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On the extremal cactus graphs for variable sum exdeg index with a fixed number of cycles

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ABSTRACT

The variable sum exdeg index, introduced by Vukičević [Croat. Chem. Acta 84 (2011) 87–91] for predicting the octanol-water partition coefficient of certain chemical compounds, of a graph G is defined as $\mathrm{SEI}_a(G) = \sum_{v \in V(G)} d_v a^{d_v}$, where a is any positive real number different from 1, $V(G)$ is the vertex set of G and d_v denotes the degree of a vertex v. A connected graph G is a cactus if and only if every edge of G lies on at most one cycle. For $n > 3$ and $k \geq 0$, let $\mathcal{C}_{n,k}$ be the class of all n-vertex cacti with k cycles. The present paper is devoted to find the graphs with minimal and maximal SEI_a values among all the members of the graph class $\mathcal{C}_{n,k}$ for $a > 1$.

KEYWORDS

Topological index; variable sum exdeg index; extremal problem; cactus graph

2010 MATHEMATICS SUBJECT CLASSIFICATION

05C07; 05C35

1. Introduction

Throughout this paper, we discuss only simple and connected graphs. Vertex set and edge of a graph G will be denoted by $V(G)$ and $E(G)$, respectively. Degree of a vertex $v \in V(G)$ will be denoted by $d_v(G)$ (or simply by d_v if the graph under consideration is clear). The (chemical) graph theoretical terminology, not defined here, can be found in some relevant standard books, like [4, 11].

In order to predict physicochemical properties of chemical compounds, graphs are usually used to model molecules [8, 11]. In molecular graphs, vertices correspond to the atoms while edges represent the covalent bonds between atoms [9, 12]. Among the various existing techniques for handling the issues of predicting physicochemical properties of chemical compounds and seeking combinatorial libraries to find molecular structures that are generally comparative to a target structure, the method involving topological indices is one of the simplest and most widely used such techniques [1, 3, 6, 16, 17]. Topological indices are actually those numerical quantities of (molecular) graph which remain same under graph isomorphism [8]. In order to predict the octanol-water partition coefficient of some particular type of molecules, Vukičević [14] devised the following topological index and called it as the *variable sum exdeg index*:

$$\mathrm{SEI}_a(G) = \sum_{v \in V(G)} d_v a^{d_v},$$

where a is any positive real number different from 1.

Due to chemical applicability of the topological index SEI_a, several papers concerning the mathematical properties of SEI_a have been appeared in literature. Vukičević [13] initiated the mathematical study of the topological index SEI_a by addressing the extremal problems for SEI_a against ten well-known graph classes. Using the definition of SEI_a, Yarahmadi and Ashrafi [15] introduced the variable sum exdeg polynomial and explored some mathematical aspects of this polynomial. For $a > 1$, Ghalavand and Ashrafi [7] solved some extremal problems for SEI_a using the concept of majorization. Ali and Dimitrov [2] gave alternative proofs of four main results proved in [7] and extended one of the theorems proved in [7]. Khalid and Ali [10] investigated the properties of the variable sum exdeg index SEI_a of trees having a fixed number of vertices and vertices with a prescribed degree. Recently, Dimitrov and Ali [5] attempted the problem of finding graphs with a fixed number of vertices and cyclomatic number (the minimum number of edges of a graph whose removal give a graph containing no cycle).

A graph G is a cactus if and only if every edge of G lies on at most one cycle. For $n \geq 4$ and $k \geq 0$, let $\mathcal{C}_{n,k}$ be the class of all n-vertex cacti with k cycles. The main purpose of this paper is to find the graphs with minimal and maximal SEI_a values among all the members of the graph class $\mathcal{C}_{n,k}$ for $a > 1$.

2. Main results

Firstly, we attempt the problem of finding graphs with minimal SEI_a value from the class $\mathcal{C}_{n,k}$ for $a > 1$. We recall that for $k = 0$ and $k = 1$ this problem has already been solved in [5, 7, 13], because the classes $\mathcal{C}_{n,0}$ and $\mathcal{C}_{n,1}$ are actually the classes of all n-vertex tree and unicyclic graphs, respectively. We note that there is a unique cactus graph for $k \geq 2$

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and $n = 5$. Thus, the aforementioned problem concerning minimal SEI_a value make sense if $n \geq 6$ for $k \geq 2$. Before moving further, we prove a lemma for SEI_a concerning the degree sequence of two graphs.

