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Extremal Problems on the Variable Sum Exdeg Index

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Abstract

The variable sum exdeg index SEI_a is a topological index which has shown to be useful in QSPR and QSAR studies. Vukičević solved several extremal problems involving this index in 2011, for values of the parameter $a > 1$, and for the case $0 < a < 1$, he left several such problems open. Some of the open problems posed by Vukičević are solved in this paper; we characterize graphs with maximum and minimum values of the SEI_a index, for $0 < a < 1/2$, in the following sets of graphs with n vertices: graphs, connected graphs, graphs with fixed minimum degree, connected graphs with fixed minimum degree, graphs with fixed maximum degree, and connected graphs with fixed maximum degree.

1 Introduction

A topological index is a single number which represents a chemical structure via the molecular graph, in graph theoretical terms, whenever it correlates with a molecular property. Hundreds of topological indices have been recognized to be useful tools in researches, especially in chemistry. Topological indices have been used to understand physicochemical properties of compounds. They usually enclose topological properties of a molecular graph in a single real number. Several topological indices were introduced by the seminal work by Wiener. They have been studied and generalized by several researchers since then (see, e.g., [2], [4], [5] and [15]). In particular, topological indices based on end-vertex degrees of edges have been studied over almost 50 years (see, e.g., [14] and [7]).

Vukičević proposed in 2011 [17] the following topological index, called the *variable sum exdeg index*, which predicts the octanol-water partition coefficient of certain compounds

$$SEI_a(G) = \sum_{uv \in E(G)} \left(a^{d_u} + a^{d_v}\right) = \sum_{u \in V(G)} d_u a^{d_u},$$

where a is a positive real number, and d_u denotes the degree of the vertex $u \in V(G)$. Among the set of 102 topological indices [9] proposed by the IAMC [8] (respectively, among the discrete Adriatic indices [16]), the best topological index predicting the octanol-water partition coefficient of octane isomers has 0.29 (respectively 0.36) coefficient of determination. The sum exdeg index $SEI_{0.37}$ allows to obtain the coefficient of determination 0.99, for predicting the aforementioned property of octane isomers [17]. Therefore, it is interesting to study mathematical properties of the SEI_a, specially for $a = 0.37$; unfortunately, usually it is difficult to obtain extremal properties for SEI_a with $1 > a > e^{-2} = 0.135335....$

Vukičević started the mathematical study of SEI_a in [18]. He found, for $a > 1$, extremal graphs with respect to the SEI_a among the sets of graphs with n vertices (1) connected, (2) trees, (3) unicyclic, (4) chemical, (5) chemical trees, (6) chemical unicyclic, (7) given maximum degree, (8) given minimum degree, (9) trees with given number of pendant vertices, and (10) connected with given number of pendant vertices. In [18] appears also, for $0 < a < 1$, the extremal graphs with respect to the SEI_a among the sets (4), (5) and (6), however extremal graphs in other seven sets of graphs was presented as open problems. Yarahmadi and Ashrafi [19] introduced the variable sum exdeg polynomial, and studied the behavior of this polynomial under some graph operations. Ghalavand and Ashrafi [6] found the extremal graphs with respect to the SEI_a, for $a > 1$, among the sets of trees and unicyclic graphs with n vertices by using the majorization technique. Also, they characterized the graphs having maximum SEI_a value, for $a > 1$, among the sets of graphs with n vertices bicyclic and tricyclic. Ali and Dimitrov in [1] extend the results from [6] for tetracyclic graphs. Khalid and Ali attacked the open problem of finding extremal trees with a fixed number of leaves with respect to SEI_a [10] for every $0 < a < 1$, but unfortunately proofs of the results, except Lemma 4.6, concerning SEI_a with $0 < a < 1$ are not correct in the reference [10], and hence these results are still needed to be prove. Recently, Dimitrov and Ali in [3] characterize, for $a > 1$ and $0 < a < e^{-2} = 0.135335...$, the n-vertex extremal graphs with fixed cyclomatic number, and for $0 < a < 1/3$ the n-vertex graphs with cyclomatic number up to four having maximal SEI_a value.

