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ORIGINAL PAPER

Minimum general sum-connectivity index of unicyclic graphs

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Abstract The general sum-connectivity index of a graph G is defined as $\chi_\alpha(G) = \sum_{\text{edges}} (d_u + d_v)^\alpha$, where d_u denotes the degree of vertex u in G and α is a real number. In this report, we determine the minimum and the second minimum values of the general sum-connectivity indices of n-vertex unicyclic graphs for non-zero $\alpha \geq -1$, and characterize the corresponding extremal graphs.

Keywords General Randić connectivity index · General product-connectivity index · General sum-connectivity index · Properties

1 Introduction

Let G be a simple graph with vertex-set $V(G)$ and edge-set $E(G)$ [1,2]. For $u \in V(G)$, $\Gamma(u)$ denotes the set of its (first) neighbors in G and the degree of u is $d_u = d_G(u) = |\Gamma(u)|$. The general Randić connectivity index (or general product-connectivity index), denoted by R_α, of G is defined as [3,4]

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

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where α is a real number. Index $R_{-1/2}$ is the (classical) Randić connectivity index (or product-connectivity index) proposed by Randić [5] in 1975, which is the most used molecular descriptor in the QSPR and QSAR modeling *e.g.*, [6–11].

Recently, the general sum-connectivity index, denoted by χ_α, of the graph G was introduced in [12], defined as

$$\chi_\alpha = \chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha.$$

Index $\chi_{-1/2}$ is the sum-connectivity index [13], which has already been studied and applied in the QSPR and QSAR modeling [13–16]. Some properties of the general sum-connectivity index, especially for trees, have already been established in [12]. We also found that in the structure-boiling point modeling for 58 aliphatic alcohols, the optimum value of α is -0.60 if the general product-connectivity index is used and is -0.85 if the general sum-connectivity index is used in the modeling. Similarly, we found that in the structure-water solubility modeling for 54 aliphatic alcohols, the optimum value of α is -0.40 if the general product-connectivity index is used and is -0.70 if the general sum-connectivity index is used in the modeling. We already established sometime ago that the optimum exponent of the product-connectivity index depends on the property considered [17] and this appears to hold also for the sum-connectivity index as well. Therefore, the properties of general sum-connectivity index warrant further studies. In this report, we determine the minimum and the second minimum values of the general sum-connectivity indices of n-vertex unicyclic graphs for non-zero $\alpha \geq -1$, and characterize the corresponding extremal graphs.

2 Preliminaries

Let P_n and C_n be respectively the path and the cycle with n vertices.

Lemma 1 [12] *Suppose that Q is a connected graph with at least two vertices. For $r \geq s \geq 1$, let G_1 be the graph obtained from Q by attaching two paths P_r and P_s to $u \in V(Q)$, and G_2 the graph obtained from Q by attaching a path P_{r+s} to u. If $\alpha > 0$, then $\chi_\alpha(G_1) > \chi_\alpha(G_2)$.*

Lemma 2 *Suppose that M is a connected graph with a vertex u of degree two, and the two neighbors of u in M are denoted by u_1 and u_2. For $r \geq 1$, let H be the graph obtained from M by attaching a path P_r to u. Denote by u' the terminal vertex of the path P_r attached to u in H. Let H_1 be the graph obtained from H by deleting the edge uu_2 and adding the edge $u'u_2$. If $\alpha > 0$ and the maximum degree of M is at most three, then $\chi_\alpha(H_1) < \chi_\alpha(H)$.*

Proof If $r = 1$, then

$$\begin{aligned}\chi_\alpha(H_1) - \chi_\alpha(H) = &\left[(d_M(u_1)+2)^\alpha - (d_M(u_1)+3)^\alpha\right] \\ &+ \left[(d_M(u_2)+2)^\alpha - (d_M(u_2)+3)^\alpha\right] < 0,\end{aligned}$$

and thus $\chi_\alpha(H_1) < \chi_\alpha(H)$. Suppose that $r \geq 2$. Then

$$\chi_\alpha(H_1) - \chi_\alpha(H) = \left[(d_M(u_1)+2)^\alpha - (d_M(u_1)+3)^\alpha\right] + \left[(d_M(u_2)+2)^\alpha - (d_M(u_2)+3)^\alpha\right] + (4^\alpha - 5^\alpha) - (3^\alpha - 4^\alpha).$$

