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On Sum-Connectivity Index of Bicyclic Graphs

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Abstract. The sum-connectivity index is a new variant of the famous Randić connectivity index usable in quantitative structure-property relationship and quantitative structure-activity relationship studies. We determine the minimum sum-connectivity index of bicyclic graphs with n vertices and matching number m, where $2 \leq m \leq \lfloor n/2 \rfloor$, the minimum and the second minimum, as well as the maximum and the second maximum sum-connectivity indices of bicyclic graphs with $n \geq 5$ vertices. The extremal graphs are characterized.

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1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $d_G(u)$ denotes the degree of u in G. The Randić connectivity index (or product-connectivity index [8, 14]) of the graph G is defined as [11]

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) d_G(v)}} .$$

The Randić connectivity index is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies, e.g., [6, 10, 12]. Its mathematical properties as well as those of its generalizations have been studied extensively as summarized in the books [5, 7].

Various variants of Randić connectivity index have been proposed in the literature, see, e.g., [1, 3, 10, 12]. One new such variant is the sum-connectivity index. For the graph G, it is defined as [14]

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}} .$$

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The sum-connectivity index has been found to be well correlated with a variety of physicochemical properties and thus belongs among the molecular structure-descriptors [12] usable in quantitative structure-property relationship and quantitative structure-activity relationship studies [8, 9]. Some mathematical properties of the sum-connectivity index have been established in [4, 14]. Recall that a connected graph on n vertices is known as a tree, a unicyclic graph and a bicyclic graph if it possesses $n-1$, n and $n+1$ edges, respectively. We obtained in [4] the minimum sum-connectivity indices of trees and unicyclic graphs respectively with given number of vertices and matching number, and determined the corresponding extremal graphs.

Study on the Randić connectivity indices of bicyclic graphs may be found in [2, 7, 13, 15].

In this paper, we obtain the minimum sum-connectivity index in the set of bicyclic graphs with n vertices and matching number m, where $2 \leq m \leq \lfloor n/2 \rfloor$. We also determine the minimum and the second minimum, as well as the maximum and the second maximum sum-connectivity indices in the set of bicyclic graphs with $n \geq 5$ vertices. The extremal graphs are characterized.

2. Preliminaries

A matching M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. A matching M of G is said to be maximum, if for any other matching M' of G, $|M'| \leq |M|$. The matching number of G is the number of edges of a maximum matching in G.

If M is a matching of a graph G and vertex $v \in V(G)$ is incident with an edge of M, then v is said to be M-saturated, and if every vertex of G is M-saturated, then M is a perfect matching.

For $2 \leq m \leq \lfloor n/2 \rfloor$, let $\mathcal{B}(n,m)$ be the set of bicyclic graphs with n vertices and matching number m.

For $3 \leq m \leq \lfloor n/2 \rfloor$, let $B_{n,m}$ be the graph obtained by identifying a vertex of two triangles, and attaching $n-2m+1$ pendent vertices (vertices of degree one) and $m-3$ paths on two vertices to the common vertex of the two triangles, see Figure 1. Obviously, $B_{n,m} \in \mathcal{B}(n,m)$.

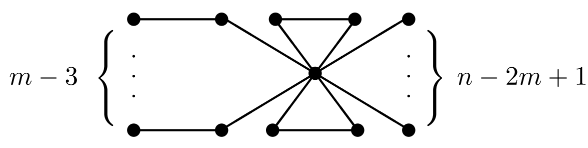

Figure 1. The graph $B_{n,m}$.

Let C_n be a cycle on $n \geq 3$ vertices. Let $\widetilde{\mathbb{B}}(n)$ be the set of bicyclic graphs on n vertices without pendent vertices, where $n \geq 4$. Let $\mathbf{B}_1^{(1)}(n)$ be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles C_a and C_b with $a+b=n$ by an edge, where $n \geq 6$. Let $\mathbf{B}_1^{(2)}(n)$ be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles C_a and C_b with $a+b<n$ by a path of length $n-a-b+1$, where $n \geq 7$. Let $\mathbf{B}_2(n)$ be the set of bicyclic graphs obtained by identifying a vertex of C_a and a vertex of C_b with $a+b=n+1$, where $n \geq 5$. Let $\mathbf{B}_3^{(1)}(n)$ be the set of bicyclic graphs obtained from C_n by adding an edge, where $n \geq 4$. Let $\mathbf{B}_3^{(2)}(n)$ be the set of bicyclic graphs obtained by joining two non-adjacent vertices of C_a with $4 \leq a \leq n-1$ by a path of length $n-a+1$, where $n \geq 5$. Obviously, $\widetilde{\mathbb{B}}(n) = \mathbf{B}_1^{(1)}(n) \cup \mathbf{B}_1^{(2)}(n) \cup \mathbf{B}_2(n) \cup \mathbf{B}_3^{(1)}(n) \cup \mathbf{B}_3^{(2)}(n)$.

Let $\mathbb{B}(n)$ be the set of bicyclic graphs on $n \geq 4$ vertices.

3. Minimum sum-connectivity index of bicyclic graphs with given matching number

First we give some lemmas that will be used.

For a graph G with $u \in V(G)$, $G-u$ denotes the graph resulting from G by deleting the vertex u (and its incident edges).

Lemma 3.1. [4] *Let G be a connected graph on n vertices with a pendent vertex u, where $n \geq 4$. Let v be the unique neighbor of u, and let w be a neighbor of v different from u.*

(i) *If $d_G(v) = 2$ and there is at most one pendent neighbor of w in G, then*

$$\chi(G) - \chi(G-u-v) \geq \frac{d_G(w)-1}{\sqrt{d_G(w)+2}} - \frac{d_G(w)-3}{\sqrt{d_G(w)+1}} - \frac{1}{\sqrt{d_G(w)}} + \frac{1}{\sqrt{3}}$$

with equality if and only if one neighbor of w has degree one, and the other neighbors of w are of degree two.

(ii) *If there are exactly k pendent neighbors of v in G, then*

$$\chi(G) - \chi(G-u) \geq \frac{d_G(v)-k}{\sqrt{d_G(v)+2}} + \frac{2k-d_G(v)}{\sqrt{d_G(v)+1}} - \frac{k-1}{\sqrt{d_G(v)}}$$

with equality if and only if k neighbors of v have degree one, and the other neighbors of v are of degree two.

Lemma 3.2. [4]

(i) *The function*

$$\frac{x-1}{\sqrt{x+2}} - \frac{x-3}{\sqrt{x+1}} - \frac{1}{\sqrt{x}}$$

is decreasing for $x \geq 2$.