In this paper, we characterize the graphs with maximum and minimum values of the SEI_a index, for $0 < a < 1/2$, in the following sets of graphs with n vertices: graphs, connected graphs, graphs with a fixed minimum degree, connected graphs with a fixed minimum degree, graphs with a fixed maximum degree, and connected graphs with a fixed maximum degree. Note that the value $a = 0.37$ belongs to this interval. These results solve the problems (1), (7) and (8) stated by Vukičević in [18], for these values of the parameter a. We can use these results for detecting chemical compounds that could satisfy desirable properties. Hence, extremal graphs should correspond to molecules with a extremal value of a desired property since there exists a property well correlated with this descriptor for some values of a, in particular, $a = 0.37$.

Our arguments allow to obtain the known results for $a > 1$, and we include them by the sake of completeness. Also, some of them are a slightly improvement of the known results (e.g., item (3) in Theorem 2.12 improves [18, Proposition 6], and item (2) in Theorem 2.18 improves [18, Proposition 4]).

In order to prove our theorems, we have obtained a result that is interesting by itself: Theorem 2.4 states that if $0 < a < 1/3$, then there exists a continuous and strictly convex function $F : [1, \infty) \to \mathbb{R}$ such that $F(k) = ka^k$ for every $k \in \mathbb{Z}^+$. This result allows to extend to $0 < a < 1/3$ every optimization result for the SEI_a in the literature proved for $0 < a \leq e^{-2}$ by using majorization (i.e., Schür convexity or Karamata inequality).

Throughout this paper, $G = (V(G), E(G))$ denotes an undirected finite simple graph without isolated vertices. As usual, a forest will denote a graph without cycles, and a tree a connected forest.

2 Optimization problems for the variable sum exdeg index

We start with some technical results.

Given any function $f : \mathbb{Z}^+ \to \mathbb{R}^+$, let us define the *$f$-index*

$$I_f(G) = \sum_{u \in V(G)} f(d_u).$$

Note that if $f(t) = ta^t$, then $I_f(G) = SEI_a(G)$.

The following result is elementary. We include a proof for the sake of completeness.

Lemma 2.1. *Let us consider $a > 0$, $\delta \in \mathbb{Z}^+$ and $f(t) = ta^t$.*

(1) *If $a > 1$, then f is strictly increasing and convex on $[0, \infty)$.*

(2) *If $0 < a \le e^{-1/\delta}$, then f is strictly decreasing on $[\delta, \infty)$.*

(3) *If $0 < a \le e^{-2/\delta}$, then f is strictly convex on $[\delta, \infty)$. In particular, if $a \le e^{-2}$, then f is strictly convex on $[1, \infty)$.*

Proof. Since $f'(t) = a^t + ta^t \log a$ and $f''(t) = 2a^t \log a + ta^t (\log a)^2$, if $a > 1$, then f is strictly increasing and convex on $[0, \infty)$.

If $0 < a < 1$, then f is strictly decreasing on $[-1/\log a, \infty)$. If $0 < a \le e^{-1/\delta}$, then $-1/\log a \le \delta$ and f is strictly decreasing on $[\delta, \infty)$.

If $0 < a < 1$, then f is strictly convex on $[-2/\log a, \infty)$. If $0 < a \le e^{-2/\delta}$, then $-2/\log a \le \delta$ and f is strictly convex on $[\delta, \infty)$. ■

Proposition 2.2. *If $0 < a < 1/2$, then $f(t) = ta^t$ satisfies $f(a) > f(b)$ whenever $a < b$ where a and b are positive integers.*

Proof. If $0 < a \le e^{-1/2}$, then Lemma 2.1 gives that f is strictly decreasing on $[2, \infty)$. Since $1/2 < e^{-1/2} = 0.60653...$, it suffices to check that $a = f(1) > f(2) = 2a^2$, and this holds since $0 < a < 1/2$. ■

Lemma 2.3. *Let us consider $f : \{1\} \cup [2, \infty) \to \mathbb{R}$ such that f is strictly convex on $[2, \infty)$. If $2f(2) < f(1) + f(3)$, then there exists $F : [1, \infty) \to \mathbb{R}$ such that $F = f$ on $\{1\} \cup \{2\} \cup [3, \infty)$ and F is continuous and strictly convex on $[1, \infty)$.*

Proof. Since f is strictly convex on $[2, \infty)$, we have

$$f(3) - f(2) < f'_-(3) = \lim_{h \to 0^-} \frac{f(3+h) - f(3)}{h}.$$

By hypothesis, $f(2)-f(1)<f(3)-f(2)$, and so,

$$\varepsilon=\frac{1}{2\pi}\min\left\{f(3)-f(2)-\big(f(2)-f(1)\big),2f'_-(3)-2\big(f(3)-f(2)\big)\right\}>0.$$

Let us define the function F as follows:

$$F(t)=\begin{cases}\big(f(2)-f(1)\big)(t-1)+f(1)-\varepsilon\sin\pi(t-1) & \text{if } t\in[1,2]\,,\\ \big(f(3)-f(2)\big)(t-2)+f(2)-\varepsilon\sin\pi(t-2) & \text{if } t\in[2,3]\,,\\ f(t) & \text{if } t\geq 3\,.\end{cases}$$

It is clear that $F=f$ on $\{1\}\cup\{2\}\cup[3,\infty)$.

