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VARIABLE SUM EXDEG INDICES OF CACTUS GRAPHS

Jianwei Du and Xiaoling Sun

Abstract. For a graph G, the variable sum exdeg index $SEI_a(G)$ is defined as $\sum_{u\in V(G)} d_G(u)a^{d_G(u)}$, where $a \in (0,1)\cup(1,+\infty)$. In this work, we determine the minimum and maximum variable sum exdeg indices (for $a > 1$) of n-vertex cactus graphs with k cycles or p pendant vertices. Furthermore, the corresponding extremal cactus graphs are characterized.

1. Introduction

Topological indices are mathematical descriptors reflecting some structural characteristics of organic molecules on the molecular graphs, and they play an important role in pharmacology, chemistry, etc. (see [8,9,17]). For a graph G, the variable sum exdeg index (denoted by SEI_a) was proposed by Vukičević [20] and is expressed by:

$$SEI_a(G) = \sum_{uv\in E(G)} (a^{d_G(u)} + a^{d_G(v)}) = \sum_{v\in V(G)} d_G(v)a^{d_G(v)},$$

where $a \neq 1$ is an arbitrary positive real number and $d_G(u)$ is the degree of vertex u in G. This graph invariant has a good correlation with the octanol-water partition coefficient [20], and was used to study the octane isomers given by the International Academy of Mathematical Chemistry (IAMC) [18,21,22]. Yarahmadi and Ashrafi [26] proposed a polynomial form of this graph invariant which is applied in nanoscience. By using the technique of majorization, Ghalavand and Ashrafi [7] provided the maximal and minimal variable sum exdeg indices (for $a > 1$) of trees, unicyclic graphs, bicyclic graphs and tricyclic graphs.

We only deal with simple connected graphs in this work. Let $G = (V(G), E(G))$ be the graph having vertex set $V(G)$ and edge set $E(G)$. Denoted by $N_G(v)$ the neighbours of vertex $v \in V(G)$. We use n_i to denote the number of vertices with degree i. Denoted by $G - uv$ and $G + uv$ the graph arisen from G by deleting the edge $uv \in E(G)$ and the graph arisen from G by adding an

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edge $uv \notin E(G)$ $(u, v \in V(G))$, respectively. The subgraph of G resulted by deleting a vertex $x \in V(G)$ and its incident edge(s) is denoted by $G - x$. For $X \subseteq V(G)$, let us denote the subgraph of G obtained by deleting the vertices of X and the edges incident with them by $G - X$. A graph G is called a cactus graph if no two cycles of G have any common edge. As usual, we use P_n, S_n and C_n to denote the n-vertex path, the n-vertex star and the n-vertex cycle, respectively.

Let $P_r = x_0x_1 \cdots x_r$ $(r \geq 1)$ be a path of graph G with $d_G(x_1) = \cdots = d_G(x_{r-1}) = 2$ (unless $r = 1$). If $d_G(x_0) \geq 3, d_G(x_r) = 1$, then P_r is called a pendant path of G; if $d_G(x_0), d_G(x_r) \geq 3$, then P_r is called an internal path of G. The k cyclic graph G is the graph whose cyclomatic number is $k = |E(G)| - |V(G)| + 1$. If a (real-valued) function f (definition domain is $X \subseteq R$, where R denotes the set of real numbers) satisfies the inequality $f(sx_1 + tx_2) < sf(x_1) + tf(x_2)$ for all $x_1, x_2 \in X$ and $s \geq 0$, $t \geq 0$, $s + t = 1$, we call f a strictly convex function.

Let $\mathscr{C}_1(n, k)$ and $\mathscr{C}_2(n, p)$ be the n-vertex cactus graphs with k cycles and p pendant vertices, respectively. Obviously, $\mathscr{C}_1(n, 0)$ and $\mathscr{C}_1(n, 1)$ are trees and unicyclic graphs, respectively. We can see [5] for other terminologies and notations.

Cactus graphs represent important class of molecules [13, 14], so some topological indices (such as the famous Randić index, Wiener index, Zagreb indices, Harary index and Szeged index, etc.) of cactus graphs are studied (see [1–4, 6, 10–16, 23–25]). Inspired by these, we study the variable sum exdeg index of cactus graphs. In this work, the minimum and maximum variable sum exdeg indices (for $a > 1$) of n-vertex cactus graphs with k cycles or p pendant vertices are determined. And the corresponding extremal graphs are characterized.