(ii) *For integer $a \geq 1$, the function*

$$\frac{x-a}{\sqrt{x+2}} + \frac{2a-x}{\sqrt{x+1}} - \frac{a-1}{\sqrt{x}}$$

is decreasing for $x \geq a+1$.

Lemma 3.3. [4] *Let G be a connected graph with $uv \in E(G)$, where $d_G(u), d_G(v) \geq 2$, and u and v have no common neighbor in G. Let G_1 be the graph obtained from G by deleting the edge uv, identifying u and v, which is denoted by w, and attaching a pendent vertex to w. Then $\chi(G) > \chi(G_1)$.*

Lemma 3.4. *For $m \ge 3$,*

$$m + \frac{4}{\sqrt{6}} - \frac{3}{2} > \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1,$$

and for $m \ge 5$,

$$\left(\frac{1}{2} + \frac{1}{\sqrt{6}}\right) m - \frac{1}{2} - \frac{2}{\sqrt{6}} + \sqrt{2} > \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1.$$

Proof. Let

$$f(m) = \left(m + \frac{4}{\sqrt{6}} - \frac{3}{2}\right) - \left(\frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1\right)$$

for $m \ge 3$, and let

$$g(m) = \left[\left(\frac{1}{2} + \frac{1}{\sqrt{6}}\right) m - \frac{1}{2} - \frac{2}{\sqrt{6}} + \sqrt{2}\right] - \left(\frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1\right)$$

for $m \ge 5$. Note that $f''(m) = g''(m) = -\frac{3}{4}(m+3)^{-5/2} + (\frac{1}{4}m + \frac{13}{4})(m+4)^{-5/2} > 0$. Then $f'(m) \ge f'(3) > 0$, implying that $f(m) \ge f(3) > 0$, and $g'(m) \ge g'(5) > 0$, implying that $g(m) \ge g(5) > 0$. ∎

Lemma 3.5. *For $m \ge 3$,*

$$-\frac{m+1}{\sqrt{m+4}} + \frac{m-1}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} \ge -\frac{4}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}$$

with equality if and only if $m = 3$.

Proof. Let $f(m) = (m+2)^{-1/2} + m(m+3)^{-1/2}$ for $m \ge 3$. Then $f''(m) = \frac{3}{4}(m+2)^{-5/2} - (\frac{1}{4}m + 3)(m+3)^{-5/2} < 0$, implying that $f(m) - f(m+1)$ is increasing on m. It is easily seen that

$$\begin{aligned} -\frac{m+1}{\sqrt{m+4}} + \frac{m-1}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} &= f(m) - f(m+1) \\ &\ge f(3) - f(4) \\ &= -\frac{4}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}} \end{aligned}$$

with equality if and only if $m = 3$. ∎

Let H_6 be the graph obtained by attaching a pendent vertex to every vertex of a triangle. For $2 \le m \le \lfloor n/2 \rfloor$, let $U_{n,m}$ be the unicyclic graph obtained by attaching $n - 2m + 1$ pendent vertices and $m - 2$ paths on two vertices to one vertex of a triangle.

Lemma 3.6. [4] *Let G be a unicyclic graph with $2m$ vertices and perfect matching, where $m \ge 3$. Suppose that $G \ne H_6$. Then*

$$\chi(G) \ge \frac{m}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} + \frac{m-2}{\sqrt{3}} + \frac{1}{2}$$

with equality if and only if $G = U_{2m,m}$.

For an edge uv of the graph G (the complement of G, respectively), $G - uv$ ($G + uv$, respectively) denotes the graph resulting from G by deleting (adding, respectively) the edge uv.

Lemma 3.7. *Let $G \in \mathcal{B}(2m, m)$ and no pendent vertex has neighbor of degree two, where $m \geq 3$. Then*

$$\chi(G) \geq \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1$$

with equality if and only if $m = 3$ and $G = B_{6,3}$.

Proof. Let

$$f(m) = \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1.$$

Since $G \in \mathcal{B}(2m, m)$ and no pendent vertex has neighbor of degree two, G is obtainable by attaching some pendent vertices to a graph in $\widetilde{\mathbb{B}}(k)$, where $m \leq k \leq 2m$, and any two pendent vertices have no common neighbor (if $k = 2m$, then no pendent vertex is attached).

Case 1. There is no vertex of degree two in G. Then either $k = m$, G is obtainable by attaching a pendent vertex to every vertex of a graph in $\widetilde{\mathbb{B}}(m)$, or $k = m+1$, G is obtainable by attaching a pendent vertex to every vertex with degree two of a graph in $\mathbf{B}_1^{(1)}(m+1) \cup \mathbf{B}_3^{(1)}(m+1)$. By direct calculation, we find that

$$\chi(G) = \frac{5}{\sqrt{6}} + 1 > f(3)$$

for $m = 3$,

$$\chi(G) \geq \frac{1}{\sqrt{8}} + \frac{4}{\sqrt{7}} + \frac{2}{\sqrt{5}} + 1 > f(4)$$

for $m = 4$, and

$$\chi(G) \geq \left(\frac{1}{2} + \frac{1}{\sqrt{6}}\right) m - \frac{1}{2} - \frac{2}{\sqrt{6}} + \sqrt{2}$$

for $m \geq 5$. Thus by Lemma 3.4, we have $\chi(G) > f(m)$.

Case 2. There is a vertex, say u, of degree two in G. Denote by v and w the two neighbors of u in G. Then one of the two edges incident with u, say $uv \in M$, where M is a perfect matching of G. Suppose that there is no vertex of degree two in any cycle of G. Since no pendent vertex has neighbor of degree two in G, u lies on the path joining the two disjoint cycles of G. For $G_1 = G - uw + vw \in \mathcal{B}(2m, m)$, the number of vertices of degree two in G_1 is less than that in G and thus by Lemma 3.3, $\chi(G_1) < \chi(G)$. Repeating the operation from G to G_1, we finally get a graph $G^* \in \mathcal{B}(2m, m)$, which has no vertex of degree two, such that $\chi(G) > \chi(G^*)$, and thus the result follows from Case 1. Now suppose that u lies on some cycle of G. Consider $G' = G - uw$, which is a unicyclic graph with perfect matching. If $G' = H_6$, then G is obtained from H_6 by adding an edge either between two pendent vertices, and thus

$$\chi(G) = \frac{3}{\sqrt{6}} + \frac{2}{\sqrt{5}} + 1,$$

or between two neighbors of a vertex of degree three, one of which being a pendent vertex, and thus

$$\chi(G) = \frac{2}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{1}{2}.$$