Since f is continuous on $(2,\infty)$, F is continuous on $[1,\infty)$. We have

$$F'(t)=\begin{cases}f(2)-f(1)-\varepsilon\pi\cos\pi(t-1) & \text{if } t\in(1,2)\,,\\ f(3)-f(2)-\varepsilon\pi\cos\pi(t-2) & \text{if } t\in(2,3)\,,\\ f'(t) & \text{if } t>3 \text{ and there exists } f'(t)\,,\end{cases}$$

and

$$F''(t)=\begin{cases}\varepsilon\pi^2\sin\pi(t-1) & \text{if } t\in(1,2)\,,\\ \varepsilon\pi^2\sin\pi(t-2) & \text{if } t\in(2,3)\,,\\ f''(t) & \text{if } t>3 \text{ and there exists } f''(t)\,.\end{cases}$$

Since

$$F'_-(2)=f(2)-f(1)+\varepsilon\pi\leq f(3)-f(2)-\varepsilon\pi=F'_+(2),$$

$$F'_-(3)=f(3)-f(2)+\varepsilon\pi\leq f'_-(3)=F'_+(3),$$

$f''>0$ on $(1,2)\cup(2,3)$, and f is continuous and strictly convex on $[3,\infty)$, F is strictly convex on $[1,\infty)$. ■

Theorem 2.4. *If $0<a<1/3$, then there exists a continuous and strictly convex function $F:[1,\infty)\to\mathbb{R}$ such that $F(k)=ka^k$ for every $k\in\mathbb{Z}^+$.*

Proof. Let us consider the function $f(t)=ta^t$. Since $0<a<1/3<e^{-1}$, Lemma 2.1 gives that f is strictly convex on $[2,\infty)$. Since $0<a<1/3$, we have $2f(2)=4a^2<a+3a^3=f(1)+f(3)$. Thus, Lemma 2.3 gives the result. ■

Note that Theorem 2.4 allows to extend to $0<a<1/3$ every optimization result for the SEI_a with $0<a\leq e^{-2}$ in the literature proved by using majorization (Schür convexity or Karamata inequality), e.g., the results in [6], and Theorems 2.4 and 2.5 in [3].

Proposition 2.5. *Let G be a graph with minimum degree at least δ, and $v,w\in V(G)$ with $vw\notin E(G)$.*

(1) *If $a>1$, then $SEI_a(G+\{vw\})>SEI_a(G)$.*

(2) *If $0<a\leq e^{-1/\delta}$ for $\delta\geq 2$ or $0<a<1/2$ for $\delta=1$, then $SEI_a(G+\{vw\})<SEI_a(G)$.*

Proof. If $u \notin \{v, w\}$, then its degree in $G + \{vw\}$ is d_u; also, the degree of v (respectively, w) in $G + \{vw\}$ is $d_v + 1$ (respectively, $d_w + 1$). Hence, $G + \{vw\}$ is a graph with minimum degree at least δ. Consider $f(t) = ta^t$. Thus, Lemma 2.1 and Proposition 2.2 give that $f(d_v + 1) + f(d_w + 1) > f(d_v) + f(d_w)$ if $a > 1$, $f(d_v + 1) + f(d_w + 1) < f(d_v) + f(d_w)$ if $0 < a \le e^{-1/\delta}$ for $\delta \ge 2$ or $0 < a < 1/2$ for $\delta = 1$. These facts finish the proof. ■

Note that item (1) in Proposition 2.5 is known.

If $0 < \delta < \Delta$ are integers, we say that a graph G is (Δ, δ)-*quasi-regular* if there exists $v \in V(G)$ with $d_v = \delta$ and $d_u = \Delta$ for every $u \in V(G) \setminus \{v\}$; G is (Δ, δ)-*pseudo-regular* if there exists $v \in V(G)$ with $d_v = \Delta$ and $d_u = \delta$ for every $u \in V(G) \setminus \{v\}$.