2. Variable sum exdeg indices of cactus graphs with k cycles for $a > 1$

Lemma 2.1 ([21]). *Let $f_a(x) = xa^x$, where $x \geq 1, a > 1$. Then*
(i) *$f_a(x)$ is strictly monotone increasing in x;*
(ii) *$f_a(x)$ is strictly convex.*

By (ii) of Lemma 2.1, we can obtain the following Lemma 2.2 immediately.

Lemma 2.2. *Let x_1, y_1, x_2, y_2 be positive integers with $x_1 + x_2 = y_1 + y_2$ and $|x_1 - x_2| < |y_1 - y_2|$. Then for $a > 1$, we have*

$$x_1a^{x_1} + x_2a^{x_2} < y_1a^{y_1} + y_2a^{y_2}.$$

Let $\boldsymbol{\mathscr{C}}_{n,k}$ be the cactus graph arisen from the star S_n by adding k mutually independent edges, as shown in Fig. 1.

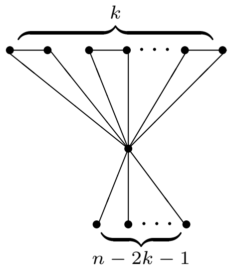

Fig. 1. The graph $\mathscr{C}_{n,k}$.

Lemma 2.3 ([21])**.** *Let T be a tree of order n. Then*

$$2(n-2)a^2 + 2a \leq SEI_a(T) \leq (n-1)a^{n-1} + (n-1)a$$

for $a > 1$, with the left equality if and only if $T \cong P_n$, and with the right equality if and only if $T \cong S_n$.

Lemma 2.4 ([21])**.** *Let U be a unicyclic graph of order n. Then*

$$2na^2 \leq SEI_a(U) \leq (n-1)a^{n-1} + 4a^2 + (n-3)a$$

for $a > 1$, with the left equality if and only if $U \cong C_n$, and with the right equality if and only if $U \cong \mathscr{C}_{n,1}$.

Theorem 2.5. *Let $G \in \mathscr{C}_1(n,k)$. Then*

$$SEI_a(G) \leq (n-1)a^{n-1} + 4ka^2 + (n-2k-1)a$$

for $a > 1$, with equality if and only if $G \cong \mathscr{C}_{n,k}$.

Proof. Choose $G \in \mathscr{C}_1(n,k)$ such that G has the maximum SEI_a for $a > 1$. If $k = 0$, by Lemma 2.3, the result holds. Thus in what follows, we always suppose $k \geq 1$. Let C be a cycle of G. Denote $V_C^* = \{x \mid d_G(x) \geq 3, x \in V(C)\}$.

Claim 1. $|V_C^*| = 1$.

To the contrary assume $|V_C^*| \geq 2$. Then there exist $x, y \in V_C^*$ such that $d_G(y) \geq d_G(x) \geq 3$. Denote $N_G(x) \setminus V(C) = \{x_1, x_2, \ldots, x_r\}$, where $r \geq 1$. Since $G \in \mathscr{C}_1(n,k)$ and $x, y \in V(C)$, then $N_G(y) \cap \{x_1, x_2, \ldots, x_r\} = \emptyset$. Let $H_1 = G - \{xx_1, xx_2, \ldots, xx_r\} + \{yx_1, yx_2, \ldots, yx_r\}$. Clearly, $H_1 \in \mathscr{C}_1(n,k)$. By Lemma 2.2,

$$\begin{aligned} SEI_a(H_1) - SEI_a(G) &= (d_G(y)+r)a^{d_G(y)+r} + (d_G(x)-r)a^{d_G(x)-r} \\ &\quad - d_G(x)a^{d_G(x)} - d_G(y)a^{d_G(y)} > 0 \end{aligned}$$

for $a > 1$, a contradiction.

Claim 2. If xy is an edge which is not contained in any cycle of G, then $d_G(x) = 1$ or $d_G(y) = 1$.

On the contrary suppose $d_G(y) \geq d_G(x) \geq 2$. Denote $N_G(x) \setminus \{y\} = \{x_1, x_2, \ldots, x_s\}$, where $s \geq 1$. Since $G \in \mathscr{C}_1(n,k)$ and xy is not contained in any cycle of G, then $N_G(y) \cap \{x_1, x_2, \ldots, x_s\} = \emptyset$. Let $H_2 = G - \{xx_1, xx_2, \ldots, xx_s\}$

$+\{yx_1, yx_2, \ldots, yx_s\}$. Clearly, $H_2 \in \mathscr{C}_1(n,k)$. The rest proof is similar to Claim 1.

