_3) = \{y_2, x_3, y_4\}$, respectively, where x_n, x_3 are pendant vertices and $d_G(y_{n-1}), d_G(y_4) \geq 2$.

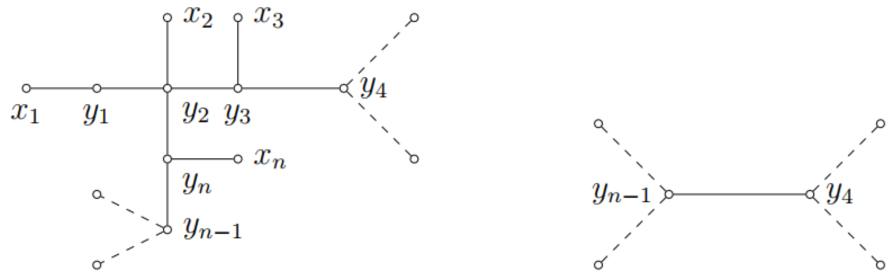
Let $\gamma_3 \coloneqq G + \{y_{n-1} y_4\} \backslash \{x_1, y_1, y_2, x_2, x_n, y_n, x_3, y_3\}$ and let $M_3 = M \backslash \{x_n y_n, x_1 y_1, x_2 y_2, x_3 y_3\}$. We have $\gamma_3 \in \beta^1_{2(n-4)}$, and M_3 is a *perfect matching* of γ_3; see Figure 9. Now by induction hypothesis, we have

$$\begin{aligned} SDD(G) &= SDD(\gamma_3) + S_{(1,2)} + S_{(2,4)} + S_{(1,4)} + 2S_{(3,4)} + 2S_{(1,3)} \\ &\quad + S_{(3,d_G(y_{n-1}))} + S_{(3,d_G(y_4))} - S_{(d_G(y_{n-1}),d_G(y_4))}. \end{aligned}$$

Since $d_G(y_{n-1}), d_G(y_4) \geq 2$ and $S_{(3,2)} > S_{(3,4)} > S_{(z,z)}$, where $z \geq 2$. Then, we have

$$SDD(G) \leq \Psi(n-4) + \frac{269}{12} \leq \Psi(n) - \frac{1}{12} < \Psi(n).$$

This follows from Equation 4.



(a) G (b) Υ_3

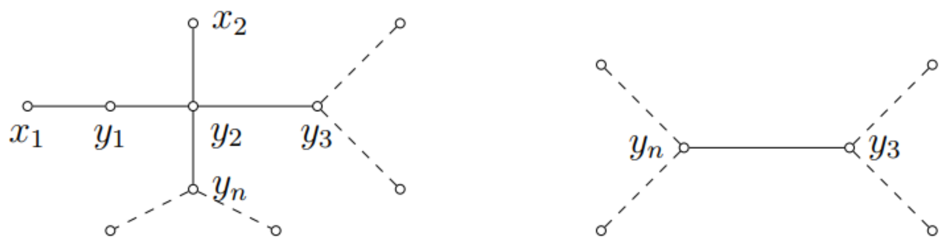
Figure 9: Illustration for the Case (B)(b).

(c) When $d_G(y_n) \geq 3$ and $d_G(y_3) = 4$. Let $\gamma_4 \coloneqq G + \{y_n y_3\} \backslash \{x_1, y_1, x_2, y_2\}$ and $M_4 = M \backslash \{x_1 y_1, x_2 y_2\}$. Note that $\gamma_4 \in \beta^1_{2(n-2)}$ and M_4 is a *perfect matching* of γ_4; see Figure 10. By induction hypothesis, we have

$$SDD(G) = SDD(\gamma_4) + S_{(1,2)} + S_{(2,4)} + S_{(1,4)} + S_{(3,4)} + S_{(4,4)} - S_{(3,4)}$$
$$\leq \Psi(n-2) + \frac{45}{4} \leq \Psi(n),$$

which follows from Equation 4.

Hence in that subcase result is true.



(a) G (b) Υ_4

Figure 10: Illustration for the Case (B)(c).

SUBCASE (1.1)(IV).2: If no pendant vertex has a degree two neighbor in $G \in \beta^1_{2n}$.

Since G is a bicyclic graph where each of its non-pendant vertex has a pendant neighbor, it follows immediately that G is isomorphic to one of the graphs in the subcollection Q^1_1, Q^1_2, as shown in Figures 5(a) and 5(b), that is $G \cong Q^1_1$ or $G \cong Q^1_2$.

By direct computation, we find that $SDD(Q^1_1) = \frac{1}{6}(32n + 25)$, and $SDD(Q^1_2) = \frac{1}{6}(32n + 26)$.

(a) If n is even, then from Equation 4, we have

$$\Psi(n) - SDD(Q^1_1) = \frac{1}{8}(45n + 26) - \frac{1}{6}(32n + 25)$$
$$= \frac{1}{24}(7n - 22) > 0, \text{ since } n \geq 6.$$

(b) If n is odd, then from Equation 4, we have

$$\Psi(n) - SDD(Q_2^1) = \frac{1}{8}(45n + 25) - \frac{1}{6}(32n + 25)$$
$$= \frac{1}{24}(7n - 25) > 0, \text{ since } n \geq 6.$$

This implies the result is true in this subcase.

SUBCASE (1.2) If $G \in \beta_{2n}^3$ and each non-pendant vertex of G has a pendant neighbor.