In either case, $\chi(G) > f(3)$. Suppose that $G' \neq H_6$. Then by Lemma 3.6,

$$\chi(G') \geq \frac{m}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} + \frac{m-2}{\sqrt{3}} + \frac{1}{2}.$$

Note that $2 \leq d_G(v), d_G(w) \leq 5$ and w has at most one pendent neighbor. By Lemmas 3.2(i) and 3.5, we have

$$\begin{aligned}
\chi(G) &= \chi(G') + \frac{1}{\sqrt{d_G(w)+2}} + \left(\frac{1}{\sqrt{d_G(v)+2}} - \frac{1}{\sqrt{d_G(v)+1}}\right) \\
&\quad + \sum_{xw \in E(G')} \left(\frac{1}{\sqrt{d_G(w)+d_G(x)}} - \frac{1}{\sqrt{d_G(w)+d_G(x)-1}}\right) \\
&\geq \chi(G') + \frac{1}{\sqrt{d_G(w)+2}} + \left(\frac{1}{\sqrt{2+2}} - \frac{1}{\sqrt{2+1}}\right) \\
&\quad + \left[\frac{1}{\sqrt{d_G(w)+1}} - \frac{1}{\sqrt{d_G(w)+1-1}}\right. \\
&\quad \left. + (d_G(w)-2)\left(\frac{1}{\sqrt{d_G(w)+2}} - \frac{1}{\sqrt{d_G(w)+2-1}}\right)\right] \\
&= \chi(G') + \left(\frac{d_G(w)-1}{\sqrt{d_G(w)+2}} - \frac{d_G(w)-3}{\sqrt{d_G(w)+1}} - \frac{1}{\sqrt{d_G(w)}}\right) + \frac{1}{2} - \frac{1}{\sqrt{3}} \\
&\geq \left(\frac{m}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} + \frac{m-2}{\sqrt{3}} + \frac{1}{2}\right) \\
&\quad + \left(\frac{5-1}{\sqrt{5+2}} - \frac{5-3}{\sqrt{5+1}} - \frac{1}{\sqrt{5}}\right) + \frac{1}{2} - \frac{1}{\sqrt{3}} \\
&= \frac{m}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} + \frac{m-2}{\sqrt{3}} + 1 - \frac{1}{\sqrt{3}} + \left(\frac{4}{\sqrt{7}} - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{5}}\right) \\
&\geq \frac{m}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} + \frac{m-2}{\sqrt{3}} + 1 - \frac{1}{\sqrt{3}} \\
&\quad + \left(\frac{m+1}{\sqrt{m+4}} - \frac{m-1}{\sqrt{m+3}} - \frac{1}{\sqrt{m+2}}\right) \\
&= f(m)
\end{aligned}$$

with equalities if and only if $d_G(v) = 2$, $d_G(w) = 5$, $G' = U_{2m,m}$ and $m = 3$, i.e., $G = B_{6,3}$.

By combining Cases 1 and 2, the result follows. ∎

Lemma 3.8. *Let $G \in \mathcal{B}(6,3)$. Then*

$$\chi(G) \geq \frac{4}{\sqrt{7}} + \frac{1}{\sqrt{6}} + 1$$

with equality if and only if $G = B_{6,3}$.

Proof. If G has a pendent vertex whose neighbor is of degree two, then G is the graph obtained from the unique bicyclic graph on four vertices by attaching a path on two vertices to either a vertex of degree three, or a vertex of degree two, and thus it is easily seen that $\chi(G) > 4/\sqrt{7} + 1/\sqrt{6} + 1$. Otherwise, by Lemma 3.7, $B_{6,3}$ is the unique graph with the minimum sum-connectivity index. ∎

Now we consider the sum-connectivity index of bicyclic graphs with perfect matching. There is a unique bicyclic graph with four vertices, and its matching number is two.

Theorem 3.1. *Let $G \in \mathcal{B}(2m, m)$, where $m \geq 3$. Then*

$$\chi(G) \geq \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1$$

with equality if and only if $G = B_{2m,m}$.

Proof. Let

$$f(m) = \frac{m+1}{\sqrt{m+4}} + \frac{1}{\sqrt{m+3}} + \frac{m-3}{\sqrt{3}} + 1.$$

We prove the result by induction on m. If $m = 3$, then the result follows from Lemma 3.8.

Suppose that $m \geq 4$ and the result holds for graphs in $\mathcal{B}(2m-2, m-1)$. Let $G \in \mathcal{B}(2m, m)$ with a perfect matching M. If there is no pendent vertex with neighbor of degree two in G, then by Lemma 3.7, $\chi(G) > f(m)$. Suppose that G has a pendent vertex u whose neighbor v is of degree two. Then $uv \in M$ and $G - u - v \in \mathcal{B}(2m-2, m-1)$. Let w be the neighbor of v different from u. Since $|M| = m$, we have $d_G(w) \leq m+2$. Note that there is at most one pendent neighbor of w in G. Then by Lemma 3.1(i), Lemma 3.2(i) and the induction hypothesis,

$$\begin{aligned}
\chi(G) &\geq \chi(G-u-v) + \frac{d_G(w)-1}{\sqrt{d_G(w)+2}} - \frac{d_G(w)-3}{\sqrt{d_G(w)+1}} - \frac{1}{\sqrt{d_G(w)}} + \frac{1}{\sqrt{3}} \\
&\geq f(m-1) + \frac{(m+2)-1}{\sqrt{(m+2)+2}} - \frac{(m+2)-3}{\sqrt{(m+2)+1}} - \frac{1}{\sqrt{m+2}} + \frac{1}{\sqrt{3}} \\
&= f(m)
\end{aligned}$$

with equalities if and only if $G - u - v = B_{2m-2,m-1}$ and $d_G(w) = m+2$, i.e., $G = B_{2m,m}$. ∎

In the following we consider the sum-connectivity indices of graphs in the set of bicyclic graphs with n vertices and matching number m. We first consider the case $m \geq 3$.

Lemma 3.9. [15] *Let $G \in \mathcal{B}(n, m)$ with $n > 2m \geq 6$, and G has at least one pendent vertex. Then there is a maximum matching M and a pendent vertex u such that u is not M-saturated.*

Theorem 3.2. *Let $G \in \mathcal{B}(n, m)$, where $3 \leq m \leq \lfloor n/2 \rfloor$. Then*

$$\chi(G) \geq \frac{m+1}{\sqrt{n-m+4}} + \frac{n-2m+1}{\sqrt{n-m+3}} + \frac{m-3}{\sqrt{3}} + 1$$

with equality if and only if $G = B_{n,m}$.