By Claims 1 and 2, it follows that all pendant edges and cycles of G have a vertex in common. Next, we will prove that each cycle of G is of length 3.

Assume there is a cycle C' of G with length at least 4. Let $C' = z_1z_2 \cdots z_tz_1$, where $t \geq 4$. Suppose without loss of generality that $d_G(z_1) \geq d_G(z_i)$, $i = 2, 3, \ldots, t$. It is evident that $d_G(z_1) \geq 2$. Let $G' = G - z_2z_3 + z_1z_3$. Then $G' \in \mathscr{C}_1(n,k)$. By Lemma 2.2,

$$\begin{aligned} SEI_a(G') - SEI_a(G) &= (d_G(z_1)+1)a^{d_G(z_1)+1} + a \\ &\quad - d_G(z_1)a^{d_G(z_1)} - 2a^2 > 0 \end{aligned}$$

for $a > 1$, a contradiction.

Thus all cycles of G are of length 3 and this implies that $G \cong \boldsymbol{\mathscr{C}}_{n,k}$. $\square$

Let $G \in \mathscr{C}_1(n,k)$. By Lemmas 2.3 and 2.4, the minimum $SEI_a(G)$ $(a > 1)$ had been determined for $k = 0, 1$. In the following, we assume $k \geq 2$.

Theorem 2.6. *Let $G \in \mathscr{C}_1(n,k)$ and $n = 2k + l$, where $k \geq 2$. Then*

$$SEI_a(G) \geq \begin{cases} 4(k-l)a^4 + 6(l-1)a^3 + 2(k+2)a^2, & \text{if } 1 \leq l \leq k-1, \\ 6(k-1)a^3 + 2(l+2)a^2, & \text{if } l \geq k \end{cases}$$

for $a > 1$, with equality if and only if G has the degree sequence $(\underbrace{4, \ldots, 4}_{k-l}, \underbrace{3, \ldots, 3}_{2l-2}, \underbrace{2, \ldots, 2}_{k+2})$ when $1 \leq l \leq k-1$, and $(\underbrace{3, \ldots, 3}_{2k-2}, \underbrace{2, \ldots, 2}_{l+2})$ when $l \geq k$.

Proof. Choose $G \in \mathscr{C}_1(n,k)$ such that G has the minimum SEI_a for $a > 1$. Let $C_1, C_2, \ldots, C_k$ be all cycles of G and $V(C) = \cup_{i=1}^{k} V(C_i)$.

Claim 3. For any $x \in V(G)$, $d_G(x) \geq 2$.

Assume there is $x \in V(G)$ with $d_G(x) = 1$. Since $G \in \mathscr{C}_1(n,k)$ and $k \geq 2$, then there are a cycle C_r $(1 \leq r \leq k)$ and a vertex $y \in V(C_r)$ such that x connects y by a path P in G and $V(C) \cap V(P) = \{y\}$. It is clear that $d_G(y) \geq 3$. Set $z \in V(C_r)$ with $yz \in E(G)$. Let $H_1 = G - yz + zx$. Then $H_1 \in \mathscr{C}_1(n,k)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G) - SEI_a(H_1) &= d_G(y)a^{d_G(y)} + a \\ &\quad - (d_G(y)-1)a^{d_G(y)-1} - 2a^2 > 0 \end{aligned}$$

for $a > 1$, a contradiction.

Claim 4. For any $x \in V(C)$, $d_G(x) \leq 4$.

Assume there are a cycle C_s $(1 \leq s \leq k)$ and a vertex $x \in V(C_s)$ such that $d_G(x) \geq 5$. Denote $N_G(x) \setminus V(C_s) = \{x_1, x_2, \ldots, x_t\}$, where $t \geq 3$. Let G_i be the components containing x_i in $G - x$, where $1 \leq i \leq t$. We prove this claim in two cases.

Case 1. There exists G_i, without loss of generality say G_1, such that $G_1 \neq G_j$ for each $2 \leq j \leq t$.

