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ORIGINAL PAPER

Minimum sum-connectivity indices of trees and unicyclic graphs of a given matching number

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Abstract The sum-connectivity index is a newly proposed molecular descriptor defined as the sum of the weights of the edges of the graph, where the weight of an edge uv of the graph, incident to vertices u and v, having degrees d_u and d_v is $(d_u + d_v)^{-1/2}$. We obtain the minimum sum-connectivity indices of trees and unicyclic graphs with given number of vertices and matching number, respectively, and determine the corresponding extremal graphs. Additionally, we deduce the n-vertex unicyclic graphs with the first and second minimum sum-connectivity indices for $n \geq 4$.

Keywords Randić connectivity index · Sum-connectivity index · Product-connectivity index · Trees · Unicyclic graphs · Matching number

1 Introduction

The Randić connectivity index [1] is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies [e.g. 2–7]. Mathematical properties of this descriptor have also been studied extensively as summarized in [8,9].

Let G be a simple graph with vertex-set $V(G)$ and edge-set $E(G)$ [10]. For $v \in V(G)$, $\Gamma(v)$ denotes the set of its (first) neighbors in G and the degree of v is

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$d_v = d_G(v) = |\Gamma(v)|$. The Randić connectivity index [1] $R = R(G)$ of the graph G is defined as

$$R = R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2}.$$

We also call this index as the product-connectivity index of G.

Recently, another connectivity index—the sum-connectivity index was proposed in [11]. The sum-connectivity index of the graph G is defined as

$$\chi = \chi(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-1/2}.$$

The sum-connectivity index and the Randić (product-)connectivity index are highly intercorrelated quantities. For example, the correlation coefficient between the sum- and product-connectivity indices for the set of 134 trees representing the lower alkanes is 0.99088 and for the set of 30 polycyclic graphs representing lower benzenoid hydrocarbons is 0.9992.

We also used both the sum-connectivity index and the product-connectivity index to approximate rather accurately the π-electron energy (E_π) of benzenoid hyrocarbons [12], the correlation coefficients between $\chi(G)$ and E_π, and $R(G)$ and E_π being 0.9999 and 0.9992, respectively. These results prompted us to study the mathematical properties of this novel variant of the connectivity index. We determined in [11] the unique tree of fixed numbers of vertices and pendant vertices (vertices of degree one) with the minimum value of the sum-connectivity index, and the n-vertex trees with the minimum, second minimum and third minimum, and the maximum, second maximum and third maximum values of the sum-connectivity index for $n \geq 7$, and discussed its properties for a class of trees representing acyclic hydrocarbons. We also determined in [13] the trees and unicyclic graphs of fixed number of vertices and maximum degree with the maximum values of the sum-connectivity index, and deduced the n-vertex unicyclic graphs with the maximum and second maximum values of sum-connectivity index for $n \geq 4$.

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_1 of G, $|M_1| \leq |M|$. 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 integers n and m with $1 \leq m \leq \left\lfloor \frac{n}{2} \right\rfloor$, let $\mathbf{T}(n, m)$ be the set of trees with n vertices and matching number m, and let $\mathbf{U}(n, m)$ be the set of unicyclic graphs with n vertices and matching number m. Obviously, $\mathbf{T}(n, 1) = \{S_n\}$ and $\mathbf{U}(n, 1) = \{C_3\}$. In the following, we assume that $2 \leq m \leq \left\lfloor \frac{n}{2} \right\rfloor$.

Recall that the minimum product-connectivity indices in $\mathbf{T}(n, m)$ and $\mathbf{U}(n, m)$ were respectively determined in [14] and [15]. In this paper, we obtain the minimum sum-connectivity indices in $\mathbf{T}(n, m)$ and $\mathbf{U}(n, m)$, respectively, and determine the corresponding extremal graphs. Additionally, we deduce the n-vertex unicyclic graphs with the first and second minimum sum-connectivity indices for $n \geq 4$.

2 Preliminaries

We first establish a few lemmas that will be used.

Lemma 2.1 *Let G be an n-vertex connected graph with a pendant 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 there are at most k pendant 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.

