Communications in Combinatorics and Optimization
Vol. 6, No. 2, 2021 pp.249-257
DOI: 10.22049/CCO.2021.26865.1152

CCO
Commun. Comb. Optim.

Research Article

On the variable sum exdeg index and cut edges of graphs

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Received: 4 July 2020; Accepted: 2 January 2021
Published Online: 4 January 2021

Abstract: The variable sum exdeg index of a graph G is defined as $SEI_a(G) = \sum_{u \in V(G)} d_G(u) a^{d_G(u)}$, where $a \neq 1$ is a positive real number, $d_G(u)$ is the degree of a vertex $u \in V(G)$. In this paper, we characterize the graphs with the extremum variable sum exdeg index among all the graphs having a fixed number of vertices and cut edges, for every $a > 1$.

Keywords: Molecular descriptor, topological index, variable sum exdeg index, cut edge, clique.

AMS Subject classification: 05C05, 05C35, 92E10

1. Introduction

We start by defining some basic notions related to graph theory. All the graphs we consider in this article are finite, simple and connected. Let G be a graph with the

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vertex set $V(G)$ and edge set $E(G)$. The vertex u is called neighbor of a vertex v if there is an edge between them. The set of neighbors of a vertex u is denoted by $N_G(u)$ and let $N_G[u] = N_G(u) \cup \{u\}$. The degree of a vertex u is denoted by $d_G(u)$ and is defined as the cardinality of the set of neighbors of u. A sequence consisting of all the vertex degrees of G is called the degree sequence of G. The minimum and maximum degree of G are denoted by $\delta(G)$ and $\Delta(G)$, respectively. We will use the notations $G-u$ and $G-uv$ for the graphs obtained from G by removing a vertex u and an edge uv, respectively. Similarly $G+uv$ is a graph obtained by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$. A pendent vertex of G is a vertex of degree 1 and a vertex with degree more than 2 is called a branching vertex. Let $P : v_0, v_1, \ldots, v_r$ be a path in G such that $d_{v_1} = d_{v_2} = \cdots = d_{v_{r-1}} = 2$ for $r \geq 2$. The path P is a pendent path of G if one of the vertices v_0, v_r is pendent and the other one is branching. The path P is said to be an internal path of G if both the vertices v_0, v_r are branching.
A cut edge in G is an edge whose deletion increase the number of components of G. Let $\mathbb{G}_n^k$ be the set of graphs on n vertices and k cut edges. We denote by K_n^k the graph arises from the complete graph K_{n-k} (on $n-k$ vertices) by joining k pendent vertices to one of its vertex. Let C_n^k be the graph arises from the cycle graph C_{n-k} (on $n-k$ vertices) by joining k pendent vertices to one of its vertex. Also, we assume that P_n^k is the graph obtained by C_{n-k} by attaching a path graph P_{k+1} (on $k+1$ vertices) to one of its vertex. For undefined terminology and notations, we refer the reader to [2].
The variable sum exdeg index of a graph G is defined as $SEI_a(G) = \sum_{u \in V(G)} d_G(u) a^{d_G(u)}$, where $a \neq 1$ is a positive real number. From the definition, it is obvious that any two graphs with the same degree sequence have also the same variable sum exdeg index. The variable sum exdeg index was firstly introduced by Vukičević [10, 11] to predict some physicochemical properties of chemical compounds. It was observed that this index is very well correlated with octanol-water partition coefficient of octane isomers. Yarahmadi and Ashrafi [13] presented the polynomial form of this index and discussed this polynomial under several graph operations. Details about the mathematical properties of the variable sum exdeg index can be found in the papers [1, 3–9, 12].
The main purpose of the present paper is to find graph(s) having maximal/minimal value of the variable sum exdeg index SEI_a among all the graphs with n vertices and k cut edges for $n \geq 4$, $k \geq 1$ and $a > 1$.

2. Some Useful Lemmas

In this section, we prove some lemmas which will be very helpful in proving our main results.