Since $G \in \mathscr{C}_1(n,k)$, by Claim 3, it follows that there is a vertex $y \in V(G_2)$ such that $d_G(y) = 2$. Let $H_2 = G - xx_1 + yx_1$. Then $H_2 \in \mathscr{C}_1(n,k)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G) - SEI_a(H_2) = d_G(x)a^{d_G(x)} + 2a^2 \\ - (d_G(x)-1)a^{d_G(x)-1} - 3a^3 > 0 \end{aligned}$$

for $a > 1$, a contradiction.

Case 2. For each i $(1 \leq i \leq t)$, there exists G_j such that $G_i = G_j$, where $i \neq j$, $1 \leq j \leq t$.

In this case, it is easy to see that $d_G(x) \geq 6$. Suppose without loss of generality that $G_1 = G_2$. Since G is a cactus graph, then x_1, x_2 are contained in a common cycle and $G_1 \neq G_3$. By Claim 3, there is $y \in V(G_3)$ such that $d_G(y) = 2$. Let $H_3 = G - xx_1 - xx_2 + yx_1 + yx_2$. Then $H_3 \in \mathscr{C}_1(n,k)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G) - SEI_a(H_3) = d_G(x)a^{d_G(x)} + 2a^2 \\ - (d_G(x)-2)a^{d_G(x)-2} - 4a^4 > 0 \end{aligned}$$

for $a > 1$, a contradiction.

Claim 5. For any $x \notin V(C)$, $d_G(x) \leq 3$.

Assume there is $x \notin V(C)$ with $d_G(x) \geq 4$. Denote $N_G(x) = \{x_1, x_2, \ldots, x_r\}$, where $r \geq 4$. Let G_i be the components containing x_i in $G - x$, where $1 \leq i \leq r$. Then for $i \neq j$, $G_i \neq G_j$. Since $G \in \mathscr{C}_1(n,k)$, by Claim 3, it follows that there is a vertex $y \in V(G_2)$ such that $d_G(y) = 2$. Let $H_4 = G - xx_1 + yx_1$. Then $H_4 \in \mathscr{C}_1(n,k)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G) - SEI_a(H_4) = d_G(x)a^{d_G(x)} + 2a^2 \\ - (d_G(x)-1)a^{d_G(x)-1} - 3a^3 > 0 \end{aligned}$$

for $a > 1$, a contradiction.

Claim 6. Let $n = 2k + l$, where $k \geq 2$ and $l \geq 1$. Then $n_4 = k - l$ when $1 \leq l \leq k-1$, and $n_4 = 0$ when $l \geq k$.

Denote $V_3^*(G) = \{x \mid d_G(x) = 3, x \notin V(C)\}$. Choose $G \in \mathscr{C}_1(n,k)$ such that $|V_3^*(G)|$ is as small as possible. Next, we will prove that $|V_3^*(G)| = 0$.

Assume there is a vertex $x \in V_3^*(G)$. Denote $N_G(x) = \{x_1, x_2, x_3\}$. By Claim 3, it follows that there is a vertex y with $d_G(y) = 2$ such that y and x_1 aren't contained in the same component in $G - x$. Let $H_5 = G - xx_1 + yx_1$. Then $H_5 \in \mathscr{C}_1(n,k)$ and $SEI_a(G) = SEI_a(H_5)$, but $|V_3^*(H_5)| < |V_3^*(G)|$, a contradiction. Thus $|V_3^*(G)| = 0$.

Since G is a cactus graph, then $n_4 = k-1$ when $l = 1$, and $n_4 \geq k - l$ when $2 \leq l \leq k-1$. Suppose $n_4 \geq k - l + 1 \geq 1$. By Claims 3, 4 and $|V_3^*(G)| = 0$, it follows that there is one cycle with length at least 4 or an internal path with length at least 2. Denote $V_4 = \{x \mid d_G(x) = 4, x \in V(G)\}$. Choose $y \in V_4$

such that $y \in V(C_i)$ ($i \in \{1, 2, \ldots, k\}$) and $(V(C_i) \setminus \{y\}) \cap V_4 = \emptyset$. By the definition of SEI_a, suppose without loss of generality that the length of C_i is at least 4. Set $C_i = v_1(= y)v_2 \cdots v_r v_1$, $r \geq 4$. Let $H_6 = G - v_1v_2 + v_rv_2$. Then $H_6 \in \mathscr{C}_1(n, k)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G) - SEI_a(H_6) = d_G(y)a^{d_G(y)} + 2a^2 \\ - (d_G(y) - 1)a^{d_G(y)-1} - 3a^3 > 0 \end{aligned}$$

for $a > 1$, a contradiction.