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

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

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

Proof (i) Denote by $v_0 = u, v_1, \ldots, v_{s-1}$ the neighbors of v in G, where $s = d_G(v)$. Assume that $d_G(v_1) = \cdots = d_G(v_r) = 1$, and $d_G(v_{r+1}), \ldots, d_G(v_{s-1}) \geq 2$, where $0 \leq r \leq k-1$. Note that $\frac{2}{\sqrt{s+1}} - \frac{1}{\sqrt{s}} - \frac{1}{\sqrt{s+2}} < 0$. Then

$$\begin{aligned}
\chi(G) &= \chi(G-u) + \frac{1}{\sqrt{s+1}} + r\left(\frac{1}{\sqrt{s+1}} - \frac{1}{\sqrt{s}}\right) \\
&\quad + \sum_{i=r+1}^{s-1}\left(\frac{1}{\sqrt{d_G(v_i)+s}} - \frac{1}{\sqrt{d_G(v_i)+s-1}}\right) \\
&\geq \chi(G-u) + \frac{1}{\sqrt{s+1}} + r\left(\frac{1}{\sqrt{s+1}} - \frac{1}{\sqrt{s}}\right) \\
&\quad +(s-1-r)\left(\frac{1}{\sqrt{2+s}} - \frac{1}{\sqrt{2+s-1}}\right) \\
&= \chi(G-u) + r\left(\frac{2}{\sqrt{s+1}} - \frac{1}{\sqrt{s}} - \frac{1}{\sqrt{s+2}}\right) \\
&\quad + \frac{s-1}{\sqrt{s+2}} - \frac{s-2}{\sqrt{s+1}} \\
&\geq \chi(G-u) + (k-1)\left(\frac{2}{\sqrt{s+1}} - \frac{1}{\sqrt{s}} - \frac{1}{\sqrt{s+2}}\right)
\end{aligned}$$

$$+\frac{s-1}{\sqrt{s+2}}-\frac{s-2}{\sqrt{s+1}}$$
$$=\chi(G-u)+\frac{s-k}{\sqrt{s+2}}+\frac{2k-s}{\sqrt{s+1}}-\frac{k-1}{\sqrt{s}}$$

with equalities if and only if $d_G(v_1)=\cdots=d_G(v_{k-1})=1$, and $d_G(v_k)=\cdots=d_G(v_{s-1})=2$.

(ii) Denote by $w_0=v, w_1,\ldots,w_{t-1}$ the neighbors of w in G, where $t=d_G(w)$. Assume that $d_G(w_{r+1}),\ldots,d_G(w_{t-1})\geq 2$, where $r=0$ or 1, and $d_G(w_1)=1$ if $r=1$. Note that $\frac{2}{\sqrt{t+1}}-\frac{1}{\sqrt{t}}-\frac{1}{\sqrt{t+2}}<0$. Then

$$\begin{aligned}\chi(G)&=\chi(G-u-v)+\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{t+2}}+r\left(\frac{1}{\sqrt{t+1}}-\frac{1}{\sqrt{t}}\right)\\&\quad+\sum_{i=r+1}^{t-1}\left(\frac{1}{\sqrt{d_G(w_i)+t}}-\frac{1}{\sqrt{d_G(w_i)+t-1}}\right)\\&\geq\chi(G-u-v)+\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{t+2}}+r\left(\frac{1}{\sqrt{t+1}}-\frac{1}{\sqrt{t}}\right)\\&\quad+(t-1-r)\left(\frac{1}{\sqrt{2+t}}-\frac{1}{\sqrt{2+t-1}}\right)\\&=\chi(G-u-v)+\frac{1}{\sqrt{3}}+r\left(\frac{2}{\sqrt{t+1}}-\frac{1}{\sqrt{t}}-\frac{1}{\sqrt{t+2}}\right)\\&\quad+\frac{t}{\sqrt{t+2}}-\frac{t-1}{\sqrt{t+1}}\\&\geq\chi(G-u-v)+\frac{1}{\sqrt{3}}+\left(\frac{2}{\sqrt{t+1}}-\frac{1}{\sqrt{t}}-\frac{1}{\sqrt{t+2}}\right)\\&\quad+\frac{t}{\sqrt{t+2}}-\frac{t-1}{\sqrt{t+1}}\\&=\chi(G-u-v)+\frac{1}{\sqrt{3}}+\frac{t-1}{\sqrt{t+2}}-\frac{t-3}{\sqrt{t+1}}-\frac{1}{\sqrt{t}}\end{aligned}$$

with equalities if and only if $d_G(w_1)=1$, and $d_G(w_2)=\cdots=d_G(w_{t-1})=2$. □

Lemma 2.2 *(i) For integer $a\geq 1$, the function $f(x)=\frac{x-a}{\sqrt{x+2}}+\frac{2a-x}{\sqrt{x+1}}-\frac{a-1}{\sqrt{x}}$ is decreasing for $x\geq a+1$.*
(ii) The function $g(x)=\frac{x-1}{\sqrt{x+2}}-\frac{x-3}{\sqrt{x+1}}-\frac{1}{\sqrt{x}}$ is decreasing for $x\geq 2$.

