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Research article

On the graph connectivity and the variable sum exdeg index

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Abstract: Topological indices are important descriptors which can be used to characterize the structural properties of organic molecules from different aspects. The variable sum exdeg index $SEI_a(G)$ of a graph G is defined as $\sum_{u\in V(G)} d_G(u)a^{d_G(u)}$, where $d_G(u)$ is the degree of vertex u and a is an arbitrary positive real number different from 1. In this paper, we obtain the extremal values of the variable sum exdeg indices (for $a > 1$) in terms of the number of cut edges, or the number of cut vertices, or the vertex connectivity, or the edge connectivity of a graph. Furthermore, the corresponding extremal graphs are characterized.

Keywords: variable sum exdeg index; cut edge; cut vertex; vertex connectivity; edge connectivity
Mathematics Subject Classification: 05C07, 05C35, 92E10

1. Introduction

In this paper, we are concerned with undirected simple connected graphs only. Let $G = (V(G), E(G))$ denote a graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$.

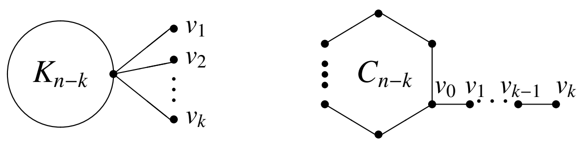
Topological indices are numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph, and they play an important role in chemistry, pharmacology, etc. (see [1–3]). The Randić index [4] (devised in 1975 for measuring the branching of molecules) and Zagreb indices [5] (appeared in 1972 within the study of total π-electron energy on molecular structure) are among the most studied topological indices. The variable sum exdeg index (denoted by SEI_a) was introduced by Vukičević [6] in 2011 and is defined as:

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

where $a \neq 1$ is an arbitrary positive real number. This graph invariant is very well correlated with octanol-water partition coefficient of octane isomers [6], and was be used to analyze the octane isomers given by the International Academy of Mathematical Chemistry (IAMC) [7–9]. Yarahmadi and Ashrafi [10] presented a polynomial form of this descriptors with some applications in nanoscience. Applying the majorization technique, Ghalavand and Ashrafi [11] obtained the maximum and minimum values of variable sum exdeg index of trees, unicyclic, bicyclic and tricyclic graphs for $a > 1$. Recent results can be found in [12–15].

Denote by $G - uv$ and $G + uv$ the graph that obtained from G by deleting the edge $uv \in E(G)$ and the graph that obtained from G by adding an edge $uv \notin E(G)$ $(u, v \in V(G))$, respectively. For $E' \subset E(G)$, let $G - E'$ be the subgraph of G obtained by deleting the edges of E'. Let $W \subset V(G)$, we use $G - W$ to denote the subgraph of G obtained by deleting the vertices of W and the edges incident with them. A cut edge of a graph is an edge whose deletion breaks the graph into two components. A cut vertex in a connected graph is a vertex whose deletion increases the number of components of the graph. A block of a graph is a maximum connected subgraph without cut vertices. We also call a block an endblock of a graph if it has at most one cut vertex in the graph as a whole. The vertex connectivity (respectively, edge connectivity) of a graph is the minimum number of vertices (respectively, minimum number of edges) whose deletion yields the resulting graph disconnected or a singleton. A clique of a graph G is a subset S of V such that any two vertices in $G[S]$ (the subgraph of G induced by S) are adjacent. As usual, we use P_n, S_n, C_n and K_n to denote the n-vertex path, the n-vertex star, the n-vertex cycle and the n-vertex complete graph, respectively.

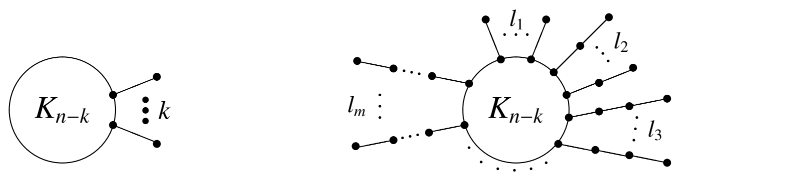
Let $P_r = x_0x_1 \cdots x_r$ $(r \geq 1)$ be a path of graph G with $d_G(x_1) = \cdots = d_G(x_{r-1}) = 2$ (unless $r = 1$). If $d_G(x_0), d_G(x_r) \geq 3$, then P_r is called an internal path of G; if $d_G(x_0) \geq 3, d_G(x_r) = 1$, then P_r is called a pendant path of G. The vertex-disjoint union of the graphs G_1 and G_2 is denoted by $G_1 \cup G_2$. Let $G_1 \vee G_2$ be the graph obtained from $G_1 \cup G_2$ by adding all possible edges from vertices of G_1 to vertices of G_2. The cyclomatic number of a connected graph G is defined as $\gamma(G) = |E(G)| - |V(G)| + 1$. A k cyclic graph is a graph whose cyclomatic number is k. For $\gamma(G) = 0$, G is a tree.



K_n^k C_n^k

Figure 1. The graphs K_n^k and C_n^k.

Let K_n^k (as shown in Figure 1) be the graph obtained by identifying one vertex of K_{n-k} with the central vertex of star S_{k+1} and C_n^k (as shown in Figure 1) be the graph obtained by attaching a pendant path P_{k+1} to one vertex of C_{n-k}. Obviously, the graph K_n^k and C_n^k are two special graphs of order n with k cut edges.



$G_{n,k}^1$ $G_{n,k}^2$ (l_t is the number of path with length t, $t = 1, 2, \cdots, m$)

Figure 2. The graphs $G_{n,k}^1$ and $G_{n,k}^2$.

The graph $G^1_{n,k}$ of order n with k cut vertices (as shown in Figure 2) is obtained from K_{n-k} by attaching at most one pendant edge to each vertex of K_{n-k}, where $0 < k \leq \frac{n}{2}$.

The graph $G^2_{n,k}$ of order n with k cut vertices (as shown in Figure 2) is obtained from K_{n-k} by attaching exactly one pendant path (with length equal or greater than one) to each vertex of K_{n-k}, where $\frac{n}{2} < k \leq n-3$, $l_1 + l_2 + \cdots + l_m = n-k$ and $l_1 + 2l_2 + \cdots + ml_m = k$ (l_t is the number of path with length t, $t = 1, 2, \cdots, m$). We can see [16] for other notations.