If $l \geq k$, by the same argument, we can prove that $n_4 = 0$.

Now we finish the proof of the theorem. If $1 \leq l \leq k-1$, by Claims 3, 4 and 5, it follows that $2 \leq d_G(u) \leq 4$ for each vertex $u \in V(G)$ and $n_i = 0$ for $i \geq 5$. By Claim 6, $n_4 = k - l$. Furthermore, since $G \in \mathscr{C}_1(n, k)$, we have

$$\begin{cases} n_2 + n_3 + n_4 = n = 2k + l, \\ 2n_2 + 3n_3 + 4n_4 = 2(n + k - 1). \end{cases}$$

Thus, we can get that $n_2 = k + 2$ and $n_3 = 2l - 2$.

If $l \geq k$, by Claims 3 and 6, it follows that $2 \leq d_G(u) \leq 3$ for each vertex $u \in V(G)$ and $n_i = 0$ for $i \geq 4$. Furthermore, since $G \in \mathscr{C}_1(n, k)$, we have

$$\begin{cases} n_2 + n_3 = n = 2k + l, \\ 2n_2 + 3n_3 = 2(n + k - 1). \end{cases}$$

Thus, we can get that $n_2 = l + 2$ and $n_3 = 2k - 2$. □

3. Variable sum exdeg indices of cactus graphs with p pendant vertices for $a > 1$

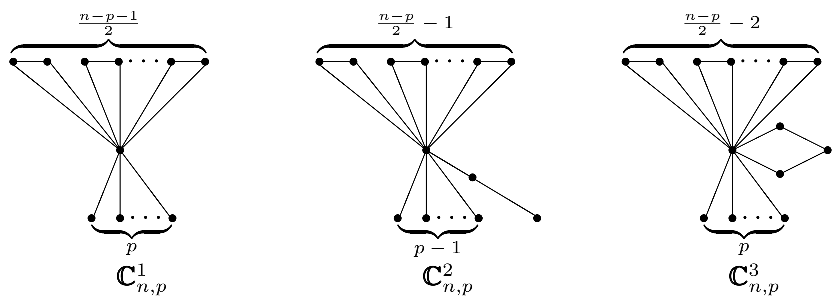

Fig. 2. The graphs $\mathbb{C}^1_{n,p}$, $\mathbb{C}^2_{n,p}$ and $\mathbb{C}^3_{n,p}$.

By the definition of SEI_a and Lemma 2.1, it is easy to obtain the following Lemmas 3.1 and 3.2.

Lemma 3.1. *Let $G \in \mathscr{C}_2(n, p)$ and G' be the graph obtained from G by transformation A_i, $i = 1, 2, 3$, as shown in Fig. 3. Then $SEI_a(G') > SEI_a(G)$ for $a > 1$.*

Lemma 3.2. *Let $G \in \mathscr{C}_2(n,p)$ and G' be the graph obtained from G by transformation A_4, as shown in Fig. 3. Then $SEI_a(G') = SEI_a(G)$ for $a > 1$.*

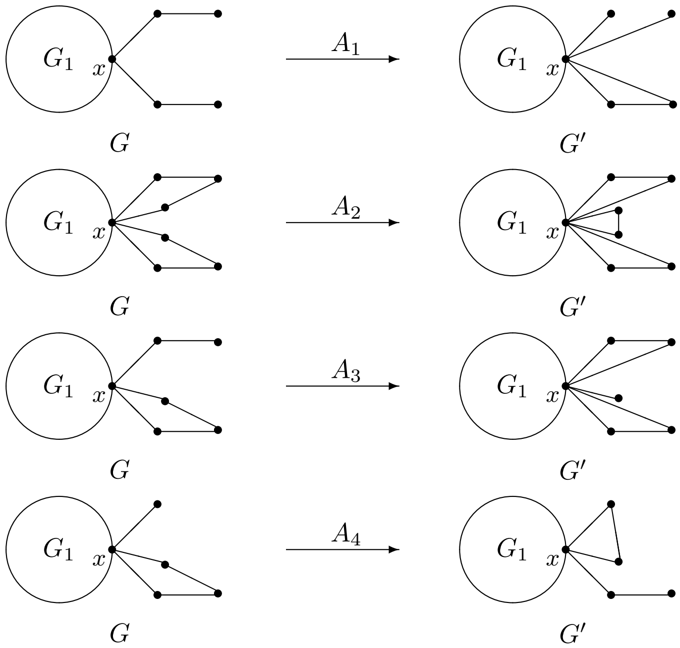

Fig. 3. Transformations A_1, A_2, A_3 and A_4

Theorem 3.3. *Let $G \in \mathscr{C}_2(n,p)$, where $n \geq 5$ and $0 \leq p \leq n-3$. Then for $a > 1$, we have*