Proof (i) Let $f_1(x)=\frac{x-1-a}{\sqrt{x+1}}+\frac{a-1}{\sqrt{x}}$. Then $f(x)=f_1(x+1)-f_1(x)$. For $x\geq a+1\geq 2$, it is easily seen that

$$f_1''(x)=-\left(\frac{1}{4}x+\frac{7}{4}+\frac{3}{4}a\right)(x+1)^{-5/2}+\frac{3}{4}(a-1)x^{-5/2}$$

$$= \frac{3}{4}\left[x^{-5/2} - (x+1)^{-5/2}\right]a - \left(\frac{1}{4}x + \frac{7}{4}\right)(x+1)^{-5/2} - \frac{3}{4}x^{-5/2}$$
$$\leq \frac{3}{4}\left[x^{-5/2} - (x+1)^{-5/2}\right](x-1) - \left(\frac{1}{4}x + \frac{7}{4}\right)(x+1)^{-5/2} - \frac{3}{4}x^{-5/2}$$
$$= \frac{3}{4}(x-2)x^{-5/2} - (x+1)^{-3/2} < 0,$$

implying that $f'(x) = f_1'(x+1) - f_1'(x) < 0$. The result follows.

(ii) Let $g_1(x) = \frac{x-2}{\sqrt{x+1}} + \frac{1}{\sqrt{x}}$. Then $g(x) = g_1(x+1) - g_1(x)$. For $x \geq 2$, it is easily seen that $g_1''(x) = -\left(\frac{1}{4}x + \frac{5}{2}\right)(x+1)^{-5/2} + \frac{3}{4}x^{-5/2} < 0$, implying that $g'(x) = g_1'(x+1) - g_1'(x) < 0$. The result follows. □

Lemma 2.3 *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 pendant vertex to w. Then $\chi(G) > \chi(G_1)$.*

Proof Let $d_x = d_G(x)$ for $x \in V(G)$. It is easily seen that

$$\chi(G) - \chi(G_1) = \sum_{xu \in E(G)\setminus\{uv\}} \left(\frac{1}{\sqrt{d_x + d_u}} - \frac{1}{\sqrt{d_x + d_u + d_v - 1}}\right) + \sum_{xv \in E(G)\setminus\{uv\}} \left(\frac{1}{\sqrt{d_x + d_v}} - \frac{1}{\sqrt{d_x + d_u + d_v - 1}}\right) > 0,$$

and then the result follows easily. □

For $2 \leq m \leq \lfloor \frac{n}{2} \rfloor$, let $T_{n,m}$ be the tree obtained by attaching $m-1$ paths on two vertices to the center of the star S_{n-2m+2}, and let $U_{n,m}$ be the unicyclic graph obtained by attaching $n-2m+1$ pendant vertices and $m-2$ paths on two vertices to one vertex of a triangle; see Fig. 1. Evidently, $T_{n,m} \in \mathbf{T}(n,m)$ and $U_{n,m} \in \mathbf{U}(n,m)$.

3 Sum-connectivity indices of trees

The following lemma is obvious.

Lemma 3.1 *Let $G \in \mathbf{T}(2m,m)$, where $m \geq 2$. Then G has a pendant vertex whose unique neighbor is of degree two.*

Lemma 3.2 [16,17] *Let $G \in \mathbf{T}(n,m)$, where $n > 2m$. Then there is a maximum matching M and a pendant vertex u of G such that u is not M-saturated.*

First, we consider the trees with a perfect matching.

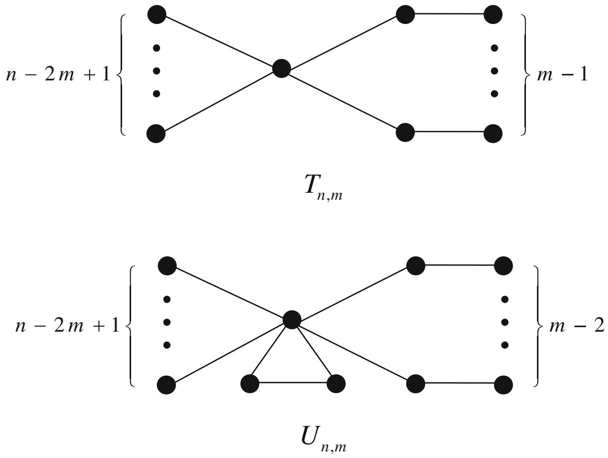

Fig. 1 The graphs $T_{n,m}$ and $U_{n,m}$

Theorem 3.1 *Let $G \in \mathbf{T}(2m, m)$, where $m \geq 2$. Then*

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

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

Proof Let $f(m) = \frac{1}{\sqrt{m+1}} + \frac{m-1}{\sqrt{m+2}} + \frac{m-1}{\sqrt{3}}$. We prove the result by induction on m. It is easily checked that $G = T_{4,2}$ if $m = 2$.