If $\alpha \geq 1$, then $x^\alpha - (x+1)^\alpha$ is nonincreasing for $x \geq 1$, and thus $\chi_\alpha(H_1) - \chi_\alpha(H) < (4^\alpha - 5^\alpha) - (3^\alpha - 4^\alpha) \leq 0$, implying that $\chi_\alpha(H_1) < \chi_\alpha(H)$. Suppose that $0 < \alpha < 1$. Note that $1 \leq d_M(u_1), d_M(u_2) \leq 3$. Then $x^\alpha - (x+1)^\alpha$ is increasing, $x^\alpha - 2(x+1)^\alpha$ is decreasing for $x \geq 1$, and thus

$$\begin{aligned}\chi_\alpha(H_1) - \chi_\alpha(H) &\leq 2\left[(3+2)^\alpha - (3+3)^\alpha\right] + (4^\alpha - 5^\alpha) - (3^\alpha - 4^\alpha)\\ &= (5^\alpha - 2\cdot 6^\alpha) - (3^\alpha - 2\cdot 4^\alpha) < 0,\end{aligned}$$

implying that $\chi_\alpha(H_1) < \chi_\alpha(H)$. □

Lemma 3 *Let G be a connected graph with $uv \in E(G)$, $d_G(u), d_G(v) \geq 2$, where 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. If $\alpha < 0$, then $\chi_\alpha(G) > \chi_\alpha(G_1)$.*

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

$$\chi_\alpha(G) - \chi_\alpha(G_1) = \sum_{xu \in E(G)\setminus\{uv\}} \left[(d_x + d_u)^\alpha - (d_x + d_u + d_v - 1)^\alpha\right] + \sum_{xv \in E(G)\setminus\{uv\}} \left[(d_x + d_v)^\alpha - (d_x + d_u + d_v - 1)^\alpha\right] > 0,$$

and thus $\chi_\alpha(G) > \chi_\alpha(G_1)$. □

Let $S_n(a, b, c)$ be the n-vertex graph obtained by attaching $a-2$, $b-2$ and $c-2$ pendant vertices to the three vertices of a triangle, respectively, where $a+b+c = n+3$ and $a \geq b \geq c \geq 2$.

Lemma 4 *Suppose that $-1 \leq \alpha < 0$. For fixed $n \geq 5$, among the graphs $S_n(a, b, c)$ with $a+b+c = n+3$ and $a \geq b \geq c \geq 2$, $S_n(n-1, 2, 2)$ and $S_n(n-2, 3, 2)$ are respectively the unique graphs with the minimum and the second minimum general sum-connectivity indices.*

Proof Since $a \geq b \geq c \geq 2$, we need only to prove $\chi_\alpha(S_n(a, b, c)) > \chi_\alpha(S_n(a+1, b-1, c))$ for $b \geq 3$. Let $f(x) = (x-3)x^\alpha + (x+c-1)^\alpha$ for $x \geq 3$. Then $f''(x) = \alpha(\alpha+1)x^{\alpha-1} - \alpha(\alpha-1)\left[3x^{\alpha-2} - (x+c-1)^{\alpha-2}\right] < 0$, implying that $f(x+1) - f(x)$ is decreasing for $x \geq 3$. Thus it is easily seen that

$$\begin{aligned}
&\chi_\alpha\left(S_n(a+1,b-1,c)\right)-\chi_\alpha\left(S_n(a,b,c)\right)\\
&\quad=\left[\chi_\alpha\left(S_n(a+1,b-1,c)\right)-\chi_\alpha\left(S_{n-1}(a,b-1,c)\right)\right]\\
&\qquad-\left[\chi_\alpha\left(S_n(a,b,c)\right)-\chi_\alpha\left(S_{n-1}(a,b-1,c)\right)\right]\\
&\quad=\left[(a-1)(a+2)^\alpha+(a+c+1)^\alpha-(a-2)(a+1)^\alpha-(a+c)^\alpha\right]\\
&\qquad-\left[(b-2)(b+1)^\alpha+(b+c)^\alpha-(b-3)b^\alpha-(b+c-1)^\alpha\right]\\
&\quad=[f(a+2)-f(a+1)]-[f(b+1)-f(b)]<0.
\end{aligned}$$

Then the result follows. □

Let $U_n(r)$ be the n-vertex (unicyclic) graph obtained by attaching r pendant vertices to a pendant vertex of $S_{n-r}(n-r-1,2,2)$, where $1\le r\le n-4$.

Lemma 5 *Suppose that* $-1\le\alpha<0$. *For fixed* $n\ge 5$, *if* $\chi_\alpha\left(U_n(r)\right)$ *is minimum for* $1\le r\le n-4$, *then* $r=1$ *or* $n-4$.