Lemma 2.6. *Consider integers $2 \le k < n$.*

(1) *If kn is even, then there is a Hamiltonian k-regular graph with n vertices.*

(2) *If kn is odd, then there are a connected $(k, k-1)$-quasi-regular graph with n vertices and a connected $(k+1, k)$-pseudo-regular graph with n vertices.*

Proof. Let us consider the cycle graph C_n. If $k = 2$, then it suffices to choose $G = C_n$. Assume now that $k \ge 3$. Let $G_1(n, k)$ be the graph obtained from C_n by adding the edges $\{uv : 2 \le d_{C_n}(u, v) \le \lfloor k/2 \rfloor\}$, where $\lfloor t \rfloor$ denotes the greatest integer less than or equal to t. Note that $G_1(n, k)$ has n vertices with degree $2\lfloor k/2 \rfloor$. Also, $G_1(n, k)$ is Hamiltonian, since it contains C_n.

If k is even, then $2\lfloor k/2 \rfloor = k$ and this gives (1).

If k is odd and n is even, then let $G_2(n, k)$ be the graph obtained from $G_1(n, k)$ by adding the edges $\{uv : d_{C_n}(u, v) = n/2\}$. Thus, $G_2(n, k)$ is a Hamiltonian $(2\lfloor k/2 \rfloor + 1)$-regular graph with n vertices. Since k is odd, $2\lfloor k/2 \rfloor + 1 = k$ and this finishes the proof of (1).

Finally, assume that kn is odd. Thus, k and n are odd, and so, $k \le n - 2$ and $n - 1$ is even. Hence, $G_2(n - 1, k)$ is Hamiltonian and k-regular with $n - 1$ vertices. Let us consider $w \notin V(G_2(n-1, k))$ and a Hamiltonian cycle C in $G_2(n-1, k)$. Choose $(k-1)/2$ non-incident edges $e_1, \dots, e_{(k-1)/2}$ in C, and define the graph $G_3(n, k)$ by

$$\begin{aligned} V(G_3(n, k)) &= V(G_2(n - 1, k)) \cup \{w\}, \\ E(G_3(n, k)) &= E(G_2(n - 1, k)) \setminus \{e_1, \dots, e_{(k-1)/2}\} \\ &\qquad \cup \{wv : v \text{ is an endpoint of } e_i \text{ for some } i = 1, \dots, (k-1)/2\}. \end{aligned}$$

Hence, $d_w = k-1$ and $d_u = k$ for every $u \in V(G_2(n-1,k)) = V(G_3(n,k)) \setminus \{w\}$. Thus, $G_3(n,k)$ is $(k,k-1)$-quasi-regular with n vertices. Finally, $G_3(n,k)$ is connected since the cycle

$$\begin{aligned} &C \setminus \{e_1, \dots, e_{(k-1)/2}\} \\ &\quad \cup \{wv : \, v \text{ is an endpoint of } e_i \text{ for some } i = 1, \dots, (k-1)/2\,\} \end{aligned}$$

contains every vertex of this graph.

If we choose $(k+1)/2$ non-incident edges in C, instead of $(k-1)/2$, in the definition of the graph $G_3(n,k)$, then we obtain a connected $(k+1,k)$-pseudo-regular graph with n vertices. ■

We start with the easiest optimization problem for SEI_a.

Proposition 2.7. *Given a positive integer n, let $\mathcal{G}(n)$ (respectively, $\mathcal{G}_c(n)$) be the collection of n-vertex graphs (respectively, connected graphs).*

(1) *If $a > 1$, then the unique graph that maximizes the SEI_a index in $\mathcal{G}_c(n)$ or $\mathcal{G}(n)$ is the complete graph K_n.*

(2) *If $a > 1$, then the unique graph that minimizes the SEI_a index in $\mathcal{G}_c(n)$ is the path graph P_n.*

(3) *If $a > 1$ and n is even, then the unique graph that minimizes the SEI_a index in $\mathcal{G}(n)$ is the disjoint union of $n/2$ path graphs P_2. If $a > 1$ and n is odd, then the unique graph that minimizes the SEI_a index in $\mathcal{G}(n)$ is the disjoint union of $(n-3)/2$ path graphs P_2 and a path graph P_3.*

(4) *If $0 < a < 1/2$, then the unique graph that minimizes the SEI_a index in $\mathcal{G}_c(n)$ or $\mathcal{G}(n)$ is the complete graph K_n.*