Suppose that $m \geq 3$ and the result holds for trees in $\mathbf{T}(2m-2, m-1)$. Let $G \in \mathbf{T}(2m, m)$ with a perfect matching M. By Lemma 3.1, there exists a pendant vertex u in G adjacent to a vertex v of degree two. Then $uv \in M$ and $G-u-v \in \mathbf{T}(2m-2, m-1)$. Let w be the neighbor of v different from u. Since $|M| = m$ and every pendant vertex is M-saturated, we have $d_G(w) \leq m$. Note that there is at most one neighbor of w with degree one. By Lemma 2.1 (ii), Lemma 2.2 (ii) and the induction hypothesis,

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

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

Now, we consider the trees with a given matching number.

Theorem 3.2 *Let $G \in \mathbf{T}(n, m)$, where $2 \leq m \leq \left\lfloor \frac{n}{2} \right\rfloor$. Then*

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

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

Proof Let $f(n,m) = \frac{n-2m+1}{\sqrt{n-m+1}} + \frac{m-1}{\sqrt{n-m+2}} + \frac{m-1}{\sqrt{3}}$. 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 trees in $\mathbf{T}(n-1,m)$. Let $G \in \mathbf{T}(n,m)$. By Lemma 3.2, there is a maximum matching M and a pendant vertex u of G such that u is not M-saturated. Then $G - u \in \mathbf{T}(n-1,m)$. 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 $d_G(v)-1 \le n-1-m$, i.e., $d_G(v) \le n-m$. Let r be the number of pendant neighbors of v in G, where $1 \le r \le d_G(v)-1$. Note that at least $r-1$ pendant neighbors of v are not M-saturated, and there are $n-2m$ vertices are not M-saturated in G. Then $r \le n-2m+1$. By Lemma 2.1 (i) with $k = n-2m+1$, Lemma 2.2 (i) and the induction hypothesis,

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

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

4 Sum-connectivity indices of unicyclic graphs

In this section, we determine the unicyclic graph of a given matching number with the minimum sum-connectivity index.

For a unicyclic graph G with cycle C_s, the forest formed from G by deleting the edges of C_s consists of s vertex-disjoint trees, each containing a vertex on C_s, which is called the root of this tree in G. These trees are called the branches of G.

Lemma 4.1 [18] *Let* $G \in \mathbf{U}(2m,m)$, *where* $m \ge 3$, *and let* T *be a branch of* G *with root* r. *If* $u \in V(T)$ *is a pendant vertex that is furthest from the root* r *with* $d_G(u,r) \ge 2$, *then* u *is adjacent to a vertex of degree two.*

Lemma 4.2 [19] *Let* $G \in \mathbf{U}(n,m)$, *where* $n > 2m$, *and* $G \ne C_n$. *Then there is a maximum matching* M *and a pendant vertex* u *of* G *such that* u *is not* M*-saturated.*

For integer $m \ge 3$, let $\mathbf{U}_1(m)$ be the set of graphs in $\mathbf{U}(2m,m)$ containing a pendant vertex whose neighbor is of degree two. Let $\mathbf{U}_2(m) = \mathbf{U}(2m,m) \backslash \mathbf{U}_1(m)$.

Lemma 4.3 *Let $G \in \mathbf{U}_2(m)$, where $m \geq 4$. Then* $\chi(G) > \frac{m}{\sqrt{m+3}} + \frac{1}{\sqrt{m+2}} + \frac{m-2}{\sqrt{3}} + \frac{1}{2}$.

Proof By Lemma 4.1, $G \in \mathbf{U}_2(m)$ implies that G is a graph of maximum degree two or three obtained by attaching some pendant vertices to a cycle C_k, where $m \leq k \leq 2m$. Let G_1 be a graph in $\mathbf{U}_2(m)$ with the minimum sum-connectivity index. Let M be a perfect matching and C the unique cycle of G_1. Suppose that $m+1 \leq k \leq 2m$. Then there is at least one edge, say xy, on C such that $xy \in M$. Note that $d_{G_1}(x), d_{G_1}(y) = 2$. Denote by x_1 the neighbor of x on C different from y. For $G_2 = G_1 - \{xx_1\} + \{x_1y\} \in \mathbf{U}_2(m)$, we have by Lemma 2.3 that $\chi(G_2) < \chi(G_1)$, a contradiction. Thus, $k = m$, i.e., each vertex on C is of degree three. Then

$$\chi(G_1) = \frac{m}{\sqrt{1+3}} + \frac{m}{\sqrt{3+3}} = \left(\frac{1}{2} + \frac{1}{\sqrt{6}}\right)m.$$