(i) *If $n-p$ is odd,*

$$SEI_a(G) \leq (n-1)(a^{n-1} + 2a^2) + (a - 2a^2)p$$

with equality if and only if $G \cong \mathbb{C}^1_{n,p}$, where $\mathbb{C}^1_{n,p}$ is shown in Fig. 2.

(ii) *If $n-p$ is even,*

$$SEI_a(G) \leq (n-2)a^{n-2} + 2(n-1)a^2 + (a - 2a^2)p$$

with equality if and only if $G \cong \mathbb{C}^2_{n,p}$ or $\mathbb{C}^3_{n,p}$, where $\mathbb{C}^2_{n,p}$ and $\mathbb{C}^3_{n,p}$ are shown in Fig. 2.

Proof. Choose $G \in \mathscr{C}_2(n,p)$ such that G has the maximum SEI_a for $a > 1$. Next, some claims will be given.

Claim 1. For each path of G, which don't lie on any cycle, must be a pendant path.

Assume there is a internal path $P = x_1x_2\cdots x_t$ ($t \geq 2$) which don't lie on any cycle in G. Suppose without loss of generality that $d_G(x_1) \geq d_G(x_t)$. Denote

$y \in (N_G(x_t) \setminus \{x_{t-1}\})$. Let $G_1 = G - x_t y + x_1 y$. Obviously, $G_1 \in \mathscr{C}_2(n,p)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G_1) - SEI_a(G) = (d_G(x_1)+1)a^{d_G(x_1)+1} + (d_G(x_t)-1)a^{d_G(x_t)-1} \\ - d_G(x_1)a^{d_G(x_1)} - d_G(x_t)a^{d_G(x_t)} > 0 \end{aligned}$$

for $a > 1$, a contradiction.

Claim 2. Each pendant path of G is of length at least 2.

Assume there is a pendant path $P = y_0 y_1 \cdots y_s$ with length $s \geq 3$ in G, where $d_G(y_0) \geq 3$, $d_G(y_s) = 1$. Let $G_2 = G - y_2 y_3 + \{y_0 y_2, y_0 y_3\}$. Obviously, $G_2 \in \mathscr{C}_2(n,p)$. By Lemma 2.1, we have

$$SEI_a(G_2) - SEI_a(G) = (d_G(y_0)+2)a^{d_G(y_0)+2} - d_G(y_0)a^{d_G(y_0)} > 0$$

for $a > 1$, a contradiction.

Claim 3. No cycle of G is of length greater than 4.

Assume there is a cycle $C = z_0 z_1 \cdots z_r z_0$ with length $r \geq 4$ in G. Let $G_3 = G - z_2 z_3 + \{z_0 z_2, z_0 z_3\}$. Obviously, $G_3 \in \mathscr{C}_2(n,p)$. By Lemma 2.1, we have

$$SEI_a(G_3) - SEI_a(G) = (d_G(z_0)+2)a^{d_G(z_0)+2} - d_G(z_0)a^{d_G(z_0)} > 0$$

for $a > 1$, a contradiction.

Claim 4. If G contains at least two cycles, then all cycles have a common vertex.

On the contrary, choose C_1 and C_2 are a pair of vertex disjoint cycles such that the length of the path connecting C_1 and C_2 is as small as possible. Let $P = u_0 u_1 \cdots u_l$ ($l \geq 1$) be the path connecting C_1 and C_2, where $u_0 \in V(C_1)$ and $u_l \in V(C_2)$. Suppose without loss of generality that $d_G(u_0) \geq d_G(u_l)$. Denote $N_{C_2}(u_l) = \{v_1, v_2\}$. We prove this claim in two cases.

Case 1. All edges of P lie on some cycle C_3 of G.