(5) *If $0 < a < 1/2$ and a graph maximizes the SEI_a index in $\mathcal{G}_c(n)$, then it is a tree.*

(6) *If $0 < a < 1/3$, then the unique graph that maximizes the SEI_a index in $\mathcal{G}_c(n)$ is the star graph S_n.*

(7) *If $0 < a < 1/2$ and n is even, then the unique graph that maximizes the SEI_a index in $\mathcal{G}(n)$ is the disjoint union of $n/2$ path graphs P_2. If $0 < a < 1/2$ and n is odd, then the unique graph that maximizes the SEI_a index in $\mathcal{G}(n)$ is the disjoint union of $(n-3)/2$ path graphs P_2 and a path graph P_3.*

Proof. Proposition 2.5 gives (1), (3), (4), (5) and (7).

[3, Lemma 2.1] gives that if a tree with n vertices has maximal variable sum exdeg index for some $0 < a < 1/3$, then it has maximum degree $n-1$. This fact and (5) gives (6).

[18, Corollary 9] gives (2). ■

Note that items (1) and (2) in Proposition 2.7 are known [18, Proposition 4 and Corollary 9].

Proposition 2.7 has the following consequence.

Proposition 2.8. *Let G be a graph with n vertices.*

(1) *If $a > 1$, then*

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

and the equality is attained if and only if G is the complete graph K_n.

(2) *If $a > 1$ and G is connected, then*

$$SEI_a(G) \geq 2(n-2)a^2 + 2a,$$

and the equality is attained if and only if G is the path graph P_n.

(3) *If $a > 1$ and n is even, then*

$$SEI_a(G) \geq na,$$

and the equality is attained if and only if G is the disjoint union of $n/2$ path graphs P_2.

If $a > 1$ and n is odd, then

$$SEI_a(G) \geq (n-1)a + 2a^2,$$

and the equality is attained if and only if G is the disjoint union of $(n-3)/2$ path graphs P_2 and a path graph P_3.

(4) *If $0 < a < 1/2$, then*

$$SEI_a(G) \geq n(n-1)a^{n-1},$$

and the equality is attained if and only if G is the complete graph K_n.

(5) *If $0 < a < 1/3$ and G is connected, then*

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

and the equality is attained if and only if G is the star graph S_n.

(6) *If* $0 < a < 1/2$ *and* n *is even, then*

$$SEI_a(G) \le na,$$

and the equality is attained if and only if G *is the disjoint union of* $n/2$ *path graphs* P_2*.*

If $0 < a < 1/2$ *and* n *is odd, then*

$$SEI_a(G) \le (n-1)a + 2a^2,$$

and the equality is attained if and only if G *is the disjoint union of* $(n-3)/2$ *path graphs* P_2 *and a path graph* P_3*.*

Note that items (1) and (2) in Proposition 2.8 are known [18, Proposition 4 and Corollary 9].

Corollary 2.9. *Let* G *be a graph with* n *vertices.*

(1) *Then*

$$SEI_{1/2}(G) \ge \frac{n(n-1)}{2^{n-1}},$$

and the equality is attained if G *is the complete graph* K_n*.*

(2) *If* G *is connected, then*

$$SEI_{1/3}(G) \le \frac{n-1}{3^{n-1}} + \frac{n-1}{3},$$

and the equality is attained if G *is the star graph* S_n*.*

(3) *Then*

$$SEI_{1/2}(G) \le \frac{n}{2},$$

and the equality is attained for each even n *if* G *is the disjoint union of* $n/2$ *path graphs* P_2*, and for each odd* n *if* G *is the disjoint union of* $(n-3)/2$ *path graphs* P_2 *and a path graph* P_3*.*

Proof. If we consider the value $\delta = 1$ and we take limits as $a \to (1/2)^-$ in the items (4) and (6) and as $a \to (1/3)^-$ in the item (5) of Theorem 2.8, then we obtain the desired inequalities.

Since the equality in (1) is attained if $G = K_n$ for every $0 < a < 1/2$, by continuity it has the equality for $a = 1/2$ at $G = K_n$.