Let $h(x) = \left(\frac{1}{2} + \frac{1}{\sqrt{6}}\right)x - \left(\frac{x}{\sqrt{x+3}} + \frac{1}{\sqrt{x+2}} + \frac{x-2}{\sqrt{3}} + \frac{1}{2}\right)$. It is easily seen that $\frac{1}{2}(x+2)^{-3/2} - \left(\frac{1}{2}x + 3\right)(x+3)^{-3/2}$ is increasing for $x \geq 4$, and thus

$$\begin{aligned} h'(x) &= \frac{1}{2}(x+2)^{-3/2} - \left(\frac{1}{2}x + 3\right)(x+3)^{-3/2} + \frac{1}{2} + \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{3}} \\ &\geq \frac{1}{2}(4+2)^{-3/2} - \left(\frac{1}{2}\cdot 4 + 3\right)(4+3)^{-3/2} + \frac{1}{2} + \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{3}} > 0, \end{aligned}$$

i.e., $h(x)$ is increasing for $x \geq 4$, implying that $h(m) \geq h(4) > 0$. The result follows. □

Let H_6 be the unicyclic graph obtained by attaching a pendant vertex to every vertex of a triangle. It may be easily checked that the following lemma holds.

Lemma 4.4 *Among the graphs in $\mathbf{U}(6, 3)$, H_6 is the unique graph with the minimum sum-connectivity index $\frac{3}{\sqrt{6}} + \frac{3}{2}$, and $U_{6,3}$ is the unique graph with the second minimum sum-connectivity index $\frac{3}{\sqrt{6}} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}} + \frac{1}{2}$.*

In the following, if G is a graph in $\mathbf{U}_1(m)$ with a perfect matching M, then denote by u a pendant vertex whose neighbor v is of degree two in G, and denote by w the neighbor of v different from u. Obviously, $uv \in M$ and $G - u - v \in \mathbf{U}(2m-2, m-1)$. Since $|M| = m$, we have $d_G(w) \leq m+1$. Note that there is at most one neighbor of w with degree one.

Lemma 4.5 *Let $G \in \mathbf{U}(8, 4)$. Then $\chi(G) \geq \frac{4}{\sqrt{7}} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{1}{2}$ with equality if and only if $G = U_{8,4}$.*

Proof If $G \in \mathbf{U}_2(4)$, then by Lemma 4.3, we have $\chi(G) > \frac{4}{\sqrt{7}} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{1}{2}$. Suppose that $G \in \mathbf{U}_1(4)$. Then $G - u - v \in \mathbf{U}(6, 3)$. If $G - u - v \neq H_6$, then by

Lemma 2.1 (ii), Lemma 2.2 (ii) and Lemma 4.4,

$$\begin{aligned}\chi(G) &\geq \chi(G-u-v)+\frac{1}{\sqrt{3}}+\frac{d_G(w)-1}{\sqrt{d_G(w)+2}}-\frac{d_G(w)-3}{\sqrt{d_G(w)+1}}-\frac{1}{\sqrt{d_G(w)}}\\ &\geq \left(\frac{3}{\sqrt{6}}+\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}+\frac{1}{2}\right)+\frac{1}{\sqrt{3}}+\frac{5-1}{\sqrt{5+2}}-\frac{5-3}{\sqrt{5+1}}-\frac{1}{\sqrt{5}}\\ &= \frac{4}{\sqrt{7}}+\frac{1}{\sqrt{6}}+\frac{2}{\sqrt{3}}+\frac{1}{2}\end{aligned}$$

with equalities if and only if $G-u-v=U_{6,3}$ and $d_G(w)=5$, i.e., $G=U_{8,4}$. If $G-u-v=H_6$, then $d_G(w)\leq 4$, and by Lemma 2.1 (ii), Lemma 2.2 (ii) and Lemma 4.4,

$$\begin{aligned}\chi(G) &\geq \chi(H_6)+\frac{1}{\sqrt{3}}+\frac{d_G(w)-1}{\sqrt{d_G(w)+2}}-\frac{d_G(w)-3}{\sqrt{d_G(w)+1}}-\frac{1}{\sqrt{d_G(w)}}\\ &\geq \left(\frac{3}{\sqrt{6}}+\frac{3}{2}\right)+\frac{1}{\sqrt{3}}+\frac{4-1}{\sqrt{4+2}}-\frac{4-3}{\sqrt{4+1}}-\frac{1}{\sqrt{4}}\\ &= \sqrt{6}-\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{3}}+1>\frac{4}{\sqrt{7}}+\frac{1}{\sqrt{6}}+\frac{2}{\sqrt{3}}+\frac{1}{2}.\end{aligned}$$

The result follows. □

Now we are ready to prove our results.