Lemma 1. *Let $s, t \in V(G)$ and let $s_1, s_2, \ldots, s_n \in N(s) \setminus N(t)$ and $t_1, t_2, \ldots, t_m \in N(t) \setminus N(s)$, where $1 \leq n \leq d_G(s)$, $1 \leq m \leq d_G(t)$. Let $G' = G \setminus \{tt_1, tt_2, \ldots, tt_m\} + \{st_1, st_2, \ldots, st_m\}$ and $G'' = G \setminus \{ss_1, ss_2, \ldots, ss_n\} + \{ts_1, ts_2, \ldots, ts_n\}$. Also, assume that*

$a > 1$.

(1) if $d_G(s) \geq d_G(t)$*, then* $SEI_a(G') > SEI_a(G)$,

(2) if $d_G(s) \leq d_G(t)$*, then* $SEI_a(G'') > SEI_a(G)$.

Proof. Note that $d_{G'}(s) = d_G(s) + m$, $d_{G'}(t) = d_G(t) - m$, $d_{G''}(s) = d_G(s) - n$ and $d_{G''}(t) = d_G(t) + n$ and for any vertex $w \in V(G) \setminus \{s, t\}$, we have $d_G(w) = d_{G'}(w) = d_{G''}(w)$. By definition of variable sum exdeg index, we have

$$\begin{aligned} SEI_a(G') - SEI_a(G) &= d_{G'}(s)a^{d_{G'}(s)} - d_G(s)a^{d_G(s)} + d_{G'}(t)a^{d_{G'}(t)} \\ &\quad - d_G(t)a^{d_G(t)} \\ &= (d_G(s) + m)a^{d_G(s)+m} - d_G(s)a^{d_G(s)} \\ &\quad + (d_G(t) - m)a^{d_G(t)-m} - d_G(t)a^{d_G(t)} \\ &= d_G(s)(a^{d_G(s)+m} - a^{d_G(s)}) + d_G(t)(a^{d_G(t)-m} - a^{d_G(t)}) \\ &\quad + m(a^{d_G(s)+m} - a^{d_G(t)-m}). \end{aligned}$$

Using Mean Value Theorem, we get

$$\begin{aligned} SEI_a(G') - SEI_a(G) &= md_G(s)a^{n_1}(1 + \ln a) - md_G(t)a^{n_2}(1 + \ln a) \\ &\quad + m(a^{d_G(s)+m} - a^{d_G(t)-m}) \\ &= m(1 + \ln a)(a^{n_1}d_G(s) - a^{n_2}d_G(t)) \\ &\quad + m(a^{d_G(s)+m} - a^{d_G(t)-m}) \end{aligned} \tag{1}$$

where $d_G(s) < n_1 < d_G(s) + m$ and $d_G(t) - m < n_2 < d_G(t)$.
Similarly, using the definition and Mean Value Theorem, we have,

$$\begin{aligned} SEI_a(G'') - SEI_a(G) &= d_{G''}(t)a^{d_{G''}(t)} - d_G(t)a^{d_G(t)} + d_{G''}(s)a^{d_{G''}(s)} \\ &\quad - d_G(s)a^{d_G(s)} \\ &= (d_G(t) + n)a^{d_G(t)+n} - d_G(t)a^{d_G(t)} \\ &\quad + (d_G(s) - n)a^{d_G(s)-n} - d_G(s)a^{d_G(s)} \\ &= d_G(t)(a^{d_G(t)+n} - a^{d_G(t)}) + d_G(s)(a^{d_G(s)-n} - a^{d_G(s)}) \\ &\quad + n(a^{d_G(t)+n} - a^{d_G(s)-n}) \\ &= n(1 + \ln a)(a^{n_1'}d_G(t) - a^{n_2'}d_G(s)) \\ &\quad + n(a^{d_G(t)+n} - a^{d_G(s)-n}) \end{aligned} \tag{2}$$

where $d_G(t) < n_1' < d_G(t) + n$ and $d_G(s) - n < n_2' < d_G(s)$.
If $a \in (1, \infty)$ and $d_G(s) \geq d_G(t)$, then $n_1 > n_2$ and from Equation (1) it follows that $SEI_a(G') > SEI_a(G)$. Similarly, when $d_G(s) \leq d_G(t)$, then $n_1' > n_2'$ and from Equation (2) it follows that $SEI_a(G'') > SEI_a(G)$. □