Proof. Let

$$f(n,m) = \frac{m+1}{\sqrt{n-m+4}} + \frac{n-2m+1}{\sqrt{n-m+3}} + \frac{m-3}{\sqrt{3}} + 1.$$

We prove the result by induction on n. If $n = 2m$, then the result follows from Theorem 3.1. Suppose that $n > 2m$ and the result holds for graphs in $\mathcal{B}(n-1,m)$. Let $G \in \mathcal{B}(n,m)$.

Suppose that there is no pendent vertex in G. Then $G \in \widetilde{\mathbb{B}}(n)$ and $n = 2m+1$. It is easily seen that there are exactly three values for $\chi(G)$, and thus we have

$$\chi(G) \geq \chi(H) = m - 1 + \frac{4}{\sqrt{6}}$$

with $H \in \mathbf{B}_2(2m+1)$. Let

$$\begin{aligned} g(m) &= \left(m - 1 + \frac{4}{\sqrt{6}}\right) - f(2m+1,m) \\ &= \left(m - 1 + \frac{4}{\sqrt{6}}\right) - \left(\frac{m+1}{\sqrt{m+5}} + \frac{2}{\sqrt{m+4}} + \frac{m-3}{\sqrt{3}} + 1\right) \end{aligned}$$

for $m \geq 3$. Then

$$g''(m) = \left(\frac{1}{4}m + \frac{17}{4}\right)(m+5)^{-5/2} - \frac{3}{2}(m+4)^{-5/2} > 0,$$

and thus $g'(m) \geq g'(3) > 0$, implying that $g(m) \geq g(3) > 0$, i.e., $m - 1 + 4/\sqrt{6} > f(2m+1,m)$. Then $\chi(G) > f(2m+1,m)$.

Suppose that there is at least one pendent vertex in G. By Lemma 3.9, there is a maximum matching M and a pendent vertex u of G such that u is not M-saturated. Then $G-u \in \mathcal{B}(n-1,m)$. Let v be the unique neighbor of u. Since M is a maximum matching, M contains one edge incident with v. Note that there are $n+1-m$ edges of G outside M. Then $d_G(v) - 1 \leq n+1-m$, i.e., $d_G(v) \leq n-m+2$. Let s be the number of pendent neighbors of v in G. Since at least $s-1$ pendent neighbors of v are not M-saturated, we have $s-1 \leq n-2m$, i.e., $s \leq n-2m+1$. By Lemma 3.1(ii), Lemma 3.2(ii) and the induction hypothesis,

$$\begin{aligned} \chi(G) &\geq \chi(G-u) + \frac{d_G(v)-s}{\sqrt{d_G(v)+2}} + \frac{2s-d_G(v)}{\sqrt{d_G(v)+1}} - \frac{s-1}{\sqrt{d_G(v)}} \\ &\geq f(n-1,m) + \frac{(n-m+2)-(n-2m+1)}{\sqrt{(n-m+2)+2}} \\ &\quad + \frac{2(n-2m+1)-(n-m+2)}{\sqrt{(n-m+2)+1}} - \frac{(n-2m+1)-1}{\sqrt{n-m+2}} \\ &= f(n,m) \end{aligned}$$

with equalities if and only if $G-u = B_{n-1,m}$, $s = n-2m+1$ and $d_G(v) = n-m+2$, i.e., $G = B_{n,m}$. ∎

Now we consider the sum-connectivity indices of bicyclic graphs with matching number two. Let $B_n(a,b)$ be the graph obtained by attaching $a-3$ and $b-3$ pendent vertices to the two vertices of degree three of the unique bicyclic graph on four vertices, respectively, where $a \geq b \geq 3$, $a+b = n+2$ and $n \geq 4$.

Lemma 3.10. *Among the graphs in $\mathcal{B}(n,2)$ with $n \geq 6$, $B_n(n-1,3)$ and $B_n(n-2,4)$ are respectively the unique graphs with the minimum and the second minimum sum-connectivity indices, which are equal to*

$$\frac{1}{\sqrt{n+2}} + \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{n+1}} + \frac{2}{\sqrt{5}}$$

and

$$\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}},$$

respectively.

Proof. Let $G \in \mathcal{B}(n,2)$. Then G may be of three types:
(a) $G = B_n(a,b)$ with $a \geq b \geq 3$. Suppose that $a \geq b \geq 4$. Let $f(x) = (x-4)x^{-1/2} + 2(x+1)^{-1/2}$ for $x \geq 3$. Then $f''(x) = -((1/4)x+3)x^{-5/2} + (3/2)(x+1)^{-5/2} < 0$, implying that $f(x+1) - f(x)$ is decreasing for $x \geq 3$. It is easily seen that

$$\begin{aligned}
&\chi(B_n(a+1,b-1)) - \chi(B_n(a,b)) \\
&= [\chi(B_n(a+1,b-1)) - \chi(B_{n-1}(a,b-1))] \\
&\quad - [\chi(B_n(a,b)) - \chi(B_{n-1}(a,b-1))] \\
&= \left(\frac{a-4}{\sqrt{a+2}} - \frac{a-3}{\sqrt{a+1}} + \frac{2}{\sqrt{a+3}}\right) - \left(\frac{b-5}{\sqrt{b+1}} - \frac{b-4}{\sqrt{b}} + \frac{2}{\sqrt{b+2}}\right) \\
&= [f(a+2) - f(a+1)] - [f(b+1) - f(b)] < 0,
\end{aligned}$$

and thus, $\chi(B_n(a,b)) > \chi(B_n(a+1,b-1))$ for $a \geq b \geq 4$. It follows that $B_n(n-1,3)$ and $B_n(n-2,4)$ are respectively the unique graphs with the minimum and the second minimum sum-connectivity indices, which are equal to

$$\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n+1}} + \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{5}}$$

and

$$\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}},$$

respectively.
(b) G is the graph obtained by attaching $n-4$ pendent vertices to a vertex of degree two of the unique bicyclic graph on four vertices. Then

$$\begin{aligned}
\chi(G) &= \frac{2}{\sqrt{n+1}} + \frac{n-4}{\sqrt{n-1}} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{5}} \\
&> \chi(B_n(n-2,4)) = \frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}},
\end{aligned}$$

since

$$\chi(G) - \chi(B_n(n-2,4)) = [g(n-1) - g(n)] + \frac{1}{\sqrt{5}} - \frac{1}{\sqrt{6}} > 0,$$

where

$$g(x) = \frac{1}{\sqrt{x+2}} + \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+1}}$$

is decreasing for $x \geq 5$.