Theorem 4.1 *Let $G\in\mathbf{U}(2m,m)$, where $m\geq 2$.*

(i) If $m=3$, then $\chi(G)\geq\frac{3}{\sqrt{6}}+\frac{3}{2}$ with equality if and only if $G=H_6$.

(ii) If $m\neq 3$, then

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

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

Proof The case $m=2$ may be checked directly since $\mathbf{U}(4,2)=\{C_4,U_{4,2}\}$, and the case $m=3$ follows from Lemma 4.4.

Suppose that $m\geq 4$. Let $g(m)=\frac{m}{\sqrt{m+3}}+\frac{1}{\sqrt{m+2}}+\frac{m-2}{\sqrt{3}}+\frac{1}{2}$. We prove the result by induction on m. If $m=4$, then the result follows from Lemma 4.5. Suppose that $m\geq 5$ and the result holds for graphs in $\mathbf{U}(2m-2,m-1)$. Let $G\in\mathbf{U}(2m,m)$. If $G\in\mathbf{U}_2(m)$, then by Lemma 4.3, $\chi(G)>g(m)$. If $G\in\mathbf{U}_1(m)$, then by Lemma 2.1 (ii), Lemma 2.2 (ii) and the induction hypothesis,

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

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

Theorem 4.2 *Let $G \in \mathbf{U}(n, m)$, where $2 \leq m \leq \lfloor \frac{n}{2} \rfloor$.*

(i) If $(n, m) = (6, 3)$, then $\chi(G) \geq \frac{3}{\sqrt{6}} + \frac{3}{2}$ with equality if and only if $G = H_6$.
(ii) If $(n, m) \neq (6, 3)$, then

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

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

Proof The case $(n, m) = (6, 3)$ follows from Lemma 4.4. Suppose that $(n, m) \neq (6, 3)$. Let

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

It was shown in [13] that the cycle C_n is the unique n-vertex unicyclic graph with the maximum sum-connectivity index. Thus, we only need to consider $G \neq C_n$. If $n > 2m$, then by Lemma 4.2, there exists a pendant vertex x and a maximum matching M such that x is not M-saturated in G. Let $G \in \mathbf{U}(n, m)$. Then $G - x \in \mathbf{U}(n - 1, m)$. Let y be the unique neighbor of x. Since M contains one edge incident with y, and there are $n - m$ edges of G outside M, we have $d_G(y) \leq n - m + 1$. Let r be the number of pendant neighbors of y in G, where $1 \leq r \leq d_G(y) - 1$. Note that at least $r - 1$ pendant neighbors of y are not M-saturated, and there are $n - 2m$ vertices are not M-saturated in G. Then $r \leq n - 2m + 1$. We prove the result by induction on n.

Suppose that $m = 3$. If $n = 7$, then $G - x \in \mathbf{U}(6, 3)$: if $G - x \neq H_6$, then by Lemma 2.1 (i) with $k = n - 2m + 1 = 2$, Lemma 2.2 (i) and Lemma 4.4,

$$\begin{aligned}
\chi(G) &\geq \chi(G - x) + \frac{d_G(y) - 2}{\sqrt{d_G(y) + 2}} + \frac{2 \cdot 2 - d_G(y)}{\sqrt{d_G(y) + 1}} - \frac{2 - 1}{\sqrt{d_G(y)}} \\
&\geq \left(\frac{3}{\sqrt{6}} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{3}} + \frac{1}{2}\right) + \frac{5 - 2}{\sqrt{5 + 2}} + \frac{4 - 5}{\sqrt{5 + 1}} - \frac{2 - 1}{\sqrt{5}} \\
&= \frac{3}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{2}
\end{aligned}$$

with equalities if and only if $G - x = U_{6,3}$, $\quad d_G(y) = 5$ and $r = 2$, i.e., $G = U_{7,3}$, while if $G - x = H_6$, then $d_G(y) \leq 4$, and thus by Lemma 2.1 (i), Lemma 2.2 (i) and

Lemma 4.4,

$$\begin{aligned}\chi(G) &\geq \chi(G-x) + \frac{d_G(y)-2}{\sqrt{d_G(y)+2}} + \frac{2\cdot 2 - d_G(y)}{\sqrt{d_G(y)+1}} - \frac{2-1}{\sqrt{d_G(y)}}\\ &\geq \left(\frac{3}{\sqrt{6}}+\frac{3}{2}\right) + \frac{4-2}{\sqrt{4+2}} + \frac{4-4}{\sqrt{4+1}} - \frac{2-1}{\sqrt{4}}\\ &= \frac{5}{\sqrt{6}} + 1 > \frac{3}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{2}.\end{aligned}$$