2. Preliminaries

Lemma 2.1. *[7] Let $f_a(x) = xa^x$, where $x \geq 1, a > 1$. Then*
(i) *$f_a(x)$ is an increasing function for each $a > 1$;*
(ii) *$f''_a(x) > 0$ and $f_a(x)$ is a convex function for each $a > 1$.*

By Lemma 2.1 and the definition of variable sum exdeg index, the following Lemma 2.2 is obvious.

Lemma 2.2. *Let $G = (V, E)$ be a simple connected graph. Then*
(i) *If $e = uv \notin E(G)$, $u, v \in V(G)$, $SEI_a(G) < SEI_a(G+e)$ for $a > 1$;*
(ii) *If $e \in E(G)$, $SEI_a(G) > SEI_a(G-e)$ for $a > 1$.*

Lemma 2.3. *Let*

$$f(x, y) = (x+y-1)a^{x+y-1} + a - xa^x - ya^y,$$

where $x, y \geq 2$ and $a > 1$. Then $f(x, y) > 0$.

Proof. If $y \geq 2$ is fixed, by Lemma 2.1, we have

$$\frac{\partial f(x, y)}{\partial x} = a^{x+y-1} - a^x + [(x+y-1)a^{x+y-1} - xa^x] \ln a > 0.$$

So $f(x, y)$ is strictly monotone increasing in x. By symmetry, if $x \geq 2$ is fixed, then $f(x, y)$ is strictly monotone increasing in y. Thus, by Jensen inequality for the function xa^x, which is strictly convex for $a > 1$, we have $f(x, y) \geq f(2, 2) = 3a^3 + a - 2 \cdot 2a^2 > 0$. □

Lemma 2.4. *Let*

$$g(x) = f_a(x+r) - f_a(x) = (x+r)a^{x+r} - xa^x,$$

where $x \geq 2$, $r \geq 1$ and $a > 1$. Then $g(x)$ is strictly monotone increasing in x.

Proof. Note that for $a > 1$,

$$g'(x) = a^{x+r} - a^x + [(x+r)a^{x+r} - xa^x] \ln a > 0.$$

So $g(x)$ is strictly monotone increasing in x. □

Lemma 2.5. *Let*

$$\begin{aligned} g(x, y) =& (x-1)[(x+y-3)a^{x+y-3} - (x-1)a^{x-1}] + a - (y-1)a^{y-1} \\ &+ (y-2)[(x+y-3)a^{x+y-3} - (y-1)a^{y-1}], \end{aligned}$$

where $x \geq 2$, $y \geq 3$ and $a > 1$. Then $g(x, y) \geq 0$.

Proof. Since for $a > 1$,

$$\begin{aligned}\frac{\partial g(x,y)}{\partial x} =&[(x+y-3)a^{x+y-3} - (x-1)a^{x-1}] \\ &+ (x-1)\{a^{x+y-3} - a^{x-1} + [(x+y-3)a^{x+y-3} - (x-1)a^{x-1}]\ln a\} \\ &+ (y-2)[a^{x+y-3} + (x+y-3)a^{x+y-3}\ln a] > 0.\end{aligned}$$

So $g(x,y)$ is strictly monotone increasing in x. Thus, $g(x,y) \geq g(2,y) = 0$. □

Lemma 2.6. *Let*

$$\begin{aligned}h(x,y) =&(x-1)[(x+y-3)a^{x+y-3} - (x-1)a^{x-1}] + 2a^2 - ya^y \\ &+ (y-2)[(x+y-3)a^{x+y-3} - (y-1)a^{y-1}],\end{aligned}$$

where $x, y \geq 3$ *and* $a > 1$. *Then* $h(x,y) > 0$.

Proof. Note that

$$\frac{\partial h(x,y)}{\partial x} = \frac{\partial g(x,y)}{\partial x} > 0.$$

So $h(x,y)$ is strictly monotone increasing in x. Thus, $h(x,y) \geq h(3,y) = ya^y - 2a^2 + (y-2)[ya^y - (y-1)a^{y-1}] > 0$. □

Lemma 2.7. *Let*

$$\begin{aligned}l(x,y) =&(x-1)[(x+y-3)a^{x+y-3} - (x-1)a^{x-1}] + (x+y-2)a^{x+y-2} + 4a^2 \\ &+ (y-2)[(x+y-3)a^{x+y-3} - (y-1)a^{y-1}] - xa^x - 2ya^y,\end{aligned}$$

where $x, y \geq 3$ *and* $a > 1$. *Then* $l(x,y) > 0$.

Proof. It can be seen that

$$\begin{aligned}\frac{\partial l(x,y)}{\partial x} =&[(x+y-3)a^{x+y-3} - (x-1)a^{x-1}] \\ &+ (x-1)\{a^{x+y-3} - a^{x-1} + [(x+y-3)a^{x+y-3} - (x-1)a^{x-1}]\ln a\} \\ &+ (y-2)[a^{x+y-3} + (x+y-3)a^{x+y-3}\ln a] \\ &+ a^{x+y-2} + (x+y-2)a^{x+y-2}\ln a - a^x - xa^x \ln a \\ &> a^{x+y-2} - a^x + [(x+y-2)a^{x+y-2} - xa^x]\ln a > 0.\end{aligned}$$

So $l(x,y)$ is strictly monotone increasing in x. Thus, $l(x,y) \geq l(3,y) = (y-2)[ya^y - (y-1)a^{y-1}] + (y+1)a^{y+1} - 3a^3 > 0$. □

3. Variable sum exdeg indices of graphs with given number of cut edges for $a > 1$

We use $\mathbf{G}_E(n,k)$ to denote the set of graphs on n vertices with k cut edges. If $k = n-1$, $\mathbf{G}_E(n, n-1)$ is a tree and trees with extremal variable sum exdeg index had been obtained in [7] and [11]. For a connected graph on n vertices having the cyclomatic number at least one, the number of its cut edges is at most $n-3$. Therefore, in this section, we always assume that G has k cut edges with $1 \leq k \leq n-3$.

3.1. The largest variable sum exdeg index of a graph with given number of cut edges for $a > 1$

First, we provide some graph transformations on graphs with given number of cut edges which will increase the variable sum exdeg index for $a > 1$.

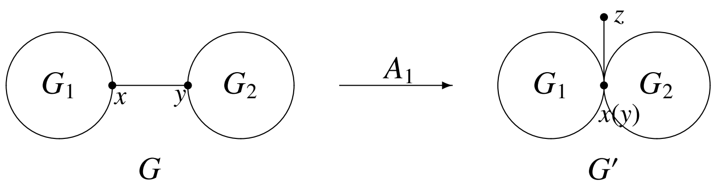


Figure 3. Transformation A_1.