(c) G is the graph obtained by attaching some pendent vertices to one or two vertices of degree three of the unique bicyclic graph on five vertices in $\mathbf{B}_3^{(2)}(5)$, and by Lemma 3.3 and the arguments in case (a), $\chi(G) > \chi(B_n(n-2,4))$. Now the result follows easily. ∎

4. Minimum sum-connectivity index of bicyclic graphs

In this section, we determine the minimum and the second minimum sum-connectivity indices of bicyclic graphs with $n \geq 5$ vertices.

Theorem 4.1. *Among the graphs in $\mathbb{B}(n)$ with $n \geq 5$, $B_n(n-1,3)$ is the unique graph with the minimum sum-connectivity index, which is equal to*

$$\frac{1}{\sqrt{n+2}} + \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{n+1}} + \frac{2}{\sqrt{5}},$$

the graph obtained by attaching a pendent vertex to a vertex of degree two of the unique bicyclic graph on four vertices for $n = 5$ is the unique graph with the second minimum sum-connectivity index, which is equal to

$$\frac{3}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{1}{2},$$

$B_n(n-2,4)$ for $n = 6,7$ is the unique graph with the second minimum sum-connectivity index, which is equal to

$$\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}},$$

and $B_{n,3}$ for $n \geq 8$ is the unique graph with the second minimum sum-connectivity index, which is equal to

$$\frac{4}{\sqrt{n+1}} + \frac{n-5}{\sqrt{n}} + 1.$$

Proof. There are five graphs in $\mathbb{B}(5)$. Thus, the case $n = 5$ may be checked directly. Suppose in the following that $n \geq 6$.

Let $G \in \mathbb{B}(n)$ and m the matching number of G, where $2 \leq m \leq \lfloor n/2 \rfloor$. If $m = 2$, then by Lemma 3.10, $\chi(G) \geq \chi(B_n(n-1,3))$ with equality if and only if $G = B_n(n-1,3)$. If $m = 3$, then by Theorem 3.2, $\chi(G) \geq \chi(B_{n,3})$ with equality if and only if $G = B_{n,3}$. If $m \geq 4$, then by Theorem 3.2 and Lemma 3.3, $\chi(G) \geq \chi(B_{n,m}) > \chi(B_{n,m-1}) > \cdots > \chi(B_{n,3})$. Let

$$f(x) = \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+1}}$$

for $x \geq 6$. Then

$$f''(x) = \frac{3}{4}x^{-5/2} - \frac{3}{4}(x+1)^{-5/2} > 0,$$

implying that $f(x+1) - f(x)$ is increasing for $x \geq 6$. Note that

$$\begin{aligned} &\chi(B_{n,3}) - \chi(B_n(n-1,3)) \\ &= \left(\frac{4}{\sqrt{n+1}} + \frac{n-5}{\sqrt{n}} + 1\right) - \left(\frac{1}{\sqrt{n+2}} + \frac{n-4}{\sqrt{n}} + \frac{2}{\sqrt{n+1}} + \frac{2}{\sqrt{5}}\right) \end{aligned}$$

$$= f(n+1) - f(n) + 1 - \frac{2}{\sqrt{5}}$$
$$\geq f(7) - f(6) + 1 - \frac{2}{\sqrt{5}} > 0.$$

Thus $B_n(n-1,3)$ is the unique graph with the minimum sum-connectivity index.

Suppose that $G \neq B_n(n-1,3)$. If $m = 2$, then by Lemma 3.10, $\chi(G) \geq \chi(B_n(n-2,4))$ with equality if and only if $G = B_n(n-2,4)$. By the arguments as above, the second minimum sum-connectivity index of graphs in $\mathbb{B}(n)$ is precisely achieved by the minimum one of $\chi(B_{n,3})$ and $\chi(B_n(n-2,4))$. If $n = 6,7$, then $\chi(B_{n,3}) > \chi(B_n(n-2,4))$. Suppose that $n \geq 8$. Let

$$g(x) = \frac{1}{\sqrt{x+1}} - \frac{3}{\sqrt{x}} - \frac{x-5}{\sqrt{x-1}}$$

for $x \geq 8$. Then

$$g''(x) = \frac{3}{4}(x+1)^{-5/2} + \left[\left(\frac{1}{4}x + \frac{11}{4}\right)(x-1)^{-5/2} - \frac{9}{4}x^{-5/2}\right] > 0,$$

implying that $g(x) - g(x+1)$ is decreasing for $x \geq 8$. Note that

$$\begin{aligned}
&\chi(B_{n,3}) - \chi(B_n(n-2,4)) \\
&= \left(\frac{4}{\sqrt{n+1}} + \frac{n-5}{\sqrt{n}} + 1\right) - \left(\frac{1}{\sqrt{n+2}} + \frac{2}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}\right) \\
&= -\frac{1}{\sqrt{n+2}} + \frac{4}{\sqrt{n+1}} + \frac{n-7}{\sqrt{n}} - \frac{n-5}{\sqrt{n-1}} + 1 - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{5}} \\
&= g(n) - g(n+1) + 1 - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{5}} \\
&\leq g(8) - g(9) + 1 - \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{5}} < 0,
\end{aligned}$$

and then $\chi(B_{n,3}) < \chi(B_n(n-2,4))$. Thus $B_n(n-2,4)$ for $n = 6,7$ and $B_{n,3}$ for $n \geq 8$ are the unique graphs with the second minimum sum-connectivity index among graphs in $\mathbb{B}(n)$. ∎

5. Maximum sum-connectivity index of bicyclic graphs

In this section, we determine the maximum and the second maximum sum-connectivity indices of bicyclic graphs with $n \geq 5$ vertices. Let P_n be the path on n vertices.