Lemma 2. *Let $C_m = s_0s_1 \dots s_{m-1}s_0$ and $C_n = t_0t_1 \dots t_{n-1}t_0$ be two cycle in G such that C_m is connected with C_n by a path P_l $(l \geq 2)$, and the end vertices of this path are s_0 and t_1. Suppose the vertex u_i (respectively v_j) on the cycle C_m (respectively C_n) in G is either of degree 2 or has a subgraph G_i (respectively H_j)attached, $0 \leq i \leq m-1$, $0 \leq j \leq n-1$. Let $G' = G - \{s_0s_1, t_0t_1, t_1t_2\} + \{s_0t_2, t_0s_1\}$, then $SEI_a(G') < SEI_a(G)$*

Proof. Observe that $d_{G'}(s_0) = d_G(s_0)$, $d_{G'}(s_1) = d_G(s_1)$, $d_{G'}(t_0) = d_G(t_0)$, $d_{G'}(t_2) = d_G(t_2)$, $d_{G'}(t_1) = d_G(t_1) - 2$ and $d_{G'}(u) = d_G(u)$ for any vertex $u \in V' = V \setminus \{s_0, s_1, t_0, t_1, t_2\}$. By using the definition of variable sum exdeg index and mean value theorem, we get

$$\begin{aligned} SEI_a(G) - SEI_a(G') &= d_G(t_1)a^{d_G}(t_1) - d_{G'}(t_1)a^{d_{G'}}(t_1) \\ &= d_G(t_1)a^{d_G}(t_1) - (d_G(t_1) - 2)a^{d_G - 2}(t_1) \\ &= 2d_G(t_1)a^{n_1}(1 + \ln a) + 2a^{d_G(t_1)-2}, \end{aligned} \tag{3}$$

where $d_G(t_1) - 2 < n_1 < d_G(t_1)$. Observe that $d_G(t_1) \geq 3$ and hence $1 < n_1 < d_G(t_1)$. Therefore, from Equation (3), we have $SEI_a(G) > SEI_a(G')$ □

Lemma 3. *Let G be a graph with $u, v \in V(G)$ such that $uv \notin E(G)$, then $SEI_a(G+uv) > SEI_a(G)$.*

Proof. Let $V' = V \setminus \{u, v\}$, then by definition of variable sum exdeg index we get

$$\begin{aligned} SEI_a(G + uv) - SEI_a(G) &= (d(u) + 1)a^{d(u)+1} + (d(v) + 1)a^{d(u)+1} \\ &- (d(u)a^{d(u)} + d(v)a^{d(v)}) \\ &= (1 + \ln a)(d(u)a^{n_1} + d(v)a^{n_2}) + a^{d(u)+1} \\ &+ a^{d(v)+1} \end{aligned} \tag{4}$$

where $d(u) < n_1 < d(u) + 1, d(v) < n_2 < d(v) + 1$. Form Equation (4) it is clear that

$$SEI_a(G + uv) > SEI_a(G).$$

□

3. Main Results

Let $K_{1,k}$ be the a star graph with vertex set $V(K_{1,k}) = \{u_0, u_1, \dots, u_k\}$ with center vertex u_0. Let $K(b_0, \{b_1, b_2, \dots, b_k\})$ be a graph obtained from $K_{1,k}$ by replacing u_i by clique K_{b_i}, where $b_i \geq 1$ for $i = 0, 1, 2, \dots, k$. Now represent

$$K_{n,k} = \{K(b_0, \{b_1, b_2, \dots, b_k\}) : b_i \geq 1 (0 \leq i \leq k) \text{ and } \sum_{i=0}^{k} b_i = n\}.$$

Clearly, it is easy to observe that $K_n^k = \{K(n-k, \{\underbrace{1,1,\ldots,1}\})\}$. Let $G \in \mathbb{G}_n^k$ and $E = \{e_1, e_2, \ldots, e_k\}$ be the set of cut edges of G.
In this section, we calculate the maximum and minimum value of variable sum exdeg index for connected graphs with n vertices and k cut edges. We get the maximum sum exdeg index value at K_n^k and minimum sum exdeg index value at P_n^k.