Let $G_4 = G - \{u_l v_1, u_l v_2\} + \{u_0 v_1, u_0 v_2\}$. Obviously, $G_4 \in \mathscr{C}_2(n,p)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G_4) - SEI_a(G) = (d_G(u_0)+2)a^{d_G(u_0)+2} + (d_G(u_l)-2)a^{d_G(u_l)-2} \\ - d_G(u_0)a^{d_G(u_0)} - d_G(u_l)a^{d_G(u_l)} > 0 \end{aligned}$$

for $a > 1$, a contradiction.

Case 2. All edges of P do not lie on any cycle of G.

Let $G_5 = G - u_l v_1 + u_0 v_1$. Obviously, $G_5 \in \mathscr{C}_2(n,p)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G_5) - SEI_a(G) = (d_G(u_0)+1)a^{d_G(u_0)+1} + (d_G(u_l)-1)a^{d_G(u_l)-1} \\ - d_G(u_0)a^{d_G(u_0)} - d_G(u_l)a^{d_G(u_l)} > 0 \end{aligned}$$

for $a > 1$, a contradiction again.

If G has at least two cycles, we use z to denote the common vertex of all cycles.

Claim 5. If G has at least two cycles, then no non-trivial tree attached to a cycle C on a vertex $z' \in V(C)$, $z' \neq z$.

Denote $N_G(z') \setminus V(C) = \{w_1, w_2, \ldots, w_k\}$ and $N_G(z) \setminus V(C) = \{v_1, v_2, \ldots, v_r\}$.

If $d_G(z) \geq d_G(z')$, let $G_6 = G - \{z'w_1, z'w_2, \ldots, z'w_k\} + \{zw_1, zw_2, \ldots, zw_k\}$. Obviously, $G_6 \in \mathscr{C}_2(n,p)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G_6) - SEI_a(G) = (d_G(z) + k)a^{d_G(z)+k} + (d_G(z') - k)a^{d_G(z')-k} \\ - d_G(z)a^{d_G(z)} - d_G(z')a^{d_G(z')} > 0 \end{aligned}$$

for $a > 1$, a contradiction.

If $d_G(z) < d_G(z')$, let $G_7 = G - \{zv_1, zv_2, \ldots, zv_r\} + \{z'v_1, z'v_2, \ldots, z'v_r\}$. Obviously, $G_7 \in \mathscr{C}_2(n,p)$. By Lemma 2.2, we have

$$\begin{aligned} SEI_a(G_6) - SEI_a(G) = (d_G(z) - r)a^{d_G(z)-r} + (d_G(z') + r)a^{d_G(z')+r} \\ - d_G(z)a^{d_G(z)} - d_G(z')a^{d_G(z')} > 0 \end{aligned}$$

for $a > 1$, a contradiction again.

Now, we complete the proof of the theorem. By Lemmas 3.1 and 3.2, it can be seen that G satisfies the following properties:

(i) There exists at most one pendant path of length 2;

(ii) There exists at most one cycle of length 4;

(iii) G doesn't have a pendant path of length 2 and a cycle of length 4 simultaneously.

Moreover, combining Claims 1-5, it follows that $G \cong \mathbb{C}^1_{n,p}$, $\mathbb{C}^2_{n,p}$ or $\mathbb{C}^3_{n,p}$. $\square$

By a simple calculation,we have

$$SEI_a(\mathbb{C}^1_{n,p}) > SEI_a(\mathbb{C}^2_{n,p}) = SEI_a(\mathbb{C}^3_{n,p}).$$

So we can obtain the following corollary immediately.

Corollary 3.4. *Let $G \in \mathscr{C}_2(n,p)$, where $n \geq 5$ and $0 \leq p \leq n-3$. Then for $a > 1$, we have*

$$SEI_a(G) \leq (n-1)(a^{n-1} + 2a^2) + (a - 2a^2)p$$

with equality if and only if $G \cong \mathbb{C}^1_{n,p}$.

It is evident that for $a > 1$, $g(p) = (n-1)(a^{n-1} + 2a^2) + (a - 2a^2)p$ is decreasing in p. Then $g(p) \leq g(0) = (n-1)(a^{n-1} + 2a^2)$. Thus, we have the following corollary.

Corollary 3.5. *Let G be a cactus graph of order n, where $n \geq 5$. Then for $a > 1$, we have*

$$SEI_a(G) \leq (n-1)(a^{n-1} + 2a^2)$$

with equality if and only if $G \cong \mathbb{C}^1_{n,0}$.