Lemma 5.1. [14] *For a connected graph Q with at least two vertices and a vertex $u \in V(Q)$, let G_1 be the graph obtained from Q by attaching two paths P_a and P_b to u, G_2 the graph obtained from Q by attaching a path P_{a+b} to u, where $a \geq b \geq 1$. Then $\chi(G_1) < \chi(G_2)$.*

Lemma 5.2. *Suppose that M is a connected graph with $u \in V(M)$ and $2 \leq d_M(u) \leq 4$. Let H be the graph obtained from M by attaching a path P_a to u. Denote by u_1 and u_2 the two neighbors of u in M, and u' the pendent vertex of the path attached to u in H. Let $H' = H - uu_2 + u'u_2$.*

(i) *If $d_M(u) = 2$ and the maximum degree of M is at most five, then $\chi(H') > \chi(H)$.*

(ii) *If $d_M(u)=3$, and there are at least two neighbors of u in M with degree two and $d_M(u_2)=2$, then $\chi(H')>\chi(H)$.*

(iii) *If $d_M(u)=4$ and all the neighbors of u in M are of degree two, then $\chi(H')>\chi(H)$.*

Proof. (i) If $a=1$, then

$$\begin{aligned}
&\chi(H')-\chi(H)\\
&=\left(\frac{1}{\sqrt{d_M(u_1)+2}}+\frac{1}{\sqrt{d_M(u_2)+2}}\right)-\left(\frac{1}{\sqrt{d_M(u_1)+3}}+\frac{1}{\sqrt{d_M(u_2)+3}}\right)\\
&>0.
\end{aligned}$$

If $a\geq 2$, then

$$\begin{aligned}
&\chi(H')-\chi(H)\\
&=\left(\frac{1}{\sqrt{d_M(u_1)+2}}-\frac{1}{\sqrt{d_M(u_1)+3}}\right)+\left(\frac{1}{\sqrt{d_M(u_2)+2}}-\frac{1}{\sqrt{d_M(u_2)+3}}\right)\\
&\quad+1-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{5}}\\
&\geq\left(\frac{1}{\sqrt{5+2}}-\frac{1}{\sqrt{5+3}}\right)+\left(\frac{1}{\sqrt{5+2}}-\frac{1}{\sqrt{5+3}}\right)+1-\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{5}}>0.
\end{aligned}$$

(ii) There are two neighbors of u with degree two, let d_1 be the degree of the third neighbor of u in M. If $a=1$, then since $\frac{1}{2}+\frac{1}{\sqrt{5}}-\frac{2}{\sqrt{6}}>0$, we have

$$\begin{aligned}
&\chi(H')-\chi(H)\\
&=\left(\frac{1}{\sqrt{d_1+3}}+\frac{1}{2}+\frac{2}{\sqrt{5}}\right)-\left(\frac{1}{\sqrt{d_1+4}}+\frac{2}{\sqrt{6}}+\frac{1}{\sqrt{5}}\right)\\
&=\left(\frac{1}{\sqrt{d_1+3}}-\frac{1}{\sqrt{d_1+4}}\right)+\frac{1}{2}+\frac{1}{\sqrt{5}}-\frac{2}{\sqrt{6}}>0.
\end{aligned}$$

If $a\geq 2$, then since

$$1+\frac{2}{\sqrt{5}}-\frac{3}{\sqrt{6}}-\frac{1}{\sqrt{3}}>0,$$

we have

$$\begin{aligned}
&\chi(H')-\chi(H)\\
&=\left(\frac{1}{\sqrt{d_1+3}}+1+\frac{2}{\sqrt{5}}\right)-\left(\frac{1}{\sqrt{d_1+4}}+\frac{3}{\sqrt{6}}+\frac{1}{\sqrt{3}}\right)\\
&=\left(\frac{1}{\sqrt{d_1+3}}-\frac{1}{\sqrt{d_1+4}}\right)+1+\frac{2}{\sqrt{5}}-\frac{3}{\sqrt{6}}-\frac{1}{\sqrt{3}}>0.
\end{aligned}$$

(iii) If $a=1$, then

$$\chi(H')-\chi(H)=\left(\frac{1}{2}+\frac{4}{\sqrt{6}}\right)-\left(\frac{4}{\sqrt{7}}+\frac{1}{\sqrt{6}}\right)>0.$$

If $a \geq 2$, then

$$\chi(H') - \chi(H) = \left(1 + \frac{4}{\sqrt{6}}\right) - \left(\frac{5}{\sqrt{7}} + \frac{1}{\sqrt{3}}\right) > 0.$$

The proof is now completed. ∎

Let $\mathbb{B}_1(n)$ be the set of connected graphs on $n \geq 6$ vertices with exactly two vertex-disjoint cycles. Let $\mathbb{B}_2(n)$ be the set of connected graphs on $n \geq 5$ vertices with exactly two cycles of a common vertex. Let $\mathbb{B}_3(n)$ be the set of connected graphs on $n \geq 4$ vertices with exactly two cycles with at least one edge in common. Obviously, $\mathbb{B}(n) = \mathbb{B}_1(n) \cup \mathbb{B}_2(n) \cup \mathbb{B}_3(n)$. For $u, v \in V(G)$, let $d_G(u, v)$ be the distance between u and v in G.

Lemma 5.3. *Among the graphs in $\mathbb{B}_1(n)$ with $n \geq 7$, the graphs in $\mathbf{B}_1^{(1)}(n)$ and the graphs in $\mathbf{B}_1^{(2)}(n)$ are respectively the unique graphs with the maximum and the second maximum sum-connectivity indices, which are equal to*

$$\frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}}$$

and

$$\frac{n-5}{2} + \frac{6}{\sqrt{5}},$$

respectively.

Proof. Suppose that G is a graph in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with the maximum sum-connectivity index, and $C^{(1)}$ and $C^{(2)}$ are its two cycles. Let $x_1 \in V\left(C^{(1)}\right)$ and $y_1 \in V\left(C^{(2)}\right)$ be the two vertices such that $d_G(x_1, y_1) = \min\{d_G(x, y) : x \in V\left(C^{(1)}\right), y \in V\left(C^{(2)}\right)\}$. Let Q be the path joining x_1 and y_1. By Lemma 5.1, the vertices outside $C^{(1)}$, $C^{(2)}$ and Q are of degree one or two, the vertices on $C^{(1)}$, $C^{(2)}$ and Q different from x_1 and y_1 are of degree two or three, and $d_G(x_1), d_G(y_1) = 3$ or 4.

Suppose that $d_G(x_1, y_1) \geq 2$. If there is some vertex, say x, on $C^{(1)}$, $C^{(2)}$ or Q different from x_1 and y_1 with degree three, then making use of Lemma 5.2(i) to $H = G$ by setting $u = x$, we may get a graph in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with larger sum-connectivity index, a contradiction. Thus the vertices on $C^{(1)}$, $C^{(2)}$ and Q different from x_1 and y_1 are of degree two. If $d_G(x_1) = 4$, then making use of Lemma 5.2 (ii) to $H = G$ by setting $u = x_1$, we may get a graph in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with larger sum-connectivity index, a contradiction. Thus $d_G(x_1) = 3$. Similarly, we have $d_G(y_1) = 3$. It follows that $G \in \mathbf{B}_1^{(2)}(n)$.