Theorem 1. *Let $a > 1$, then from the class of connected graph with n vertices and k cut edges the maximum value of variable sum exdeg index (SEI_a) is obtained at K_n^k.*

Proof. To prove this theorem, we will show that if $G \in G_{n,k}$, then $SEI_a(G) \leq SEI_a(K_n^k)$ and the equality holds iff $G \cong K_n^k$. If $k = 0$, then $G = K_n$ and the theorem follows from Fact 1. Now suppose $k \geq 1$, then again by Fact 1, each component of $G - E$ is a clique. Let $K_{b_0}, K_{b_1}, K_{b_2}, \ldots, K_{b_k}$ be the components of $G - E$, where $b_0, b_1, b_2, \ldots, b_k$ are the number of vertices of each component respectively. Then $b_0 + b_1 + b_2 + \cdots + b_k = n$. Let V_{b_i} be the set of those vertices of the clique K_{b_i} which are the end vertex of cut edge in G. Let $G \in \mathbb{G}_n^k$ such that it SEI_a value is maximum. Then there are few facts which are important:

Fact 1. Let $G \in \mathbb{G}_{n,k}$ such that the value of it variable sum exdeg index is maximum, then each block of $G - E$ is a clique.
Proof. By Lemma 3, we can immediately deduce this fact.

Fact 2. $\mid V_{b_i} \mid = 1$ for $0 \leq i \leq k$.
Proof. Suppose on contrary $\mid V_{b_i} \mid > 1$ for some $0 \leq i \leq k$. Let $u, v \in V_{b_i}$ and without loss of generality we can assume that $d_G(u) \geq d_G(v)$. Take $N(v) \setminus N[u] = x_1, x_2, \ldots, x_t$. Since $v \in V_{b_i}$, so $t \geq 1$. Let $G' = G - \{vx_1, vx_2, \ldots, vx_t\} + \{ux_1, ux_2, \ldots, ux_t\}$, then $G' \in G_{n,k}$ and by Lemma 1 $SEI_a(G') > SEI_a(G)$, a contradiction. Hence $\mid V_{b_i} \mid = 1$.

Fact 3. $G \in K_{n,k}$.
Proof. Suppose $G \notin K_{n,k}$, then there exist $u \in K_{b_i}$ and $v \in K_{b_j}$ ($0 \leq i, j \leq k, i \neq j$) with $uv \in E(G)$ and $|N(u) - V(K_{b_i})| \geq 2$, $|N(v) - V(K_{b_j})| \geq 2$. Let $V_{b_i} = \{u\}$ and $V_{b_i} = \{v\}$(by Fact 2) and assume that $d_G(v) \geq d_G(u)$. Take $N(v) - N[u] = \{t_1, t_2, \ldots, t_p\}$, $(p \geq 2)$ and consider $G' = G - \{vt_1, vt_2, \ldots, vt_p\} + \{ut_1, ut_2, \ldots, ut_p\}$. Then $G' \in \mathbb{G}_n^k$ and by Lemma 1 $SEI_a(G') > SEI_a(G)$ a contradiction.
Now by Fact 2 we can assume $V_{b_i} = u_i$, where $0 \leq i \leq k$ and by Fact 3 we can assume that $u_0 u_j \in E(G)$ $(1 \leq i \leq k)$. Without loss of Generality, we can further assume that $b_k \geq b_{k-1} \geq \cdots \geq b_1 \geq 1$. Next we will show that $G \cong K(b_0, \{\underbrace{1,1,\ldots,1}, n - b_0 - k + 1\})$.

Fact 4. $G \cong K(b_0, \{\underbrace{1,1,\ldots,1}, n - b_0 - k + 1\})$.
Proof. Suppose $b_i \geq 2$ for some $1 \leq i \leq k-1$. Then $b_k \geq 2$ and $d_G(u_k) \geq d_G(u_i)$. Let $N(u_i) - \{u_0\} = \{t_1, t_2, \ldots, t_{a_i - 1}\}$ and take

$G' = G - \{u_i t_1, u_i t_2, \ldots, u_i t_{a_i - 1}\} + \{u_k t_1, u_k t_2, \ldots, u_k t_{a_i - 1}\}$. Then $G' \in \mathbb{G}_n^k$ and by Lemma 1 $SEI_a(G') > SEI_a(G)$ a contradiction.

Fact 5. $b_0 = n - k$.