Transformation A_1: Suppose G_1 is a graph with $n_1 \geq 3$ vertices and G_2 is a graph with $n_2 \geq 2$ vertices, where G_1 is 2-edge connected. Let G be a graph obtained from G_1 and G_2 by adding an edge between a vertex x of G_1 and a vertex y of G_2, as shown in Figure 3. Then xy be a non-pendant cut edge of G. Let G' be the graph obtained by identifying x of G_1 to y of G_2 and adding a pendant edge to $x(y)$, as shown in Figure 3.

Lemma 3.1. *Let G and G' be graphs in Figure 3. Then $SEI_a(G') > SEI_a(G)$ for $a > 1$.*

Proof. Let $d_G(x) = r$ and $d_G(y) = s$. By the definition of variable sum exdeg index and Lemma 2.3, we have

$$SEI_a(G') - SEI_a(G) = (r + s - 1)a^{r+s-1} + a - ra^r - sa^s > 0.$$

The proof is completed. □

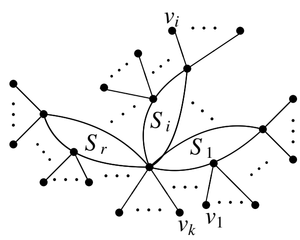


Figure 4. The graph G^*.

Remark 3.2. *For any $G \in \mathbf{G}_E(n, k)$, if necessary, by repeating the graph transformation A_1, any cut edge (non-pendant cut edge) of G can changed into pendant edge. That is, if necessary, by a series of transformation A_1, we can change G to G^* (as shown in Figure 4), where S_i $(1 \leq i \leq r)$ are 2-edge-connected graphs.*

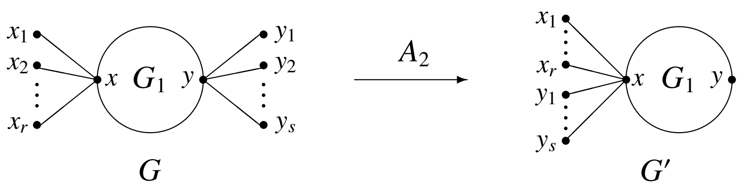


Figure 5. Transformation A_2.

Transformation A_2: Let G be a graph as shown in Figure 5, $x, y \in V(G_1)$, $x_1, x_2, \cdots, x_r$ are pendant vertices adjacent to x, and $y_1, y_2, \cdots, y_s$ are pendant vertices adjacent to y, where $d_G(y) \leq d_G(x)$. Let $G' = G - \{yy_1, yy_2, \cdots, yy_s\} + \{xy_1, xy_2, \cdots, xy_s\}$, as shown in Figure 5.

Lemma 3.3. *Let G and G' be graphs in Figure 5. Then $SEI_a(G') > SEI_a(G)$ for $a > 1$.*

Proof. In view of the definition of variable sum exdeg index and Lagrange mean value theorem, for $a > 1$, we have

$$\begin{aligned} SEI_a(G') - SEI_a(G) &= f_a(d_G(x) + s) + f_a(d_G(y) - s) - [f_a(d_G(x)) + f_a(d_G(y))] \\ &= f_a(d_G(x) + s) - f_a(d_G(x)) - [f_a(d_G(y)) - f_a(d_G(y) - s)] \\ &= s(f_a'(\xi) - f_a'(\eta)), \end{aligned}$$

where $d_G(x) < \xi < d_G(x) + s$, $d_G(y) - s < \eta < d_G(y)$.

Since $d_G(y) \leq d_G(x)$, by Lemma 2.1, then $SEI_a(G') - SEI_a(G) > 0$, i.e., $SEI_a(G') > SEI_a(G)$ for $a > 1$. □

Remark 3.4. *For any $G \in \mathbf{G}_E(n, k)$, if necessary, by repeating graph transformation A_1 and A_2, all the pendant edges are attached to the same vertex. That is, if necessary, by a series of transformation A_1 and A_2, we can change G to H_1 or H_2 (as shown in Figure 6), where S_i $(1 \leq i \leq r)$ are 2-edge-connected graphs.*

Figure 6. The graphs H_1 and H_2.

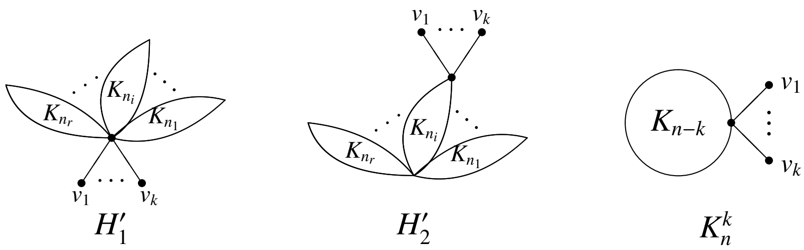


Figure 7. The graphs H_1', H_2' and K_n^k.

By Lemmas 3.1, 3.3 and Remarks 3.2, 3.4, we have the following Lemma 3.5.

Lemma 3.5. *Let $G \in \mathbf{G}_E(n, k)$. Then $SEI_a(G) \leq SEI_a(H_i)$ $(i = 1$ or $2)$ for $a > 1$, where H_1 or H_2 is a graph as shown in Figure 6, S_i $(1 \leq i \leq r)$ are 2-edge-connected graphs.*

Denoted K_{n_i} $(1 \leq i \leq r)$ to be a clique which is obtained by adding edges in S_i $(1 \leq i \leq r)$ and changing S_i into complete sub-graphs, where S_i $(1 \leq i \leq r)$ in H_1 or H_2 are 2-edge-connected graphs.

Lemma 3.6. *Suppose H'_1 or H'_2 is a graph as shown in Figure 7, where K_{n_i} $(1 \le i \le r)$ is a clique as above. Then $SEI_a(H'_i) \ge SEI_a(H_i)$ $(i = 1$ or $2)$ for $a > 1$.*

Proof. By Lemma 2.2, the result holds obviously. □

Theorem 3.7. *Let $G \in \mathbf{G}_E(n,k)$, where $1 \le k \le n-3$. Then*

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

for $a > 1$, with equality holding if and only if $G \cong K_n^k$.

Proof. Choose $G \in \mathbf{G}_E(n,k)$ such that G has the maximum variable sum exdeg index for $a > 1$. By Lemma 3.5 and 3.6, we have $SEI_a(G) \le SEI_a(H'_1)$ or $SEI_a(G) \le SEI_a(H'_2)$ for $a > 1$.