Thus, $\chi(G) \geq \frac{3}{\sqrt{7}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{2}$ with equality if and only if $G = U_{7,3}$. Suppose that $n \geq 8$ and the result holds for graphs in $\mathbf{U}(n-1, 3)$. Then by Lemma 2.1 (i), Lemma 2.2 (i), and the induction hypothesis,

$$\begin{aligned}\chi(G) &\geq \chi(G-x) + \frac{d_G(y)-(n-5)}{\sqrt{d_G(y)+2}} + \frac{2(n-5)-d_G(y)}{\sqrt{d_G(y)+1}} - \frac{(n-5)-1}{\sqrt{d_G(y)}}\\ &\geq g(n-1,3) + \frac{(n-2)-(n-5)}{\sqrt{(n-2)+2}} + \frac{2(n-5)-(n-2)}{\sqrt{(n-2)+1}} - \frac{(n-5)-1}{\sqrt{n-2}}\\ &= g(n,3)\end{aligned}$$

with equalities if and only if $G - x = U_{n-1,3}, \quad d_G(y) = n-2$ and $r = n-5$, i.e., $G = U_{n,3}$.

Suppose that $m \neq 3$. If $n = 2m$, then the result follows from Theorem 4.1. Suppose that $n > 2m$ and the result holds for graphs in $\mathbf{U}(n-1, m)$. Then by Lemma 2.1 (i) with $k = n - 2m + 1$, Lemma 2.2 (i) and the induction hypothesis,

$$\begin{aligned}\chi(G) \geq\ & \chi(G-x) + \frac{d_G(y)-(n-2m+1)}{\sqrt{d_G(y)+2}}\\ &+\frac{2(n-2m+1)-d_G(y)}{\sqrt{d_G(y)+1}}\\ &-\frac{(n-2m+1)-1}{\sqrt{d_G(y)}}\\ \geq\ & g(n-1,m) + \frac{(n-m+1)-(n-2m+1)}{\sqrt{(n-m+1)+2}}\\ &+\frac{2(n-2m+1)-(n-m+1)}{\sqrt{(n-m+1)+1}}\\ &-\frac{(n-2m+1)-1}{\sqrt{n-m+1}}\\ =\ & g(n,m)\end{aligned}$$

with equalities if and only if $G-x = U_{n-1,m}, \quad d_G(y) = n-m+1$ and $r = n-2m+1$, i.e., $G = U_{n,m}$. □

5 Small sum-connectivity indices of unicyclic graphs

Recall that we have already determined in [13] the n-vertex unicyclic graphs for $n \geq 4$ with the maximum and second maximum sum-connectivity indices. Now we determine the n-vertex unicyclic graphs for $n \geq 4$ with the minimum and second minimum sum-connectivity indices.

Let $S_n(a, b)$ be the graph obtained by attaching $a - 2$ and $b - 2$ pendant vertices to two vertices of a triangle, respectively, where $a \geq b \geq 2$ and $n = a + b - 1$.

Lemma 5.1 *Among the graphs $S_n(a, b)$ with $a \geq b \geq 2$ and $n = a + b - 1 \geq 5$, $S_n(n-1, 2)$ and $S_n(n-2, 3)$ are respectively the unique graphs with the minimum and second minimum sum-connectivity indices, which are equal to $\frac{2}{\sqrt{n+1}} + \frac{n-3}{\sqrt{n}} + \frac{1}{2}$ and $\frac{1}{\sqrt{n+1}} + \frac{1}{\sqrt{n}} + \frac{n-4}{\sqrt{n-1}} + \frac{1}{\sqrt{5}} + \frac{1}{2}$, respectively.*

Proof Actually, we only need to prove $\chi(S_n(a, b)) > \chi(S_n(a+1, b-1))$ for $a \geq b \geq 3$. Let $f(x) = (x+1)^{-1/2} + (x-3)x^{-1/2}$ for $x \geq 3$. Then $f''(x) = \frac{3}{4}(x+1)^{-5/2} - \frac{1}{4}(x+9)x^{-5/2} < 0$, implying that $f(x+1) - f(x)$ is decreasing for $x \geq 3$. Thus, it is easily seen that

$$\begin{aligned}
&\chi(S_n(a+1, b-1)) - \chi(S_n(a, b)) \\
&= \left[\chi(S_n(a+1, b-1)) - \chi(S_{n-1}(a, b-1))\right] - \left[\chi(S_n(a, b)) - \chi(S_{n-1}(a, b-1))\right] \\
&= \left(\frac{a-2}{\sqrt{a+2}} - \frac{a-2}{\sqrt{a+1}} + \frac{1}{\sqrt{a+3}}\right) - \left(\frac{b-3}{\sqrt{b+1}} - \frac{b-3}{\sqrt{b}} + \frac{1}{\sqrt{b+2}}\right) \\
&= [f(a+2) - f(a+1)] - [f(b+1) - f(b)] < 0.
\end{aligned}$$