Proof. Clearly $b_0 \leq n - k$. Suppose $b_0 < n - k$, then by Fact 4, $b_k > 1$. Let $N(u_k) - \{u_0\} = \{t_1, t_2, \ldots, t_{a_k - 1}\}$ and $N(u_0) - \{u_k\} = \{s_1, s_2, \ldots, s_{a_0 - 1}, u_1, u_2, \ldots, u_{k-1}\}$. If $d_G(u_0) \geq d_G(u_k)$, we take $G' = G - \{u_k t_1, u_k t_2, \ldots, u_k t_{a_k - 1}\} + \{u_0 t_1, u_0 t_2, \ldots, u_0 t_{a_k - 1}\}$. If $d_G(u_k) \geq d_G(u_0)$, we take $G' = G - \{u_0 s_1, u_0 s_2, \ldots, u_0 s_{a_0 - 1}, u_0 u_1, u_0 u_2, \ldots, u_0 u_{k-1}\} + \{u_k s_1, u_k s_2, \ldots, u_k s_{a_0 - 1}, u_k u_1, u_k u_2, \ldots, u_k u_{k-1}\}$. In both the cases, we have $G' \in \mathbb{G}_n^k$ and by Lemma 1 $SEI_a(G') > SEI_a(G)$ a contradiction.
Thus $b_0 = n - k$ and $G \cong K(n - k, \underbrace{1, 1, \ldots, 1}) = K_n^k$, which completes the proof. □

Now we find the graph in the class of $\mathbb{G}_n^k$ which have minimum SEI_a index value.

Lemma 4. *Let $a > 0//(a \neq 1)$ and $G \in \mathbb{G}_n^k$ such that $SEI_a(G)$ is minimum. Then each component of $G - E$ is a cycle or a pendent vertex.*

Proof. Suppose there is a component H in $G - E$ which is neither a pendent vertex nor a cycle. Then H is 2-connected graph. Let $C_t = v_1 v_2 \ldots v_{s-1} v_s v_{s+1} \ldots v_{t-1} v_t v_{t+1} \ldots v_1$ be the largest cycle in H. Also by assumption, H is not a clique. Hence there exists $v_i, v_j \in V(C_t)$ such that they are connected by a path P and $V(P) \cap V(C_t) = \{v_i, v_j\}$. Now, there are two possibilities.

(1) Suppose the length of P is 1. Take $G' = G - v_i v_j$, then by Lemma 3 $SEI_a(G) > SEI_a(G')$, a contradiction.

(2) Suppose length of P is greater or equal to 2. Let $P = v_s u_1 u_2 \ldots u_{l-1} u_l$. If $l = l$, then there does not exist $k \in \{s-1, s+1, t-1, t+1\}$ such that $u_1 v_k \in E(G)$, otherwise a cycle of length $t + 1$ appears in C_t, a contradiction. Let $G' = G - \{v_s u_1, v_t v_{t+1}\} + u_1 v_{t+1}$, then $d'_G(v_s) = d_G(v_s) - 1$, $d'_G(v_t) = d_G(v_t) - 1$ and for all $w \in V(G) - \{v_s, v_t\}$, we have $d'_G(w) = d_G(w)$. By definition of variable sum exdeg index, we have

$$\begin{aligned} SEI_a(G) - SEI_a(G') &= d_G(v_s) a^{d_G(v_s)} + d_G(v_t) a^{d_G(v_t)} \\ &\quad -((d_G(v_s) - 1) a^{d_G(v_s) - 1} + (d_G(v_t) - 1) a^{d_G(v_t) - 1}) \\ &= (1 + \ln a)(d_G(v_s) a^{n_1} + d_G(v_t) a^{n_2}) + a^{d_G(v_s) - 1} + a^{d(v_t) - 1} \end{aligned}$$

where $d_G(v_s) - 1 < n_1 < d_G(v_s), d_G(v_t) - 1 < n_2 < d_G(v_t)$. It is clear that $SEI_a(G) > SEI_a(G')$, a contradiction. Similarly, when $l \geq 2$, $\{u_1 v_{s-1}, u_1 v_{s+1}, u_l v_{t-1}, u_l v_{t+1}\} \nsubseteq E$. Let $G' = G - \{u_s v_{s-1}, v_t v_{t+1}, u_l u_{l-1}\} + \{u_l v_{t+1}, u_{l-1} v_{s-1}\}$, then in the similar way we can show that $SEI_a(G) > SEI_a(G')$, a contradiction. This completes the proof. □