Next, we prove that $r = 1$. By contradiction, assume that $r \ge 2$. Without loss of generality, suppose that there exists an edge $e = uv \notin E(G)$, $u \in V(K_{n_i})$, $v \in V(K_{n_j})$, $1 \le i, j \le r$, $i \ne j$, and u, v is not the common vertex of K_{n_i} and K_{n_j}. By Lemma 2.2, we have $SEI_a(G+e) > SEI_a(G)$ for $a > 1$, a contradiction to the choice of G. So $r = 1$, i.e., $G \cong K_n^k$. □

3.2. The smallest variable sum exdeg index of a graph with given number of cut edges for $a > 1$

First, we provide some transformations on graphs with cut edges which will decrease the variable sum exdeg index for $a > 1$.

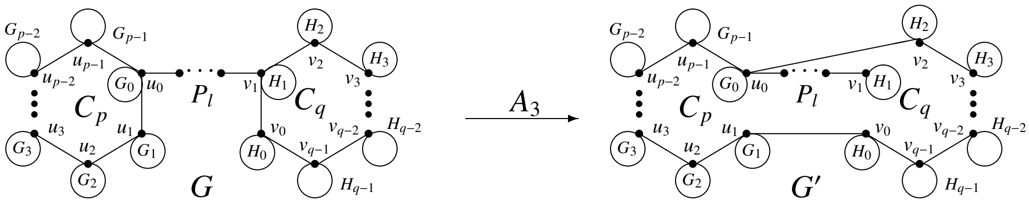


Figure 8. Transformation A_3.

Transformation A_3: Let $C_p = u_0u_1u_2\cdots u_{p-1}$ and $C_q = v_0v_1v_2\cdots v_{q-1}$ be two cycles in G (as shown in Figure 8) such that C_p connects C_q by a path P_l (with $l \ge 2$ vertices) whose end vertices are u_0, v_1, and the vertex, say u_t (resp. v_s), on the cycle C_p (resp. C_q) in G either is of degree 2 or has subgraph G_t (resp. H_s) attached, $0 \le t \le p-1$, $0 \le s \le q-1$. $G' = G - \{u_0u_1, v_1v_0, v_1v_2\} + \{u_0v_2, u_1v_0\}$, as shown in Figure 8.

Lemma 3.8. *Let G and G' be graphs in Figure 8. Then $SEI_a(G) > SEI_a(G')$ for $a > 1$.*

Proof. It is easy to see that $d_{G'}(u_0) = d_G(u_0)$, $d_{G'}(u_1) = d_G(u_1)$, $d_{G'}(v_0) = d_G(v_0)$, $d_{G'}(v_2) = d_G(v_2)$, $d_{G'}(v_1) = d_G(v_1) - 2$, and $d_{G'}(w) = d_G(w)$ for $w \in V(G)\backslash\{u_0, u_1, v_0, v_1, v_2\}$. Thus, for $a > 1$,

$$SEI_a(G) - SEI_a(G') = f_a(d_G(v_1)) - f_a(d_G(v_1) - 2) > 0.$$

The proof is completed. □

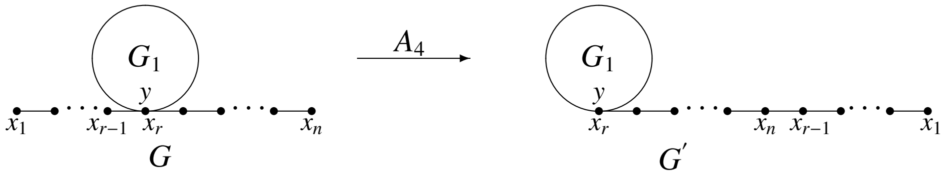


Figure 9. Transformation A_4.

Transformation A_4: Let G be a graph as shown in Figure 9, where $G_1 \ncong K_1$ and $y \in V(G_1)$. That is, we use G to denote the graph obtained from G_1 by identifying y with the vertex x_r of a path $x_1x_2 \cdots x_{r-1}x_r \cdots x_n$, $1 < r < n$. Let $G' = G - x_{r-1}x_r + x_nx_{r-1}$, as shown in Figure 9.

Lemma 3.9. *Let G and G' be graphs in Figure 9. Then $SEI_a(G) > SEI_a(G')$ for $a > 1$.*

Proof. By Lemma 2.1 and the definition of variable sum exdeg index, we have

$$\begin{aligned} SEI_a(G) - SEI_a(G') =& f_a(d_{G_1}(y) + 2) - f_a(d_{G_1}(y) + 1) - (f_a(2) - f_a(1)) \\ =& f_a'(\xi) - f_a'(\eta) > 0, \end{aligned}$$

where $d_{G_1}(y) + 1 < \xi < d_{G_1}(y) + 2$, $1 < \eta < 2$. □

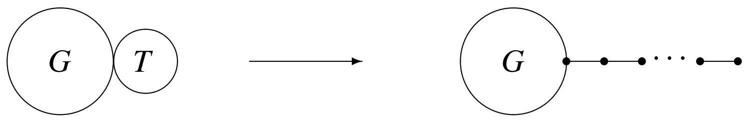


Figure 10. The graphs in Remark 3.10.

Remark 3.10. *By repeating Transformation A_5, any tree T attached to a graph G can be changed into a path as showed in Figure 10.*

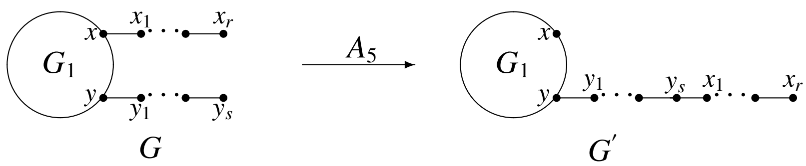


Figure 11. Transformation A_5.

Transformation A_5: Let G be a graph as shown in Figure 11, where $x, y \in V(G_1)$ and $d_{G_1}(x), d_{G_1}(y) \geq 2$. That is, we use G to denote the graph obtained from identifying x with the vertex x_0 of a path $x_0x_1 \cdots x_r$ and identifying y with the vertex y_0 of a path $y_0y_1 \cdots y_s$, where $r, s \geq 1$. $G' = G - xx_1 + y_sx_1$, as shown in Figure 11.

Lemma 3.11. *Let G and G' be graphs in Figure 11. Then $SEI_a(G) > SEI_a(G')$ for $a > 1$.*

Proof. The proof is similar to Lemma 3.9, omitted. □

Theorem 3.12. *Let $G \in \mathbf{G}_E(n,k)$, where $1 \le k \le n-3$. Then*

$$SEI_a(G) \ge 2(n-2)a^2 + 3a^3 + a$$

for $a > 1$, with equality holding if and only if $G \cong C_n^k$.