A similar argument gives the statements on equality in (2) and (3). ∎

Given integers $1 \leq \delta \leq n$, denote by K_n^δ the n-vertex graph with maximum and minimum degrees $n = 1$ and δ, respectively, obtained from the complete graph K_{n-1} and an additional vertex v in the following way: Fix δ vertices $u_1, \ldots, u_\delta \in V(K_n^\delta)$ and let $V(K_n^\delta) = V(K_{n-1}) \cup \{v\}$ and $E(K_n^\delta) = E(K_{n-1}) \cup \{u_1v, \ldots, u_\delta v\}$. Besides, denote by $\mathcal{H}_c(n, \delta)$ the family of all connected n-vertex graphs with minimum degree δ.

Theorem 2.10. *Let δ, n be two integer numbers such that $1 \leq \delta < n$. Then*

(1) *If $a > 1$, then the unique graph that maximizes the SEI_a index in $\mathcal{H}_c(n, \delta)$ is K_n^δ.*

(2) *If $a > 1$ and $\delta = 1$, then the unique graph that minimizes the SEI_a index in $\mathcal{H}_c(n, 1)$ is the path graph P_n.*

(3) *If $a > 1$, $\delta \geq 2$ and δn is even, then the unique graphs that minimize the SEI_a index in $\mathcal{H}_c(n, \delta)$ are the connected δ-regular graphs.*

(4) *If $a > 1$, $\delta \geq 2$ and δn is odd, then the unique graphs that minimize the SEI_a index in $\mathcal{H}_c(n, \delta)$ are the connected $(\delta + 1, \delta)$-pseudo-regular graphs.*

(5) *If $0 < a \leq e^{-1/\delta}$ for $\delta \geq 2$ or $0 < a < 1/2$ for $\delta = 1$, then the unique graph that minimizes the SEI_a index in $\mathcal{H}_c(n, \delta)$ is K_n^δ.*

(6) *If $0 < a < 1/2$, $\delta = 1$ and a graph maximizes the SEI_a index in $\mathcal{H}_c(n, 1)$, then it is a tree. Furthermore, if $0 < a < 1/3$, then the unique graph that maximizes the SEI_a index in $\mathcal{H}_c(n, \delta)$ is the star graph S_n.*

(7) *If $0 < a \leq e^{-1/\delta}$, $\delta \geq 2$ and δn is even, then the unique graphs that maximize the SEI_a index in $\mathcal{H}_c(n, \delta)$ are the connected δ-regular graphs.*

(8) *If $0 < a \leq e^{-1/\delta}$, $\delta \geq 2$ and δn is odd, then the unique graphs that maximize the SEI_a index in $\mathcal{H}_c(n, \delta)$ are the connected $(\delta + 1, \delta)$-pseudo-regular graphs.*

Proof. Firstly, note that Proposition 2.7 gives (2) and (6).

Assume that $0 < a \leq e^{-1/\delta}$ for $\delta \geq 2$ or $0 < a < 1/2$ for $\delta = 1$.

Given any graph $G \in \mathcal{H}_c(n, \delta) \setminus \{K_n^\delta\}$, fix a vertex $u \in V(G)$ with $d_u = \delta$. Since

$$G \neq G \cup \{vw : v, w \in V(G) \setminus \{u\} \text{ and } vw \notin E(G)\} = K_n^\delta,$$

Proposition 2.5 gives $SEI_a(K_n^\delta) < SEI_a(G)$.

Assume now that $0 < a \leq e^{-1/\delta}$ and $\delta \geq 2$.

Since $d_u \geq \delta$ for every u in $V(G)$, Proposition 2.5 gives

$$SEI_a(G) = \sum_{u \in V(G)} d_u a^{d_u} \leq \sum_{u \in V(G)} \delta a^\delta = n\delta a^\delta,$$

and the equality is attained if and only if $d_u = \delta$ for every $u \in V(G)$.

If δn is even, then Lemma 2.6 gives that there is a connected δ-regular graph with n vertices. Hence, the unique graphs that maximize the SEI_a index in $\mathcal{H}_c(n, \delta)$ are the connected δ-regular graphs.

If δn is odd, then handshaking lemma gives that there is no regular graph. Hence, there exists a vertex v with $d_v \geq \delta + 1$ and

$$SEI_a(G) = d_v a^{d_u} + \sum_{u \in V(G) \setminus \{v\}} d_u a^{d_u} \leq (n-1)\delta a^{\delta} + (\delta+1)a^{\delta+1},$$

and the equality is attained if and only if $d_u = \delta$ for every $u \in V(G) \setminus \{v\}$, and $d_v = \delta + 1$. Lemma 2.6 gives that there is a connected $(\delta+1, \delta)$-pseudo-regular graph with n vertices. Therefore, the unique graphs that maximize the SEI_a index in $\mathcal{H}_c(n, \delta)$ are the connected $(\delta + 1, \delta)$-pseudo-regular graphs.