Lemma 2.1. *Let c be a positive even integer and $d_i \geq d_j + c$. If G and G' are graphs with degree sequences $(d_1, d_2, \ldots, d_{i-1}, d_i, d_{i+1}, \ldots, d_{j-1}, d_j, d_{j+1}, \ldots, d_n)$ and $(d_1, d_2, \ldots, d_{i-1}, d_i - \frac{c}{2}, d_{i+1}, \ldots, d_{j-1}, d_j + \frac{c}{2}, d_{j+1}, \ldots, d_n)$, respectively, then $SEI_a(G) > SEI_a(G')$ for $a > 1$.*

Proof. By using the definition of the variable sum exdeg index SEI_a, we have

$$\begin{aligned} SEI_a(G) - SEI_a(G') &= d_i a^{d_i} - \left(d_i - \frac{c}{2}\right) a^{d_i - \frac{c}{2}} \\ &\quad - \left[\left(d_j + \frac{c}{2}\right) a^{d_j + \frac{c}{2}} - d_j a^{d_j}\right] \\ &\geq \frac{c}{2}\left[a^{\Theta_1}(1 + \Theta_1 \ln a) - a^{\Theta_2}(1 + \Theta_2 \ln a)\right], \end{aligned}$$

where

$$d_i - \frac{c}{2} < \Theta_1 < d_i$$

and

$$d_j < \Theta_2 < d_j + \frac{c}{2}.$$

As $d_i \geq d_j + c$, we have $\Theta_1 > \Theta_2$ and hence the desired result follows. $\square$

For a graph G, $V^* \subset V(G), E^* \subseteq E(G)$ and $E^{**} \subseteq E(\bar{G})$ where $V^* \cap \{u, v\} = \emptyset$ for all $uv \in E^{**}$, let $G - V^* - E^* + E^{**}$ be the graph obtained from G by removing the elements of V^* and E^*, and adding the edges of E^{**}, where $\bar{G}$ is the complement of G. If some of the aforementioned sets V^*, E^* and E^{**} in the notation $G - V^* - E^* + E^{**}$ are empty, we do not write those empty sets; for example, if E^* is empty then we write $G - V^* + E^{**}$ instead of $G - V^* - \emptyset + E^{**}$. The cyclomatic number $\nu(G)$ of G is the minimum number of edges of G whose removal from G gives a graph containing no cycle.

Lemma 2.2. *For $\nu \geq 1, n \geq 6$ and $a > 1$, if G has minimal SEI_a value among all the n-vertex graphs with cyclomatic number ν, then minimum degree of G is at least 2.*

Proof. Suppose to the contrary that $v \in V(G)$ is a vertex of degree 1. Since $\nu \geq 1$, let $P : vv_1v_2 \cdots v_r$ be a path in G provided that v_r is the unique vertex of degree at least 3 of P in G. Let u be a neighbor of v_r in G. If $G' \cong G - \{v_r u\} + \{uv\}$, then by using Lemma 2.1, we have $SEI_a(G) > SEI_a(G')$, which is a contradiction to the definition of G. $\square$

The following result is an immediate consequence of Lemma 2.2.

Corollary 2.3. *For $k \geq 2, n \geq 6$ and $a > 1$, if G has minimal SEI_a value among all the members of $\mathcal{C}_{n,k}$, then minimum degree of G is 2.*

For a graph G, the set of vertices adjacent to a vertex $v \in V(G)$ is denoted by $N_G(v)$.

Lemma 2.4. *For $k \geq 2, n \geq 6$ and $a > 1$, if G has minimal SEI_a value among all the members of $\mathcal{C}_{n,k}$, then every vertex of G, which does not lie on any cycle of G, has degree at most 3.*

Proof. Suppose to the contrary that $v \in V(G)$ does not lie on any cycle of G but $d_v = r \geq 4$. Let $N_G(u) = \{v_1, v_2, \ldots, v_r\}$. For $i = 1, 2, \ldots, r$, let H_i be the component of $G - v$, containing v_i. It is clear that $H_i \ncong H_j$ for $i \neq j$ (if $H_i \cong H_j$ for some $i \neq j$ then there exists a v_i-v_j path in $G - \{v\}$ and this path together with the path $v_i v v_j$ generates a cycle (in G) containing v, a contradiction). From Corollary 2.3 and the fact that G is a cactus graph, it follows that there exists a vertex $u \in V(H_2)$ of degree 2. If $G' \cong G - \{v_1 v\} + \{v_1 u\}$ then from Lemma 2.1, it follows that $SEI_a(G) > SEI_a(G')$, which is a contradiction. $\square$

Lemma 2.5. *For $k \geq 2, n \geq 6$ and $a > 1$, if G has minimal SEI_a value among all the members of $\mathcal{C}_{n,k}$ and if u is any vertex on some cycle of G, then $d_u \leq 4$.*

Proof. Let C be a cycle in G. Suppose to the contrary that there exists a vertex $v \in V(C)$ of degree at least 5. Let $N_G(v) \setminus V(C) := \{v_1, v_2, \ldots, v_r\}$. For $i = 1, 2, \ldots, r$, let H_i be the component of $G - \{v\}$, containing v_i. We claim that at most two vertices from the set $N_G(v) \setminus V(C)$ belong to the same component of $G - \{v\}$. Contrarily, without loss of generality, we assume that $H_1 \cong H_2 \cong H_3$. Then, the path v_1-v_3, containing the vertex v_2, together with the edges $v_1 v, v_3 v$, generate a cycle whose every edge lies on more than one cycle in G because $v_2 v \in E(G)$, which is a contradiction to the definition of a cactus graph.