Proof. Choose connected graph $G \in \mathbf{G}_E(n,k)$ such that it has the smallest variable sum exdeg index for $a > 1$. Let $E' = \{e_1, e_2, \cdots, e_k\}$ be the set of the cut edges of $G \in \mathbf{G}_E(n,k)$. By Lemma 2.2, it can be seen that each component of $G - E'$ is either a cycle or an isolated vertex.

Next, we prove that G contains exactly one cycle of length $n-k$. By contradiction, assume that G contains at least two cycles. Then by Lemma 3.8, we can obtain a graph $G' \in \mathbf{G}_E(n,k)$ such that $SEI_a(G') < SEI_a(G)$ for $a > 1$, a contradiction to the choice of G. Furthermore, G has k cut edges, so the length of the cycle contained in G is of $n-k$. By Lemmas 3.9, 3.11 and Remark 3.10, we have $G \cong C_n^k$. □

4. Variable sum exdeg indices of graphs with given number of cut vertices for $a > 1$

Let $\mathbf{G}_V(n,k)$ be the set of graphs on n vertices with k cut vertices. If $k = n-2$, then the only graph in $\mathbf{G}_V(n, n-2)$ is the path. Therefore, in this section, we always assume that G has k cut vertices with $1 \le k \le n-3$.

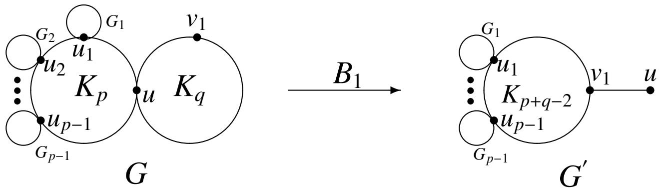


Figure 12. Transformation B_1.

Transformation B_1: Let G be a graph as shown in Figure 12, K_p and K_q be two cliques of G, where $p \ge 2$, $q \ge 3$ and K_q is an endblock. $V(K_p)$ and $V(K_q)$ have one cut vertex, say u, in common. $V(K_p) = \{u_1, u_2, \cdots, u_{p-1}, u\}$, $V(K_q) = \{v_1, v_2, \cdots, v_{q-1}, u\}$. G_i $(1 \le i \le p-1)$ is the subgraph attached to u_i $(1 \le i \le p-1)$. Let $G' = G - \{uu_1, uu_2, \cdots, uu_{p-1}, uv_2, uv_3, \cdots, uv_{q-1}\} + \{u_1v_1, u_1v_2, \cdots, u_1v_{q-1}\} + \cdots + \{u_{p-1}v_1, u_{p-1}v_2, \cdots, u_{p-1}v_{q-1}\}$, as shown in Figure 12.

Lemma 4.1. *Let G and G' be graphs in Figure 12. Then $SEI_a(G') > SEI_a(G)$ for $a > 1$.*

Proof. Note that $d_G(u) = p+q-2$, $d_{G'}(u) = 1$, $d_G(v_1) = q-1$, $d_{G'}(v_1) = p+q-2$, $d_{G'}(u_i) = d_G(u_i)+q-2$ $(i = 1, 2, \cdots, p-1)$, $d_{G'}(v_j) = p+q-3$ $(j = 2, 3, \cdots, q-1)$, and the degrees of other vertices in G_i $(1 \le i \le p-1)$ are unchanged. By the definition of variable sum exdeg index and Lemma 2.4, 2.5, for $a > 1$, we have

$$\begin{aligned}
&SEI_a(G') - SEI_a(G) \\
&= \sum_{i=1}^{p-1} f_a(d_G(u_i) + q - 2) + \sum_{j=2}^{q-1} f_a(d_G(v_j) + p - 2) + f_a(d_G(v_1) + p - 1) + f_a(1) \\
&\quad - f_a(d_G(u)) - \sum_{i=1}^{p-1} f_a(d_G(u_i)) - \sum_{j=1}^{q-1} f_a(d_G(v_j))
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{i=1}^{p-1} [f_a(d_G(u_i) + q - 2) - f_a(d_G(u_i))] + \sum_{j=2}^{q-1} [f_a(p + q - 3) - f_a(q - 1)] \\
&\quad + f_a(p - q - 2) + f_a(1) - f_a(p - q - 2) - f_a(q - 1) \\
&>(p - 1)[(p + q - 3)a^{p+q-3} - (p - 1)a^{p-1}] + a - (q - 1)a^{q-1} \\
&\quad + (q - 2)[(p + q - 3)a^{p+q-3} - (q - 1)a^{q-1}] > 0.
\end{aligned}
$$

This completes the proof. □

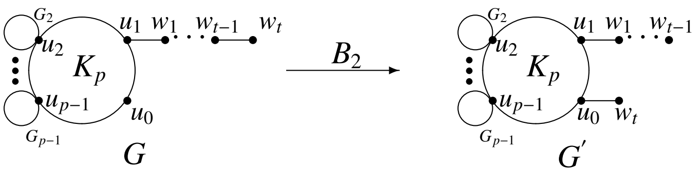


Figure 13. Transformation B_2.

Transformation B_2: Let G be a graph as shown in Figure 13, K_p be a clique of G, where $p \geq 3$. $V(K_p) = \{u_0, u_1, \cdots, u_{p-1}\}$. $P = u_1w_1 \cdots w_t$ ($t \geq 2$) is a path attached to u_1. $N_G(u_0) = \{u_1, u_2, \cdots, u_{p-1}\}$, $N_G(u_1) = \{u_0, u_2, \cdots, u_{p-1}, w_1\}$. G_i ($2 \leq i \leq p - 1$) is the subgraph attached to u_i ($2 \leq i \leq p - 1$). Let $G' = G - w_{t-1}w_t + u_0w_t$, as shown in Figure 13.