The proof in the case $a > 1$ is similar. ■

Note that item (2) in Theorem 2.10 is known [18, Proposition 8].

Analogous to $\mathcal{H}_c(n, \delta)$, we define $\mathcal{H}(n, \delta)$ as the family of all n-vertex graphs with minimum degree δ.

Remark 2.11. *If we replace $\mathcal{H}_c(n, \delta)$ with $\mathcal{H}(n, \delta)$ in the items* (1), (3), (4), (5), (7) *and* (8) *in Theorem 2.10, then the arguments in their proofs give that the same conclusion hold in these items when we remove from them the word "connected".*

Also, the argument in the proof of Theorem 2.10 allows to conclude that the following statements hold:

(2′) *If $a > 1$, $\delta = 1$ and n is even, then the unique graph that minimizes the SEI_a index in $\mathcal{H}(n, 1)$ is the disjoint union of $n/2$ path graphs P_2. If $a > 1$, $\delta = 1$ and n is odd, then the unique graph that minimizes the SEI_a index in $\mathcal{H}(n, 1)$ is the disjoint union of $(n - 3)/2$ path graphs P_2 and a path graph P_3.*

(6′) *If $0 < a < 1/2$, $\delta = 1$ and n is even, then the unique graph that maximizes the SEI_a index in $\mathcal{H}(n, 1)$ is the disjoint union of $n/2$ path graphs P_2. If $0 < a < 1/2$, $\delta = 1$ and n is odd, then the unique graph that maximizes the SEI_a index in $\mathcal{H}(n, 1)$ is the union of $(n - 3)/2$ path graphs P_2 and a path graph P_3.*

Theorem 2.10 and Remark 2.11 have the following consequence.

Theorem 2.12. *Let $G \in \mathcal{H}(n, \delta)$.*

(1) *If $a > 1$, then*

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

and the equality is attained if and only if G is K_n^{δ}.

(2) *If $a > 1$, $\delta = 1$ and $G \in \mathcal{H}_c(n, \delta)$, then*

$$SEI_a(G) \geq 2a + 2(n-2)a^2,$$

and the equality is attained if and only if G is the path graph P_n.

(3) *If $a > 1$, $\delta = 1$ and n is even, then*

$$SEI_a(G) \geq na,$$

and the equality is attained if and only if G is the disjoint union of $n/2$ path graphs P_2.

If $a > 1$, $\delta = 1$ and n is odd, then

$$SEI_a(G) \geq (n-1)a + 2a^2,$$

and the equality is attained if and only if G is the disjoint union of $(n-3)/2$ path graphs P_2 and a path graph P_3.

(4) *If $a > 1$, $\delta \geq 2$ and δn is even, then*

$$SEI_a(G) \geq n\delta a^{\delta},$$

and the equality is attained if and only if G is δ-regular.

(5) *If $a > 1$, $\delta \geq 2$ and δn is odd, then*

$$SEI_a(G) \geq (n-1)\delta a^{\delta} + (\delta+1)a^{\delta+1},$$

and the equality is attained if and only if G is $(\delta+1, \delta)$-pseudo-regular.

(6) *If $0 < a \leq e^{-1/\delta}$ for $\delta \geq 2$ or $0 < a < 1/2$ for $\delta = 1$, then*

$$SEI_a(G) \geq \delta(n-1)a^{n-1} + (n-1-\delta)(n-2)a^{n-2} + \delta a^{\delta},$$

and the equality is attained if and only if G is K_n^{δ}.

(7) *If $0 < a < 1/3$, $\delta = 1$ and $G \in \mathcal{H}_c(n, \delta)$, then*

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

and the equality is attained if and only if G *is the star graph* S_n.

(8) *If* $0 < a < 1/2$, $\delta = 1$ *and* n *is even, then*

$$SEI_a(G) \leq na,$$

and the equality is attained if and only if G *is the disjoint union of* $n/2$ *path graphs* P_2.

If $0 < a < 1/2$, $\delta = 1$ *and* n *is odd, then*

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

and the equality is attained if and only if G *is the disjoint union of* $(n-3)/2$ *path graphs* P_2 *and a path graph* P_3.