Proof It is trivial for $n=5,6$. Suppose that $n\ge 7$ and $2\le r\le n-5$. Note that $(x+1)^\alpha-x^\alpha$ is increasing for $x\ge 1$. Let $f(x)=x(x+2)^\alpha$ for $x\ge 1$. Then

$$f''(x)=\alpha(x+2)^{\alpha-2}\left[(\alpha+1)(x+2)-2(\alpha-1)\right]<0,$$

implying that $f(x+1)-f(x)$ is decreasing for $x\ge 1$. Let $s=n-4-r$. If $r\ge s+1$, then it is easily checked that

$$\begin{aligned}
&\chi_\alpha(U_n(r))-\chi_\alpha(U_{n-1}(r))\\
&\quad=n^\alpha-(n-1)^\alpha+s(s+4)^\alpha-(s-1)(s+3)^\alpha+2\left[(s+5)^\alpha-(s+4)^\alpha\right]\\
&\quad>n^\alpha-(n-1)^\alpha+s(s+4)^\alpha-(s-1)(s+3)^\alpha+2\left[(s+4)^\alpha-(s+3)^\alpha\right]\\
&\quad=n^\alpha-(n-1)^\alpha+(s+2)(s+4)^\alpha-(s+1)(s+3)^\alpha\\
&\quad=n^\alpha-(n-1)^\alpha+f(s+2)-f(s+1)\\
&\quad\ge n^\alpha-(n-1)^\alpha+f(r+1)-f(r)\\
&\quad=n^\alpha-(n-1)^\alpha+(r+1)(r+3)^\alpha-r(r+2)^\alpha\\
&\quad=\chi_\alpha(U_n(r+1))-\chi_\alpha(U_{n-1}(r)),
\end{aligned}$$

and thus $\chi_\alpha(U_n(r))>\chi_\alpha(U_n(r+1))$, implying that $\chi_\alpha(U_n(r))>\chi_\alpha(U_n(n-4))$. Suppose that $r\le s$. Then

$$\begin{aligned}
\chi_\alpha(U_n(r))-\chi_\alpha(U_n(s+2))&=2\left[(s+5)^\alpha-(s+4)^\alpha\right]\\
&\quad-2\left[(r+3)^\alpha-(r+2)^\alpha\right]>0,
\end{aligned}$$

and thus $\chi_\alpha(U_n(r))>\chi_\alpha(U_n(s+2))$. If $r=2$, then $\chi_\alpha(U_n(r))>\chi_\alpha(U_n(n-4))$. Suppose that $r\ge 3$. Note that $s+2\ge(r-2)+1$. By the above argument, $\chi_\alpha(U_n(s+2))>\chi_\alpha(U_n(s+3))$, implying that $\chi_\alpha(U_n(r))>\chi_\alpha(U_n(s+2))>\chi_\alpha(U_n(n-4))$. The result follows. □

3 Main result

Let $\mathbf{U}_n^1$ be the set of n-vertex (unicyclic) graphs obtained by attaching a path on at least two vertices to a vertex of a cycle. Let U_n^2 be the graph obtained by attaching a pendant vertex to a vertex of the cycle C_{n-1}.

Now we prove our main result.

Proposition 1 *Among the set of n-vertex unicyclic graphs with $n \geq 5$,*

- *for $\alpha > 0$, C_n is the unique graph with the minimum general sum-connectivity index, which is equal to $n \cdot 4^\alpha$, the graphs in $\mathbf{U}_n^1$ for $0 < \alpha < 1$, the graphs in $\mathbf{U}_n^1$ and U_n^2 for $\alpha = 1$, and U_n^2 for $\alpha > 1$ are the unique graphs with the second minimum general sum-connectivity index, which is equal to $3 \cdot 5^\alpha + (n-4)4^\alpha + 3^\alpha$ for $0 < \alpha < 1$, equal to $4n + 2$ for $\alpha = 1$, and equal to $2 \cdot 5^\alpha + (n-2)4^\alpha$ for $\alpha > 1$,*
- *for $-1 \leq \alpha < 0$, $S_n(n-1, 2, 2)$ and $S_n(n-2, 3, 2)$ are respectively the unique graphs with the minimum and the second minimum general sum-connectivity indices, which are equal to $2(n+1)^\alpha + (n-3)n^\alpha + 4^\alpha$ and $(n+1)^\alpha + n^\alpha + (n-4)(n-1)^\alpha + 5^\alpha + 4^\alpha$, respectively.*

Proof Let G be an n-vertex unicyclic graph.