Suppose that $d_G(x_1, y_1) = 1$. Suppose that one of x_1 and y_1, say x_1, is of degree four. Then by Lemma 5.2(i), the vertices on $C^{(1)}$ and $C^{(2)}$ different from x_1 and y_1 are of degree two. If $d_G(y_1) = 4$, then making use of Lemma 5.2(ii) to $H = G$ by setting $u = y_1$, we may get a graph in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with larger sum-connectivity index, a contradiction. Thus $d_G(y_1) = 3$. Denote by x_2 the pendent vertex of the path attached to x_1. Consider $G_1 = G - x_1y_1 + x_2y_1 \in \mathbf{B}_1^{(2)}(n)$. If $d_G(x_1, x_2) = 1$, then

$$\chi(G_1) - \chi(G) = \frac{4}{\sqrt{5}} - \left(\frac{1}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{5}}\right) > 0.$$

If $d_G(x_1, x_2) \geq 2$, then

$$\chi(G_1) - \chi(G) = \left(\frac{1}{2} + \frac{4}{\sqrt{5}}\right) - \left(\frac{1}{\sqrt{7}} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{3}}\right) > 0.$$

In either case, $\chi(G_1) > \chi(G)$ with $G_1 \in \mathbf{B}_1^{(2)}(n)$, a contradiction. Thus $d_G(x_1) = d_G(y_1) = 3$. Note that $G \notin \mathbf{B}_1^{(1)}(n)$ and by Lemma 5.2(i), there is exactly one vertex, say $x_3 \in V\left(C^{(1)}\right)$, on $C^{(1)}$ and $C^{(2)}$ different from x_1 and y_1 with degree three. Denote by x_4 the pendent vertex of the path attached to x_3. Consider $G_2 = G - x_1y_1 + x_4y_1 \in \mathbf{B}_1^{(2)}(n)$. Let d_1 be the degree of the neighbor of x_4, one neighbor of x_1 on $C^{(1)}$ is of degree two, and we denote by d_2 the degree of the other neighbor of x_1 on $C^{(1)}$, where $d_1, d_2 = 2$ or 3. We have

$$\begin{aligned}
&\chi(G_2) - \chi(G) \\
&= \left(\frac{1}{\sqrt{d_1+2}} - \frac{1}{\sqrt{d_1+1}}\right) + \left(\frac{1}{\sqrt{d_2+2}} - \frac{1}{\sqrt{d_2+3}}\right) + \frac{1}{2} - \frac{1}{\sqrt{6}} \\
&\geq \left(\frac{1}{\sqrt{2+2}} - \frac{1}{\sqrt{2+1}}\right) + \left(\frac{1}{\sqrt{3+2}} - \frac{1}{\sqrt{3+3}}\right) + \frac{1}{2} - \frac{1}{\sqrt{6}} > 0,
\end{aligned}$$

and thus, $\chi(G_2) > \chi(G)$ with $G_2 \in \mathbf{B}_1^{(2)}(n)$, which is also a contradiction.

Now we have shown that the graphs in $\mathbf{B}_1^{(2)}(n)$ are the unique graphs in $\mathbb{B}_1(n) \setminus \left\{\mathbf{B}_1^{(1)}(n)\right\}$ with the maximum sum-connectivity index. Note that for $H_1 \in \mathbf{B}_1^{(1)}(n)$ and $H_2 \in \mathbf{B}_1^{(2)}(n)$,

$$\chi(H_1) = \frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}} > \chi(H_2) = \frac{n-5}{2} + \frac{6}{\sqrt{5}}.$$

The result follows. ∎

Lemma 5.4. *Among the graphs in $\mathbb{B}_3(n)$ with $n \geq 5$, the graphs in $\mathbf{B}_3^{(1)}(n)$ and the graphs in $\mathbf{B}_3^{(2)}(n)$ are respectively the unique graphs with the maximum and the second maximum sum-connectivity indices, which are equal to*

$$\frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}}$$

and

$$\frac{n-5}{2} + \frac{6}{\sqrt{5}},$$

respectively.

Proof. Suppose that G is a graph in $\mathbb{B}_3(n) \setminus \left\{\mathbf{B}_3^{(1)}(n)\right\}$ with the maximum sum-connectivity index. Then G has exactly three cycles, let $C^{(1)}$ and $C^{(2)}$ be its two cycles such that the remaining one is of the maximum length. Let A be the set of the common vertices of $C^{(1)}$ and $C^{(2)}$. Let v_1 and v_2 be the two vertices in A such that $d_G(v_1, v_2) = \max\{d_G(x, y) : x, y \in A\}$. By Lemma 5.1, the vertices outside $C^{(1)}$ and $C^{(2)}$ are of degree one or two, the vertices on $C^{(1)}$ and $C^{(2)}$ different from v_1 and v_2 are of degree two or three, and $d_G(v_1), d_G(v_2) = 3$ or 4. Denote by v_1' (v_2', respectively) the neighbor of v_1 on $C^{(1)}$ (v_2 on $C^{(2)}$, respectively) different from the vertices in A.

If $d_G(v_1, v_2) \geq 2$, then by Lemma 5.2(i)(ii), we have $G \in \mathbf{B}_3^{(2)}(n)$.

Suppose that $d_G(v_1, v_2) = 1$. Suppose that the lengths of $C^{(1)}$ and $C^{(2)}$ are at least four. Consider $G_1 = G - \{v_1v_1', v_2v_2'\} + \{v_1'v_2, v_1v_2'\} \in \mathbb{B}_1(n) \setminus \{\mathbf{B}_1^{(1)}(n), \mathbf{B}_1^{(2)}(n)\}$. Note that

$$\begin{aligned}\chi(G_1) - \chi(G) = &\left(\frac{1}{\sqrt{d_G(v_1') + d_G(v_2)}} + \frac{1}{\sqrt{d_G(v_1) + d_G(v_2')}}\right) \\ &- \left(\frac{1}{\sqrt{d_G(v_1) + d_G(v_1')}} + \frac{1}{\sqrt{d_G(v_2) + d_G(v_2')}}\right).\end{aligned}$$

If $d_G(v_1) = d_G(v_2)$, then $\chi(G_1) = \chi(G)$. If $d_G(v_1) \neq d_G(v_2)$, then by Lemma 5.2 (i), we have $d_G(v_1') = d_G(v_2') = 2$, and thus $\chi(G_1) = \chi(G)$. In either case, we have $\chi(G_1) = \chi(G)$. By Lemma 5.3, we have $\chi(G) = \chi(G_1) < \chi(H) = (n-5)/2 + 6/\sqrt{5}$ for $H \in \mathbf{B}_1^{(2)}(n)$.