Case 1. There exists a component of $G - \{v\}$ containing exactly one vertex of $N_G(v) \setminus V(C)$.
Without loss of generality, we assume that H_1 does not contain any of the vertices $v_2, v_3, \cdots, v_r$. Then, by Corollary 2.3, there exists a vertex $u \in V(H_2)$ of degree 2. It is clear that $G' \cong G - \{vv_1\} + \{uv_1\} \in \mathcal{C}_{n,k}$. But, by Lemma 2.1, we have $SEI_a(G) > SEI_a(G')$, a contradiction.

Case 2. Every component of $G - \{v\}$ contains exactly two vertices of $N_G(v) \setminus V(C)$.
In this case, we have $d_v \geq 6$. Without loss of generality, we assume that $H_1 \cong H_2$. Clearly, $H_3 \ncong H_1$ and there exists a vertex $w \in V(H_3)$ of degree 2, by Corollary 2.3. If $G'' \cong G - \{vv_1, vv_2\} + \{wv_1, wv_2\}$ then again by Lemma 2.1, we have $SEI_a(G) > SEI_a(G'')$, a contradiction. $\square$

Lemma 2.6. *For $k \geq 2, n \geq 6$ and $a > 1$, if $G \in \mathcal{C}_{n,k}$ has a cycle of length at least 4 containing an edge, whose end vertices have degrees 2 and 4, then there exists $G' \in \mathcal{C}_{n,k}$ such that $SEI_a(G) > SEI_a(G')$.*

Proof. Let $uv \in E(G)$ be an edge on a cycle C of length at least 4 in G such that $d_u = 4$ and $d_v = 2$. Let v' $(\neq v)$ be the other neighbor of u on C. Evidently, the graph $G' \cong G - \{v'u\} + \{v'v\}$ belongs to $\mathcal{C}_{n,k}$. On the other hand, Lemma 2.1 ensures that $SEI_a(G) > SEI_a(G'')$. $\square$

Let $\mathcal{C}_{n,k}^*$ be the class of all those members of $\mathcal{C}_{n,k}$ which satisfy the following constraints

- minimum degree is 2,
- maximum degree is at most 4,
- all those vertices which do not lie on any cycle have degree at most 3,
- does not have any cycle of length at least 4 containing an edge, whose end vertices have degrees 2 and 4.

Now, we are in position to state and prove the first main result of this paper.

Theorem 2.7. *For $k \geq 2, n \geq 6$ and $a > 1$, if G has minimal SEI_a value among all the members of $\mathcal{C}_{n,k}$ then $G \in \mathcal{C}_{n,k}^*$.*

Proof. The result follows directly from Corollary 2.3 and Lemmas 2.4, 2.5, 2.6. □

The n-vertex star graph is denoted by S_n. Let $S_n^{(k)}$ be the cactus obtained from S_n by adding $k \geq 1$ mutually independent edges and take $S_n \cong S_n^{(0)}$. Next, we prove that $S_n^{(k)}$ is the unique graph with maximal SEI_a value among all the members of the graph class $\mathcal{C}_{n,k}$ for $a > 1$. In order to prove this fact, we need the following already known result.

Lemma 2.8. [2, 5, 7, 13] *Among all the n-vertex tree (unicyclic) graphs, the star ($S_n^{(1)}$, respectively) is the unique graph with maximal SEI_a value for $a > 1$.*

The following lemma will also be useful in proving the second main result of this paper.

Lemma 2.9. *Let*

$$f(x) = xa^x - (x-p)a^{x-p},$$

where $x > p \geq 1$ and $a > 1$. Then the function f is increasing.

Proof. Note that

$$f'(x) = a^x(1 + x \ln a) - a^{x-p}(1 + (x-p)\ln a).$$

The assumptions $x > p \geq 1$ and $a > 1$ give

$$a^x(1 + x\ln a) > a^x(1 + (x-p)\ln a) > a^{x-p}(1 + (x-p)\ln a).$$

Hence, $f'(x) > 0$ for all x with $x > p \geq 1$ and $a > 1$. □

Now, we are ready to prove the second main result of the present paper.