First suppose that $\alpha > 0$. If the maximum degree of G is at least four, then by Lemma 1, we may get an n-vertex unicyclic graph of maximum degree three with smaller general sum-connectivity index. Suppose that the maximum degree of G is three. If there are at least two vertices with maximum degree three, then by Lemmas 1 and 2, we may get an n-vertex unicyclic graph with exactly one vertex of degree three with smaller general sum-connectivity index. If there is exactly one vertex with maximum degree three, then either $G \in \mathbf{U}_n^1$ with $\chi_\alpha(G) = 3 \cdot 5^\alpha + (n-4)4^\alpha + 3^\alpha$, or $G = U_n^2$ with $\chi_\alpha(U_n^2) = 2 \cdot 5^\alpha + (n-2)4^\alpha$. For $H \in \mathbf{U}_n^1$, it is easily checked that $\chi_\alpha(H) < \chi_\alpha(U_n^2)$ for $0 < \alpha < 1$, $\chi_\alpha(H) = \chi_\alpha(U_n^2)$ for $\alpha = 1$, and $\chi_\alpha(H) > \chi_\alpha(U_n^2)$ for $\alpha > 1$. It follows that the graphs in $\mathbf{U}_n^1$ for $0 < \alpha < 1$, the graphs in $\mathbf{U}_n^1$ and U_n^2 for $\alpha = 1$, and U_n^2 for $\alpha > 1$ are the unique graphs with the minimum general sum-connectivity index among the n-vertex unicyclic graphs with maximum degree at least three. If the maximum degree of G is two, then $G = C_n$, and by Lemma 2, we have $\chi_\alpha(C_n) < \min\left\{\chi_\alpha(H), \chi_\alpha(U_n^2)\right\}$ for $H \in \mathbf{U}_n^1$. Now the result for $\alpha > 0$ follows easily.

Now suppose that $-1 \leq \alpha < 0$. Let C be the unique cycle of G. If the length of C is at least four, then by Lemma 3, $\chi_\alpha(G) > \chi_\alpha(S_n(a, b, c))$ with $a \geq b \geq c \geq 2$ and $b \geq 3$, and thus by Lemma 4, $\chi_\alpha(G) > \chi_\alpha(S_n(n-2, 3, 2))$. Suppose that the length of C is three. First suppose that there are at least two vertices on C with degree at least three. If there is at least one non-pendant vertex outside C, then by Lemmas 3 and 4, $\chi_\alpha(G) > \chi_\alpha(S_n(n-2, 3, 2))$. If all vertices outside C are pendant, then $G = S_n(a, b, c)$ with $a \geq b \geq c \geq 2$ and $b \geq 3$, and thus by Lemma 4, we have $\chi_\alpha(G) \geq \chi_\alpha(S_n(n-2, 3, 2))$ with equality if and only if $G = S_n(n-2, 3, 2)$. Now suppose that there is exactly one vertex on C with degree at least three. If there is at least one non-pendant vertex outside C, then since

$$\begin{aligned}\chi_\alpha(U_n(1)) - \chi_\alpha(S_n(n-2,3,2)) &= \left[3n^\alpha + (n-5)(n-1)^\alpha + 4^\alpha + 3^\alpha\right] \\ &\quad - \left[(n+1)^\alpha + n^\alpha + (n-4)(n-1)^\alpha + 5^\alpha + 4^\alpha\right] \\ &= \left[n^\alpha - (n+1)^\alpha\right] - \left[(n-1)^\alpha - n^\alpha\right] + 3^\alpha - 5^\alpha \\ &> \left[4^\alpha - (4+1)^\alpha\right] - \left[(4-1)^\alpha - 4^\alpha\right] + 3^\alpha - 5^\alpha \\ &= 2(4^\alpha - 5^\alpha) > 0\end{aligned}$$

and

$$\begin{aligned}\chi_\alpha(U_n(n-4)) - \chi_\alpha(S_n(n-2,3,2)) &= \left[n^\alpha + (n-4)(n-2)^\alpha + 2\cdot 5^\alpha + 4^\alpha\right] \\ &\quad - \left[(n+1)^\alpha + n^\alpha + (n-4)(n-1)^\alpha \right.\\ &\quad \left. + 5^\alpha + 4^\alpha\right] \\ &= \left[5^\alpha - (n+1)^\alpha\right] + (n-4)\left[(n-2)^\alpha \right.\\ &\quad \left. -(n-1)^\alpha\right] > 0,\end{aligned}$$

we have by Lemmas 3 and 5 that for some r with $1 \le r \le n-4$, $\chi_\alpha(G) \ge \chi_\alpha(U_n(r)) \ge \min\{\chi_\alpha(U_n(1)), \chi_\alpha(U_n(n-4))\} > \chi_\alpha(S_n(n-2,3,2))$. If all vertices outside C are pendant, then $G = S_n(n-1,2,2)$. Thus we have shown that $\chi_\alpha(G) > \chi_\alpha(S_n(n-2,3,2))$ if $G \ne S_n(n-2,3,2), S_n(n-1,2,2)$. Then the result for $-1 \le \alpha < 0$ follows from Lemma 4. □

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