Lemma 4.2. *Let G and G' be graphs in Figure 13. Then $SEI_a(G') > SEI_a(G)$ for $a > 1$.*

Proof. By the definition of variable sum exdeg index and Lemma 2.4, for $a > 1$, we have

$$
\begin{aligned}
SEI_a(G') - SEI_a(G) &= f_a(d_G(u_0) + 1) + f_a(d_G(w_{t-1}) - 1) - f_a(d_G(u_0)) - f_a(d_G(w_{t-1})) \\
&= pa^p - (p - 1)a^{p-1} + a - 2a^2 \\
&\geq 3a^3 + a - 2 \cdot 2a^2 > 0.
\end{aligned}
$$

The proof is completed. □

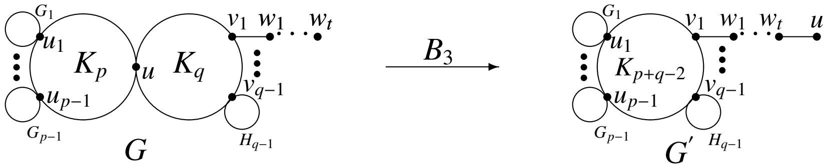


Figure 14. Transformation B_3.

Transformation B_3: Let G be a graph as shown in Figure 14, K_p and K_q be two cliques of G, where $p, q \geq 3$. $V(K_p)$ and $V(K_q)$ have one cut vertex, say u, in common. $V(K_p) = \{u_1, u_2, \cdots, u_{p-1}, u\}$, $V(K_q) = \{v_1, v_2, \cdots, v_{q-1}, u\}$. $P = v_1w_1 \cdots w_t$ ($t \geq 1$) is a path attached to v_1 and $N_G(v_1) = \{u, v_2, \cdots, v_{q-1}, w_1\}$. G_i ($1 \leq i \leq p - 1$) is the subgraph attached to u_i ($1 \leq i \leq p - 1$) and H_j ($2 \leq j \leq q - 1$) is the subgraph attached to v_j ($2 \leq j \leq q - 1$). Let $G' = G - \{uu_1, uu_2, \cdots, uu_{p-1}, uv_1, uv_2, \cdots, uv_{q-1}\} + \{w_tu\} + \{u_1v_1, u_1v_2, \cdots, u_1v_{q-1}\} + \cdots + \{u_{p-1}v_1, u_{p-1}v_2, \cdots, u_{p-1}v_{q-1}\}$, as shown in Figure 14.

Lemma 4.3. *Let G and G' be graphs in Figure 14. Then $SEI_a(G') > SEI_a(G)$ for $a > 1$.*

Proof. It can be seen that $d_G(u) = p + q - 2$, $d_{G'}(u) = 1$, $d_G(w_t) = 1$, $d_{G'}(w_t) = 2$, $d_G(v_1) = q$, $d_{G'}(v_1) = p+q-2$, $d_{G'}(u_i) = d_G(u_i)+q-2$ $(i = 1, 2, \cdots, p-1)$, $d_{G'}(v_j) = d_G(v_j)+p-2$ $(j = 2, \cdots, q-1)$, and the degrees of other vertices are unchanged. By the definition of variable sum exdeg index and Lemma 2.4, 2.6, for $a > 1$, we have

$$\begin{aligned}
&SEI_a(G') - SEI_a(G)\\
=&\sum_{i=1}^{p-1}[f_a(d_G(u_i) + q - 2) - f_a(d_G(u_i))] + \sum_{j=2}^{q-1}[f_a(d_G(v_j) + p - 2) - f_a(d_G(v_j))]\\
&+ f_a(p + q - 2) - f_a(q) - f_a(p + q - 2) + f_a(2)\\
\geq&(p - 1)[(p + q - 3)a^{p+q-3} - (p - 1)a^{p-1}] + 2a^2 - qa^q\\
&+ (q - 2)[(p + q - 3)a^{p+q-3} - (q - 1)a^{q-1}] > 0.
\end{aligned}$$

The proof is completed. □

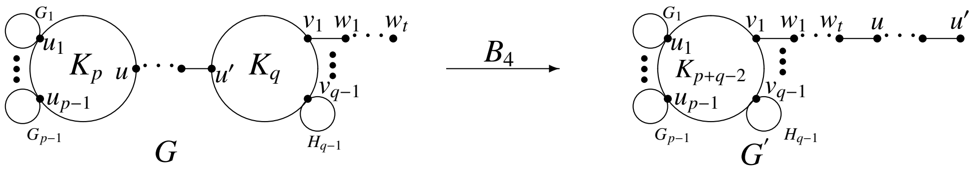


Figure 15. Transformation B_4.

Transformation B_4: Let G be a graph as shown in Figure 15, K_p and K_q be two cliques of G, where $p, q \geq 3$. K_p connects K_q by an internal path $P = u \cdots u'$ of length $s \geq 1$. $V(K_p) = \{u_1, u_2, \cdots, u_{p-1}, u\}$, $V(K_q) = \{v_1, v_2, \cdots, v_{q-1}, u'\}$. $P_{t+1} = v_1w_1 \cdots w_t$ $(t \geq 1)$ is a path attached to v_1 and $N_G(v_1) = \{u', v_2, \cdots, v_{q-1}, w_1\}$. G_i $(1 \leq i \leq p-1)$ is the subgraph attached to u_i $(1 \leq i \leq p-1)$ and H_j $(2 \leq j \leq q-1)$ is the subgraph attached to v_j $(2 \leq j \leq q-1)$. Let $G' = G - \{uu_1, uu_2, \cdots, uu_{p-1}, u'v_1, u'v_2, \cdots, u'v_{q-1}\} + \{w_tu\} + \{u_1v_1, u_1v_2, \cdots, u_1v_{q-1}\} + \cdots + \{u_{p-1}v_1, u_{p-1}v_2, \cdots, u_{p-1}v_{q-1}\}$, as shown in Figure 15.

Lemma 4.4. *Let G and G' be graphs in Figure 15. Then $SEI_a(G') > SEI_a(G)$ for $a > 1$.*

Proof. We notice that $d_G(u) = p$, $d_{G'}(u) = 2$, $d_G(u') = q$, $d_{G'}(u') = 1$, $d_G(w_t) = 1$, $d_{G'}(w_t) = 2$, $d_G(v_1) = q$, $d_{G'}(v_1) = p + q - 2$, $d_{G'}(u_i) = d_G(u_i) + q - 2$ $(i = 1, 2, \cdots, p - 1)$, $d_{G'}(v_j) = d_G(v_j) + p - 2$ $(j = 2, \cdots, q - 1)$, and the degrees of other vertices are unchanged. By the definition of variable sum exdeg index and Lemma 2.4, 2.7, for $a > 1$, we have

$$\begin{aligned}
&SEI_a(G') - SEI_a(G)\\
=&\sum_{i=1}^{p-1}[f_a(d_G(u_i) + q - 2) - f_a(d_G(u_i))] + \sum_{j=2}^{q-1}[f_a(d_G(v_j) + p - 2) - f_a(d_G(v_j))]\\
&+ f_a(p + q - 2) - f_a(q) + 2f_a(2) - f_a(p) - f_a(q)\\
\geq&(p - 1)[(p + q - 3)a^{p+q-3} - (p - 1)a^{p-1}] + (p + q - 2)a^{p+q-2} + 4a^2
\end{aligned}$$

$$+ (q-2)[(p+q-3)a^{p+q-3} - (q-1)a^{q-1}] - pa^p - 2qa^q > 0.$$

This finishes the proof. □

Lemma 4.5. *Choose $G \in \mathbf{G}_V(n,k)$ such that $SEI_a(G)$ is as large as possible for $a > 1$. Then each cut vertex of G connects exactly two blocks and each of the blocks contained in G is a clique.*