Theorem 2.10. *For $k \geq 0, n \geq 4$ and $a > 1$, $S_n^{(k)}$ is the unique graph with maximal SEI_a value among all the members of $\mathcal{C}_{n,k}$.*

Proof. Let G be any cactus graph in the collection $\mathcal{C}_{n,k}$ where $n \geq 4$ and $k \geq 0$. Then an equivalent statement of the theorem is:

$$\mathrm{SEI}_a(G) \leq f(n,k,a)$$

with equality if and only if $G \cong S_n^{(k)}$, where

$$f(n,k,a) = \mathrm{SEI}_a(S_n^{(k)}) = (n-1)a^{n-1} + 4ka^2 + (n-2k-1)a$$

and $a > 1$.

We will prove the result by using induction on $n+k$. For $k = 0$, 1, the theorem follows directly from Lemma 2.8. Also, we note that $S_5^{(2)}$ is the unique cactus graph for $n = 5$ and $k \geq 2$. Thus, we take $G \in \mathcal{C}_{n,k}$ with $k \geq 2$ and $n \geq 6$.

Case 1. Minimum degree of G is 1.
Let $u_0 \in V(G)$ be a pendent vertex adjacent to a vertex u with $N_G(u) = \{u_0, u_1, u_2, \ldots, u_{x-1}\}$. Without loss of generality, we assume that $d_{u_i} = 1$ for $0 \leq i \leq p-1$ and $d_{u_i} \geq 2$ for $p \leq i \leq x-1$. If $G' \cong G - \{u_0, u_1, u_2, \ldots, u_{p-1}\}$, then $G' \in \mathcal{C}_{n-p,k}$ with $n - p \geq 5$ (because $k \geq 2$) and

$$\mathrm{SEI}_a(G) = \mathrm{SEI}_a(G') + pa + xa^x - (x-p)a^{x-p}.$$

By inductive hypothesis, we have

$$\mathrm{SEI}_a(G) - f(n,k,a) \leq (n-p-1)a^{n-p-1} - (n-1)a^{n-1} + xa^x - (x-p)a^{x-p}$$

with equality if and only if $G' \cong S_{n-p}^{(k)}$. Thus, Lemma 2.9 ensures that

$$\mathrm{SEI}_a(G) - f(n,k,a) \leq 0.$$

with equality if and only if $G' \cong S_{n-p}^{(k)}$ and $x = n-1$.

Case 2. Minimum degree of G is at least 2.
In this case, there must exist three vertices v_1, v_2 and w on some cycle of G such that v_1 is adjacent to both the vertices $v_2, w, d_{v_1} = d_{v_2} = 2$ and $d_w = y \geq 3$. We have two possibilities.

Subcase 2.1. The vertices v_2 and w are nonadjacent.
It is clear that $G' \cong G - \{v_1\} + \{v_2w\} \in \mathcal{C}_{n-1,k}$ and $\mathrm{SEI}_a(G) = \mathrm{SEI}_a(G') + 2a^2$. Due to the inductive hypothesis, we have

$$\mathrm{SEI}_a(G) - f(n,k,a) \leq 2a^2 - a - \left[(n-1)a^{n-1} - (n-2)a^{n-2}\right],$$

with equality if and only if $G' \cong S_{n-1}^{(k)}$. However, it holds that

$$2a^2 - a - \left[(n-1)a^{n-1} - (n-2)a^{n-2}\right] = \left[a^{\Theta_1}(1 + \Theta_1 \ln a) - a^{\Theta_2}(1 + \Theta_2 \ln a)\right] < 0$$

where $1 < \Theta_1 < 2 < n-2 < \Theta_2 < n-1$. Hence

$$\mathrm{SEI}_a(G) - f(n,k,a) < 0.$$

Subcase 2.2. The vertices v_2 and w are adjacent.
We note that $G' \cong G - \{v_1, v_2\} \in \mathcal{C}_{n-2,k-1}$ and hence

$$\mathrm{SEI}_a(G) = \mathrm{SEI}_a(G') + 4a^2 + ya^y - (y-2)a^{y-2}.$$

By inductive hypothesis, we get

$$\mathrm{SEI}_a(G) - f(n,k,a) \leq (n-3)a^{n-3} - (n-1)a^{n-1} + ya^y - (y-2)a^{y-2},$$

with equality if and only if $G' \cong S_{n-2}^{(k-1)}$. Consequently, by Lemma 2.9, we have

$$\mathrm{SEI}_a(G) - f(n,k,a) \leq 0,$$

with equality if and only if $G' \cong S_{n-2}^{(k-1)}$ and $y = n-1$.

This completes the induction and hence the proof. □

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