I. If $n = 6$, then graphs of β_{12}^3 have edge-degree partition as given in Table 4. From direct observation, we have $SDD(G) \leq \Psi(6) = 37$, and equality is attained by class (VI) in Table 4. Note that the graph in class (VI) represents D_1^3; that is, equality holds if $G \in D_1^3(12)$.

Table 4: Edge-degree partition for graphs in β_{12}^3.

Classes	e_{12}	e_{13}	e_{14}	e_{23}	e_{24}	e_{33}	e_{34}	e_{44}	SDD
I	0	4	2	0	0	1	6	0	36.33
II	0	4	2	0	0	2	4	1	36.166
III	1	2	3	0	1	0	4	2	36.75
IV	1	2	3	0	1	1	2	3	36.58
V	1	2	3	1	0	0	3	3	36.33
VI	**2**	**0**	**4**	**0**	**2**	**0**	**0**	**5**	**37**

II. If $n = 7$, then graphs of β_{14}^3 have edge-degree partition as given in Table 5. From Table 5, $SDD(G) \leq \Psi(7) = 42.5$, and equality is attained by the graphs in class (VIII) of Table 5, whose edge-degree partition represents $D_1^3(14)$; that is, equality holds if $G \in D_1^3(14)$. Thus the results hold for $n = 6$ and $n = 7$.

Table 5: Edge-degree partition for graphs in β_{14}^3.

Classes	e_{12}	e_{13}	e_{14}	e_{23}	e_{24}	e_{33}	e_{34}	e_{44}	SDD
I	0	5	2	0	0	2	6	0	41.66
II	0	5	2	0	0	3	4	1	41.5
III	1	3	3	0	1	0	6	1	42.25
IV	1	3	3	0	1	1	4	2	42.08
V	1	3	3	1	0	0	5	2	41.83
VI	1	3	3	1	0	1	3	3	41.66
VII	2	1	4	1	1	0	1	5	40.08
VIII	**2**	**1**	**4**	**0**	**2**	**0**	**2**	**4**	**42.5**

III. For $n \geq 8$, we prove by induction by assuming that the result holds for β_{2m}^3, $8 \leq m < n$, where each non-pendant vertex of $G \in \beta_{2m}^3$ has a pendant neighbor.

Let M be the *perfect matching* of $G \in \beta_{2n}^{3}$ where each non-pendant vertex of G has a pendant neighbor. Let $x_1, \dots, x_n$ be the pendant vertices adjacent to the vertices $y_1, \dots, y_n$, respectively, where $d_G(y_i) \geq 2$, $i = 1,2, \dots, n$. Note that $\{x_i y_i\} \in M$, for $i = 1,2, \dots, n$. Similar to Case (1.1)(iv), we consider the following two subcases to complete the proof.

(a) If $G \in \beta_{2n}^{3}$ has a vertex $y \in \{y_1, \dots, y_n\}$ such that $d_G(y) = 2$.
Proof of this subcase is similar to Subcase (1.1)(iv).1.

(b) If no pendant vertex has a degree two neighbor in $G \in \beta_{2n}^{3}$.
In this subcase, we find that G is isomorphic to one of the graphs in the subcollection Q_1^3, Q_2^3, that is, either $G \cong Q_1^3$ (see Figure. 5(c)) or $G \cong Q_2^3$ (see Figure. 5(d)). By direct computation, we have that

$$SDD(Q_1^3) = \frac{1}{6}(32n + 25), \text{ and } SDD(Q_2^3) = \frac{1}{6}(32n + 26),$$

i. If n is even, then from Equation 4, we have

$$\Psi(n) - SDD(Q_1^3) = \frac{1}{24}(7n - 22) > 0, \text{ since } n \geq 4.$$

ii. If n is odd, then from Equation 4, we have

$$\Psi(n) - SDD(Q_2^3) = \frac{1}{24}(7n - 26) > 0, \text{ since } n \geq 4.$$

Hence, if each non-pendant vertex of a bicyclic graph $G \in \beta_{2n}$ has a pendant neighbor, then $SDD(G) \leq \Psi(n)$.

Case (2) Suppose G has at most $n - 1$ pendant vertex, then G has at least one vertex not adjacent to a vertex of degree one.

From Lemma 2.2, it is immediate that the contribution of a vertex in the *SDD* index is maximum if that vertex has a pendant neighbor. Further, in Case (1), we have shown that $SDD(G) \leq \Psi(n)$, when each non-pendant vertex of a bicyclic graph G has a pendent neighbor, implying $SDD(G) \leq \Psi(n)$, if G has at the most $n - 1$ vertex.

Hence, to summarize, if $G \in \beta_{2n}^{1}$, then $SDD(G) \leq \Psi(n)$ and equality holds if and only if $G \in D_1^1(2n)$, $n \geq 9$. If $G \in \beta_{2n}^{2}$, then $SDD(G) < \Psi(n)$, and in that case, equality does not hold. Finally, if $G \in \beta_{2n}^{3}$, then $SDD(G) \leq \Psi(n)$ and equality holds if and only if $G \in D_1^3(2n)$, $n \geq 6$. ■

4. Conclusion

In this article, we have studied the first five minimum values of the *SDD* index attained by the bicyclic graphs having a perfect matching. One of our main contributions in this study is identifying the graphs that attain the stated bounds. Further, we have also computed an upper bound of the *SDD* index for bicyclic graphs with a maximum degree of four, which admits a perfect matching, and have shown that the given bound is tight.

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