Proof. We shall prove by contradiction. Let u be a cut vertex in G. Assume that u connects at least three connected components, say $G_1, G_2, \cdots, G_r$ ($r \geq 3$), of G. Let $G' = G + xy$, where $x \in V(G_2)\backslash\{u\}$ and $y \in V(G_3)\backslash\{u\}$. Clearly, $G' \in \mathbf{G}_V(n,k)$ and by Lemma 2.2, we have $SEI_a(G') > SEI_a(G)$ for $a > 1$, a contradiction. Thus, we get that each cut vertex connects exactly two blocks. Moreover, by Lemma 2.2, we can conclude that each block is a clique. □

In order to determine the maximum variable sum exdeg index of $\mathbf{G}_V(n,k)$, we choose connected graph $G \in \mathbf{G}_V(n,k)$ such that $SEI_a(G)$ is as large as possible for $a > 1$. By Lemma 4.5, each cut vertex of G connects exactly two cliques. We define two cliques K_p, K_q ($p, q \geq 3$) of G are adjacent, if K_p connects K_q by a path P such that P does not intersect some other clique with at least 3 vertices. By Lemma 4.5, the following Lemma 4.6 is obtained.

Lemma 4.6. *Choose $G \in \mathbf{G}_V(n,k)$ such that $SEI_a(G)$ is as large as possible for $a > 1$. If two cliques K_p, K_q with $p, q \geq 3$ in G are adjacent, then the path connecting K_p and K_q is either of length 0 or an internal path.*

Lemma 4.7. *Choose $G \in \mathbf{G}_V(n,k)$ such that $SEI_a(G)$ is as large as possible for $a > 1$. If K_q is an endblock of G, then $q = 2$.*

Proof. We prove this lemma by contradiction. Suppose that $q \geq 3$, let K_p ($p \geq 2$) be a clique such that $V(K_p)$, $V(K_q)$ have one cut vertex, say u, in common. By Lemma 4.5, u is not a cut vertex of some other clique. From Lemma 4.1, G can be changed to G' by transformation B_1 with a larger variable sum exdeg index for $a > 1$, which contradicts the choice of G. Hence, $q = 2$. □

Choose $G \in \mathbf{G}_V(n,k)$ such that $SEI_a(G)$ is as large as possible for $a > 1$. By Lemma 4.5, we assume that $K_{n_1}, K_{n_2}, \cdots, K_{n_r}$ are all cliques of G.

Lemma 4.8. *Choose $G \in \mathbf{G}_V(n,k)$ such that $SEI_a(G)$ is as large as possible for $a > 1$. Let $K_{n_1}, K_{n_2}, \cdots, K_{n_r}$ are all of the cliques contained in G. Then there is only one clique K_{n_i} with $n_i \geq 3$.*

Proof. To the contrary, suppose that there are two cliques K_p, K_q ($p \neq q$ and $p, q \in \{n_1, n_2, \cdots, n_r\}$) such that K_p is adjacent to K_q, where $p, q \geq 3$. By Lemma 4.7, it can be seen that K_p and K_q are not endblocks. Furthermore, by Lemma 4.5, we can choose two such blocks such that at least one of them have a pendant path attached to one of its vertices. Without loss of generality, we assume that K_q is one of such cliques and v_1 is attached by one pendant path, say $P_{t+1} = v_1 w_1 \cdots w_t$ ($t \geq 1$). By Lemma 4.6, we can see that K_p and K_q have exactly one cut vertex in common or K_p connects K_q by an internal path P of length $s \geq 1$. Next, We discuss in two cases.

Case 1. K_p and K_q have exactly one cut vertex, say u, in common.

By Lemma 4.3, G can be changed to G' by transformation B_3 with a larger variable sum exdeg index for $a > 1$, which is a contradiction to the choice of G.

Case 2. The internal path $P = u \cdots u'$ is of length $s \geq 1$.

By Lemma 4.4, G can be changed to G' by transformation B_4 with a larger variable sum exdeg index for $a > 1$, which contradicts the assumption of G.

The proof is completed. □

Lemma 4.9. *Choose $G \in \mathbf{G}_V(n, k)$ such that $SEI_a(G)$ is as large as possible for $a > 1$. Let K_p be the only clique with $p \geq 3$. Then $p = n - k$.*

Proof. In view of Lemma 4.5 and 4.8, it can be concluded that in G, there are $k + 1$ cliques and k of them are isomorphic to K_2. Since G has k cut vertices, and each cut vertex belongs to two cliques, then $2k + p - k = n$. Thus, $p = n - k$. □

Denote $\mathbf{G}_{n,k} = \{G | G \in \mathbf{G}_V(n, k)$ is obtained by attaching at most one pendant path to each vertex of $K_{n-k}\}$. Then it is not difficult to see that $\{G^1_{n,k}, G^2_{n,k}\} \subset \mathbf{G}_{n,k}$.