Then the result follows easily. □

Theorem 5.1 *Among the n-vertex unicyclic graphs, $U_{n,2} = S_n(n-1, 2)$ for $n \geq 3$ is the unique graph with the minimum sum-connectivity index, which is equal to $\frac{2}{\sqrt{n+1}} + \frac{n-3}{\sqrt{n}} + \frac{1}{2}$, C_4 for $n = 4$ is the unique graph with the second minimum sum-connectivity index, which is equal to 2, and $S_n(n-2, 3)$ for $n \geq 5$ is the unique graph with the second minimum sum-connectivity index, which is equal to $\frac{1}{\sqrt{n+1}} + \frac{1}{\sqrt{n}} + \frac{n-4}{\sqrt{n-1}} + \frac{1}{\sqrt{5}} + \frac{1}{2}$.*

Proof The case $n = 3$ is trivial. Let G be an n-vertex unicyclic graph with matching number m, where $2 \leq m \leq \lfloor \frac{n}{2} \rfloor$. The cases $n = 4, 5$ may be checked directly since there are only two and five possibilities for G, respectively. Suppose that $n \geq 6$.

If $m = 2$, then by Theorem 4.2, $\chi(G) \geq \chi(U_{n,2})$ with equality if and only if $G = U_{n,2}$. Suppose that $m \geq 3$. If $(n, m) = (6, 3)$, then by Lemma 4.4 and direct calculation, we have $\chi(G) \geq \chi(H_6) > \chi(U_{6,2})$, and if $(n, m) \neq (6, 3)$, then by Theorem 4.2 and Lemma 2.3, $\chi(G) \geq \chi(U_{n,m}) > \chi(U_{n,m-1}) > \cdots > \chi(U_{n,2})$. Thus, $U_{n,2} = S_n(n-1, 2)$ is the unique graph among the n-vertex unicyclic graphs with the minimum sum-connectivity index.

By the above arguments, to determine the graphs with the second minimum sum-connectivity index, we only need to consider H_6, $U_{n,3}$ with $n \geq 7$, and the graphs in $\mathbf{U}(n,2)$ different from $U_{n,2}$. Thus, G may be of five types: (1) $G = S_n(a,b)$ with $b \geq 3$, and then by Lemma 5.1,

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

with equality if and only if $G = S_n(n-2,3)$; (2) $G = H_6$, and then by direct calculation, $\chi(G) > \chi(S_6(4,3))$; (3) $G = U_{n,3}$ with $n \geq 7$, for which

$$\chi(G) = \frac{3}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{1}{2} + \frac{1}{\sqrt{3}} > \frac{1}{\sqrt{n+1}} + \frac{1}{\sqrt{n}} + \frac{n-4}{\sqrt{n-1}} + \frac{1}{\sqrt{5}} + \frac{1}{2},$$

as it may be easily checked that for $h(x) = \frac{1}{\sqrt{x}} - \frac{1}{\sqrt{x+1}}$ with $x \geq 6$, $h''(x) = \frac{3}{4}x^{-5/2} - \frac{3}{4}(x+1)^{-5/2} > 0$, implying that $h(x) - h(x-1)$ is increasing for $x \geq 7$, and then

$$\left(\frac{3}{\sqrt{n}} + \frac{n-5}{\sqrt{n-1}} + \frac{1}{2} + \frac{1}{\sqrt{3}}\right) - \left(\frac{1}{\sqrt{n+1}} + \frac{1}{\sqrt{n}} + \frac{n-4}{\sqrt{n-1}} + \frac{1}{\sqrt{5}} + \frac{1}{2}\right)$$
$$= h(n) - h(n-1) + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{5}} \geq h(7) - h(6) + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{5}} > 0;$$

(4) G is the graph obtained by identifying a pendant vertex of S_{n-2} and a vertex of a triangle, for which,

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

(5) G is a graph obtained by attaching some pendant vertices to one vertex or two non-adjacent vertices of a quadrangle. By Lemmas 2.3 and 5.1, we have $\chi(G) > \chi(S_n(n-2,3))$. Thus, $S_n(n-2,3)$ is the unique graph among the n-vertex unicyclic graphs with the second minimum sum-connectivity index. □

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