Lemma 3.6 ([21])**.** *Let T be an n-vertex tree with p pendant vertices. Then*

$$SEI_a(T) \geq 3(p-2)a^3 + 2(n-2p+2)a^2 + pa$$

for $a > 1$, with equality if and only if T is a tree with p vertices of degree 1, $n-2p+2$ vertices of degree 2 and $p-2$ vertices of degree 3.

Theorem 3.7. *Let $G \in \mathscr{C}_2(n,p)$, where $n \geq 3$ and $0 \leq p \leq n-2$. Then for $a > 1$, we have*

(i) *If $p = 0, 1$,*

$$SEI_a(G) \geq 3pa^3 + 2(n-2p)a^2 + pa$$

with equality if and only if G has the degree sequence $(\underbrace{3,\dots,3}_{p}, \underbrace{2,\dots,2}_{n-2p}, \underbrace{1,\dots,1}_{p})$.

(ii) *If $p \geq 2$,*

$$SEI_a(G) \geq 3(p-2)a^3 + 2(n-2p+2)a^2 + pa$$

with equality if and only if G has the degree sequence $(\underbrace{3,\dots,3}_{p-2}, \underbrace{2,\dots,2}_{n-2p+2}, \underbrace{1,\dots,1}_{p})$.

Proof. Choose $G \in \mathscr{C}_2(n,p)$ such that G has the minimum SEI_a for $a > 1$.

Claim 1. For $p \leq 1$, G is a unicyclic graph.

For $p = 0$ or 1, G must have at least one cycle since otherwise G is a tree with $p \geq 2$. Suppose there exist at least two cycles in G.

If G contains two cycles $C_1 = x_1x_2\cdots x_rx_1$ and $C_2 = y_1y_2\cdots y_sy_1$ having a common vertex, without loss of generality say $x = x_1 = y_1$, let $G_1 = G - \{xx_2, xy_2\} + \{x_2y_2\}$. Clearly, $G_1 \in \mathscr{C}_2(n,p)$ and $d_{G_1}(x) = d_G(x) - 2$. By Lemma 2.1, we have $SEI_a(G_1) < SEI_a(G)$ for $a > 1$, a contradiction. Otherwise, choose two cycles C_1' and C_2' such that C_1' connecting C_2' by a path $P = z_1z_2\cdots z_t$, where $V(C_1') \cap V(P) = \{z_1\}$, $V(C_2') \cap V(P) = \{z_t\}$ and P has no common vertices with any other cycles except C_1' and C_2'. Denote $N_{C_1'}(z_1) = \{u_1, u_2\}$ and $N_{C_2'}(z_t) = \{v_1, v_2\}$. Let $G_1 = G - \{u_1z_1, v_1z_t\} + \{u_1v_1\}$. Clearly, $G_2 \in \mathscr{C}_2(n,p)$. By Lemma 2.1, we have $SEI_a(G_1) < SEI_a(G)$ for $a > 1$, a contradiction again.

Claim 2. For $p \geq 2$, G is a tree.

Suppose G is not a tree, let x, y be two pendant vertices and C be a cycle of G. Denote $P_1 = x_1x_2\cdots x_r$ $(x = x_1)$ is the path from x to C, and $P_2 = y_1y_2\cdots y_s$ $(y = y_s)$ is a pendant path of G, where $x_r \in V(C)$, $d_G(y_1) \geq 3$. Let $z \in \big(V(C) \cap N_C(x_r)\big) \setminus \{y_1\}$ and $G_2 = G - \{x_rz, y_1y_2\} + \{zy_2\}$. Clearly, $G_1 \in \mathscr{C}_2(n,p)$. By Lemma 2.1, we have $SEI_a(G_2) < SEI_a(G)$ for $a > 1$, a contradiction.

By Claims 1, 2 and Lemma 3.6, the theorem holds. □

4. Conclusions

In [21], Vukičević proposed that mathematical properties of the variable sum exdeg index deserves further study since it can be applied in detecting the chemical compounds that may have desirable properties. Namely, if one can find some properties well-correlated with this descriptor for some value of a, then extremal graphs should correspond to molecules with minimum or maximum value of that property. Furthermore, one such property has already been found (see [19]). Since cactus graphs represent some important class of molecules, so our results are meaningful.

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Jianwei Du
School of Science
North University of China
Taiyuan, 030051, P. R. China
Email address: jianweidu@nuc.edu.cn

Xiaoling Sun
School of Science
North University of China
Taiyuan, 030051, P. R. China
Email address: sunxiaoling@nuc.edu.cn