Suppose that at least one of $C^{(1)}$ and $C^{(2)}$, say $C^{(1)}$, is of length three. Since $G \notin \mathbf{B}_3^{(1)}(n)$, there are some vertices outside $C^{(1)}$ and $C^{(2)}$. By Lemma 5.2(i)(ii), the subgraph induced by the vertices outside $C^{(1)}$ and $C^{(2)}$ is a path, say P_k, which is attached to $x \in V\left(C^{(1)}\right) \cup V\left(C^{(2)}\right)$. Suppose that $x \neq v_1'$. Denote by v_3 the neighbor of x outside $C^{(1)}$ and $C^{(2)}$. Consider $G_2 = G - xv_3 + v_1'v_3 \in \mathbb{B}_3(n) \setminus \left\{\mathbf{B}_3^{(1)}(n)\right\}$. If $x = v_1$ or v_2, then

$$\chi(G_2) - \chi(G) = \left(\frac{1}{\sqrt{d_G(v_3) + 3}} - \frac{1}{\sqrt{d_G(v_3) + 4}}\right) + \left(\frac{1}{\sqrt{6}} - \frac{1}{\sqrt{7}}\right) > 0,$$

and thus $\chi(G_2) > \chi(G)$, a contradiction. Hence $x \in V\left(C^{(2)}\right) \setminus \{v_1, v_2\}$, and the length of $C^{(2)}$ is at least four. Note that one neighbor of x on $C^{(2)}$ is of degree two. Denote by d_1 the degree of the other neighbor of x on $C^{(2)}$, where $d_1 = 2$ or 3. Then

$$\begin{aligned}\chi(G_2) - \chi(G) &= \left(\frac{1}{\sqrt{d_1 + 2}} - \frac{1}{\sqrt{d_1 + 3}}\right) + \frac{1}{2} + \frac{2}{\sqrt{6}} - \frac{3}{\sqrt{5}} \\ &\geq \left(\frac{1}{\sqrt{3 + 2}} - \frac{1}{\sqrt{3 + 3}}\right) + \frac{1}{2} + \frac{2}{\sqrt{6}} - \frac{3}{\sqrt{5}} > 0,\end{aligned}$$

and thus $\chi(G_2) > \chi(G)$, which is also a contradiction. Thus, $x = v_1'$. If $k = 1$, then

$$\chi(G) = \frac{n-5}{2} + \frac{3}{\sqrt{6}} + \frac{2}{\sqrt{5}} + \frac{1}{2},$$

and if $k \geq 2$, then

$$\chi(G) = \frac{n-6}{2} + \frac{3}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \frac{1}{\sqrt{3}}.$$

In either case, we have

$$\chi(G) < \frac{n-5}{2} + \frac{6}{\sqrt{5}}.$$

Now we have shown that the graphs in $\mathbf{B}_3^{(2)}(n)$ are the unique graphs in $\mathbb{B}_3(n) \setminus \left\{\mathbf{B}_3^{(1)}(n)\right\}$ with the maximum sum-connectivity index. Note that for $H_1 \in \mathbf{B}_3^{(1)}(n)$

and $H_2 \in \mathbf{B}_3^{(2)}(n)$,

$$\chi(H_1) = \frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}} > \chi(H_2) = \frac{n-5}{2} + \frac{6}{\sqrt{5}}.$$

The result follows. ∎

Theorem 5.1. *Among the graphs in $\mathbb{B}(n)$ with $n \geq 5$, the graph in $\mathbf{B}_3^{(1)}(5)$ and the graph in $\mathbf{B}_3^{(2)}(5)$ for $n = 5$ are respectively the unique graphs with the maximum and the second maximum sum-connectivity indices, the graphs in $\mathbf{B}_1^{(1)}(6) \cup \mathbf{B}_3^{(1)}(6)$ and the graph in $\mathbf{B}_3^{(2)}(6)$ for $n = 6$ are respectively the unique graphs with the maximum and the second maximum sum-connectivity indices, the graphs in $\mathbf{B}_1^{(1)}(n) \cup \mathbf{B}_3^{(1)}(n)$ and the graphs in $\mathbf{B}_1^{(2)}(n) \cup \mathbf{B}_3^{(2)}(n)$ for $n \geq 7$ are respectively the unique graphs with the maximum and the second maximum sum-connectivity indices, where*

$$\chi(G) = \frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}}$$

for $G \in \mathbf{B}_1^{(1)}(n) \cup \mathbf{B}_3^{(1)}(n)$ and

$$\chi(H) = \frac{n-5}{2} + \frac{6}{\sqrt{5}}$$

for $H \in \mathbf{B}_1^{(2)}(n) \cup \mathbf{B}_3^{(2)}(n)$.

Proof. Suppose that G is a graph in $\mathbb{B}_2(n)$ with the maximum sum-connectivity index, and $C^{(1)}$ and $C^{(2)}$ are its two cycles. Let u be the unique common vertex of $C^{(1)}$ and $C^{(2)}$. By Lemma 5.1, the vertices outside $C^{(1)}$ and $C^{(2)}$ are of degree one or two, the vertices on $C^{(1)}$ and $C^{(2)}$ different from u are of degree two or three, and $d_G(u) = 4$ or 5. Moreover, by Lemma 5.2(i), the vertices on $C^{(1)}$ and $C^{(2)}$ different from u are of degree two. If $d_G(u) = 5$, then making use of Lemma 5.2(iii) to $H = G$, we may get a graph in $\mathbb{B}_2(n)$ with larger sum-connectivity index, a contradiction. Thus $d_G(u) = 4$, i.e., $G \in \mathbf{B}_2(n)$.

Note that for $H_1 \in \mathbf{B}_1^{(1)}(n)$, $H_1' \in \mathbf{B}_1^{(2)}(n)$, $H_2 \in \mathbf{B}_2(n)$, $H_3 \in \mathbf{B}_3^{(1)}(n)$ and $H_3' \in \mathbf{B}_3^{(2)}(n)$,

$$\begin{aligned}
\chi(H_1) = \chi(H_3) &= \frac{n-4}{2} + \frac{1}{\sqrt{6}} + \frac{4}{\sqrt{5}} \\
> \chi(H_1') = \chi(H_3') &= \frac{n-5}{2} + \frac{6}{\sqrt{5}} \\
> \chi(H_2) &= \frac{n-3}{2} + \frac{4}{\sqrt{6}}.
\end{aligned}$$

Then the result follows from Lemmas 5.3 and 5.4. ∎

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