Lemma 4.10. *Let $H \in \mathbf{G}_{n,k}$. Then for $a > 1$, the maximum value of $SEI_a(H)$ is obtained at the graph in $G^1_{n,k}$ or $G^2_{n,k}$.*

Proof. Choose $H \in \mathbf{G}_{n,k}$ such that $SEI_a(H)$ is as large as possible for $a > 1$. If $H \cong G^1_{n,k}$ or $G^2_{n,k}$, the lemma holds. Otherwise, $H \in \mathbf{G}_{n,k} \backslash \{G^1_{n,k}, G^2_{n,k}\}$. Let P, which is attached to u_0, be the shortest path of all the pendant paths in H and P', which is attached to u_1, be the longest one in H. Since $H \notin \{G^1_{n,k}, G^2_{n,k}\}$, then we have $|E(P)| = 0$ (H has no pendant path attached to u_0) and $|E(P')| \geq 2$. By Lemma 4.2, H can be changed to H' by transformation B_2 with a larger variable sum exdeg index for $a > 1$, which contradicts the assumption of H. □

Theorem 4.11. *Let $G \in \mathbf{G}_V(n, k)$, where $1 \leq k \leq n - 3$. Then*

(*i*) *if $1 \leq k \leq \frac{n}{2}$, $SEI_a(G) \leq (n - 2k)(n - k - 1)a^{n-k-1} + k(n - k)a^{n-k} + ka$ for $a > 1$, with equality holding if and only if $G \cong G^1_{n,k}$;*

(*ii*) *if $\frac{n}{2} < k \leq n - 3$, $SEI_a(G) \leq (n - k)^2(n - k - 1)a^{n-k-1} + 2(2k - n)a^2 + a(n - k)$ for $a > 1$, with equality holding if and only if $G \cong G^2_{n,k}$.*

Proof. By Lemma 4.8 and 4.9, we have $G \in \mathbf{G}_{n,k}$. By Lemma 4.10, for $a > 1$, we have $SEI_a(G) \leq SEI_a(G^1_{n,k})$ when $1 \leq k \leq \frac{n}{2}$ and $SEI_a(G) \leq SEI_a(G^2_{n,k})$ when $\frac{n}{2} < k \leq n - 3$.

The proof is finished. □

5. Variable sum exdeg indices of graphs with given vertex connectivity or edge connectivity for $a > 1$

Lemma 5.1. *Let G be a graph of order n with vertex connectivity $\kappa < n - 1$. Then there exist positive integers n_1 and n_2 such that $n_1 + n_2 = n - \kappa$ and for $a > 1$,*

$$SEI_a(G) \leq SEI_a(K_\kappa \vee (K_{n_1} \cup K_{n_2})).$$

Proof. Assume that X is a vertex cut of G with κ vertices such that $G - X$ has l components, say $G_1, G_2, \cdots, G_l$, where $l \geq 2$. Let $n_1 = |V(G_1)|$ and $n_2 = |V(G_2 \cup \cdots \cup G_l)|$. Then G is a spanning subgraph of $K_\kappa \vee (K_{n_1} \cup K_{n_2})$. By Lemma 2.2, the lemma holds immediately. □

Lemma 5.2. *Let G be a n-vertex graph with edge connectivity $\lambda < n-1$. Then there exist positive integers n_1 and n_2 such that $n_1 + n_2 = n - \kappa$, $\kappa \leq \lambda$ and for $a > 1$,*

$$SEI_a(G) \leq SEI_a(K_\kappa \vee (K_{n_1} \cup K_{n_2})).$$

Proof. Let κ be the vertex connectivity of G. Then $\kappa \leq \lambda < n-1$. From Lemma 5.1, the conclusion holds clearly. □

Lemma 5.3. *Let $G = K_s \vee (K_{n_1} \cup K_{n_2})$ and $G' = K_s \vee (K_{n_1-1} \cup K_{n_2+1})$, where $2 \leq n_1 \leq n_2$, $n_1 + n_2 = n - s$. Then for $a > 1$,*

$$SEI_a(G') > SEI_a(G).$$

Proof. In view of the definition of variable sum exdeg index, for $a > 1$, we have

$$\begin{aligned}
& SEI_a(G') - SEI_a(G) \\
=& (n_1 - 1) f_a(n_1 + s - 2) + (n_2 + 1) f_a(n_2 + s) - n_1 f_a(n_1 + s - 1) - n_2 f_a(n_2 + s - 1) \\
=& n_2 (f_a(n_2 + s) - f_a(n_2 + s - 1)) - n_1 (f_a(n_1 + s - 1) - f_a(n_1 + s - 2)) \\
& + f_a(n_2 + s) - f_a(n_1 + s - 2) \\
>& n_2 f_a'(\xi) - n_1 f_a'(\eta) \geq n_1 (f_a'(\xi) - f_a'(\eta)),
\end{aligned}$$

where $n_2 + s - 1 < \xi < n_2 + s$, $n_1 + s - 2 < \eta < n_1 + s - 1$. By Lemma 2.1, we have $SEI_a(G') - SEI_a(G) > 0$ for $a > 1$, i.e., $SEI_a(G') > SEI_a(G)$ for $a > 1$. □

Theorem 5.4. *Let G be a graph of order n with vertex connectivity κ ($\kappa < n-1$). Then*

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

for $a > 1$, with equality if and only if $G \cong K_\kappa \vee (K_1 \cup K_{n-\kappa-1})$.

Proof. Choose G such that G has the maximum variable sum exdeg index (for $a > 1$) among all graphs of order n with vertex connectivity κ. By Lemma 2.2 and 5.1, there exist positive integers n_1 and n_2 such that $n_1 + n_2 = n - \kappa$ and $G \cong K_\kappa \vee (K_{n_1} \cup K_{n_2})$. Moreover, by Lemma 5.3, $G \cong K_\kappa \vee (K_1 \cup K_{n-\kappa-1})$. □

Theorem 5.5. *Let G be a n-vertex graph with edge connectivity λ ($\lambda < n-1$). Then*

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

for $a > 1$, with equality if and only if $G \cong K_\lambda \vee (K_1 \cup K_{n-\lambda-1})$.

Proof. Choose G such that G has the maximum variable sum exdeg index (for $a > 1$) among all n-vertex graphs with edge connectivity λ. By Lemma 2.1 and 5.2, there exist positive integers $\kappa \leq \lambda$ such that $n_1 + n_2 = n - \kappa$ and $G \cong K_\kappa \vee (K_{n_1} \cup K_{n_2})$. By Lemma 5.3, we have $G \cong K_\kappa \vee (K_1 \cup K_{n-\kappa-1})$. Furthermore, $K_\kappa \vee (K_1 \cup K_{n-\kappa-1})$ is a spanning subgraph of $K_\lambda \vee (K_1 \cup K_{n-\lambda-1})$ for $\kappa \leq \lambda$, by Lemma 2.2, the result holds obviously. □

6. Conclusions

In [7], Vukičević think that mathematical properties of the variable sum exdeg index deserves further study since it can be used for the detection of chemical compounds that may have desirable properties. Inspired by [17–24], we continue to study the mathematical properties of the variable sum exdeg index and the connectivity of a graph. In this work, we present the extremal value of the variable sum exdeg indices (for $a > 1$) in terms of the number of cut edges, or the number of cut vertices, or the vertex connectivity, or the edge connectivity of a graph. Furthermore, the corresponding extremal graphs are characterized.

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Conflict of interest

The authors declare no conflict of interest.

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