Theorem 2. *Let $a > 1$ and $G \in \mathbb{G}_n^k$, then $SEI_a(G)$ attains its minimum value uniquely at $G = P_n^k$.*

Proof. Let $a > 1$ and $G \in \mathbb{G}_n^k$, we will show that $SEI_a(G) \geq SEI_a(P_n^k)$ and the equality holds iff $G \cong P_n^k$. If $k = 0$, then by Lemma 4 $G \cong C_n$ and the theorem follows. Now assume that $k \geq 1$. In the following we will prove some important fact from which the theorem follows.

Claim 1. G contains exactly one cycle of length $n - k$.
Proof. By Lemma 4, $G - E$ is either an pendent vertex or a cycle. If G contains exactly one cycle then the result follows. Hence G contains at least two cycles with no common vertex. Then by Lemma 2 there exists $G' \in \mathbb{G}_n^k$, such that $SEI_a(G') < SEI_a(G)$, a contradiction. Hence the length of cycle is $n - k$ follows from our assumption that G has k cut edges.

Claim 2. $G \cong P_n^k$.
Proof. By Lemma 1 there is only one pendent tree T attached to the cycle C_{n-k}. Assume that T is attached to C_{n-k} at u_0 and let us suppose that T is not a path. Let $P = u_0u_1 \ldots u_t$ be a longest path in T which connects u_0 with a pendent vertex say u_t. Then there exist a vertex u_j such that $d_G(u_j) \geq 3$ or $u_j = u_0$ with $d_G(u_j) \geq 4$. Take $u' \in N(u_j) \setminus P \cup C_{n-k}$ and consider $G' = G - u_ju' + u'u_t$. Clearly $G' \in \mathbb{G}_n^k$ with $d_{G'}(u_j) = d_G(u_j) - 1$, $d_{G'}(u_t) = 2$, $d_G(u_t) = 1$ and for all $w \in V(G) - \{u_j, u_t\}$, we have $d_{G'}(w) = d_G(w)$. By definition of variable sum exdeg index, we get

$$\begin{aligned} SEI_a(G') - SEI_a(G) &= (d_G(u_j) - 1)a^{d_G(u_j)-1} + 2a^2 - (d_G(u_j)a^{d_G(u_j)} + a) \\ &= 2a^2 - a - (1 + \ln a)d_G(u_j)a^{n_1} - a^{d_G(u_j)-1} \end{aligned}$$

where $d_G(u_j) - 1 < n_1 < d_G(u_j)$. As $a > 1$, this implies that $SEI_a(G') < SEI_a(G)$, a contradiction. This completes the proof. □

4. Conclusion

After simple calculations, we obtain $SEI_a(K_n^k) = (n-k-1)^2a^{n-k-1}+(n-1)a^{n-1}+ka$, and $SEI_a(P_n^k) = 2(n-2)a^2+a+3a^3$. Thus, by Theorems 1 and 2, whenever $a > 1$, we get the sharp lower and upper bounds for the variable sum exdeg index of connected graphs on n vertices with k cut edges, given in the following theorem.

Theorem 3. *Let $a > 1$ and $G \in \mathbb{G}_n^k$, then*

$$2(n-2)a^2 + a + 3a^3 \leq SEI_a(G) \leq (n-k-1)^2a^{n-k-1} + (n-1)a^{n-1} + ka$$

where the left equality holds if and only if $G \cong P_n^k$ and the right equality holds if and only if $G \cong K_n^k$.

Observe that we have not given the sharp bounds for $SEI_a(G)$ for connected graphs on n vertices and k cut edges whenever $0 < a < 1$. Hence the following research problem is open to consider.

Problem: Determine the sharp bounds for $SEI_a(G)$ for connected graphs on n vertices and k cut edges whenever $0 < a < 1$.

Acknowledgment

This research has been funded by Scientific Research Deanship at University of Ha'il, Saudi Arabia through project number RG-191323.

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