(9) *If* $0 < a \leq e^{-1/\delta}$, $\delta \geq 2$ *and* δn *is even, then*

$$SEI_a(G) \leq n\delta a^{\delta},$$

and the equality is attained if and only if G *is* δ*-regular.*

(10) *If* $0 < a \leq e^{-1/\delta}$, $\delta \geq 2$ *and* δn *is odd, then*

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

and the equality is attained if and only if G *is* $(\delta+1, \delta)$*-pseudo-regular graphs.*

Note that items (1), (2) and (4) in Theorem 2.12 is known [18, Propositions 6 and 8].

Corollary 2.13. *Let* $G \in \mathcal{H}(n, 1)$.

(1) *Then*

$$SEI_{1/2}(G) \geq \frac{n-1}{2^{n-1}} + \frac{(n-2)^2}{2^{n-2}} + \frac{1}{2},$$

and the equality in the bound is attained if $G = K_n^1$.

(2) *If* $G \in \mathcal{H}_c(n, 1)$, *then*

$$SEI_{1/3}(G) \leq \frac{n-1}{3^{n-1}} + \frac{n-1}{3},$$

and the equality is attained if and only if G *is the star graph* S_n.

(3) *Then*

$$SEI_{1/2}(G) \leq \frac{n}{2},$$

and the equality is attained for every even n *if* G *is the disjoint union of* $n/2$ *path graphs* P_2*, and for every odd* n *if* G *is a the union of* $(n-3)/2$ *path graphs* P_2 *and a path graph* P_3.

Proof. If we consider the value $\delta = 1$ and we take limits as $a \to (1/2)^-$ in the items (6) and (8) and as $a \to (1/3)^-$ in the item (7) in Theorem 2.12, then we obtain the desired inequalities.

Since the equality in (1) is attained if $G = K_n^1$ for every $0 < a < 1/2$, by continuity it is also extended to $a = 1/2$.

A similar argument gives the statements on equality in (2) and (3). ■

Let $n \geq 3$ and $2 \leq \Delta \leq n-1$. Let us define $j_0 = \left\lfloor \frac{n-2}{\Delta-1} \right\rfloor$, $\mathbf{y} = (y_1, y_2, \ldots, y_n)$ with

- $y_j = \Delta$ for every $1 \leq j \leq j_0$,
- $y_{j_0+1} = 2n - 2 - j_0\Delta - (n - j_0 - 1) = n - 1 - j_0(\Delta - 1)$,
- $y_j = 1$ for every $j_0 + 1 < j \leq n$,

and $\mathbf{z} = (z_1, z_2, \ldots, z_n)$ with

- $z_1 = \Delta$,
- $z_j = 2$ for every $1 < j \leq n - \Delta$,
- $z_j = 1$ for every $n - \Delta < j \leq n$.

Since $\sum_{j=1}^n y_j = \sum_{j=1}^n z_j = 2n - 2$, if a connected graph has degree sequence $\mathbf{y}$ or $\mathbf{z}$, then it is a tree.

Let $\mathcal{S}_{n,k}$ be the set of trees with n vertices obtained from the star graph S_{k+1} by replacing some edges with paths. Note that a tree has the degree sequence $\mathbf{z}$ if and only if it belongs to $\mathcal{S}_{n,\Delta}$.

Denote by $\mathcal{T}_{n,\Delta}$ be the set of trees with degree sequence $\mathbf{y}$.

Recall that given any function $f : [1, \infty) \to \mathbb{R}$, we define the index

$$I_f(G) = \sum_{u \in V(G)} f(d_u).$$

In [11] appears the following result (see [12] and [13] for related results).

Theorem 2.14. *If T is a tree with $n \geq 3$ vertices and maximum degree $\Delta \geq 2$, $j_0 = \left\lfloor \frac{n-2}{\Delta-1} \right\rfloor$ and $f : [1, \infty) \to \mathbb{R}$ is a strictly convex function, then*

$$f(\Delta) + (n - \Delta - 1)f(2) + \Delta f(1) \leq I_f(T) \leq j_0 f(\Delta) + f(n - 1 - j_0(\Delta - 1)) + (n - j_0 - 1)f(1).$$

Moreover, the lower bound is attained if and only if T belongs to $\mathcal{S}_{n,\Delta}$, and the upper bound is attained if and only if T belongs to $\mathcal{T}_{n,\Delta}$.

Given integers $2 \le \Delta < n$, define by $\mathcal{I}_c(n,\Delta)$ the set of all connected n-vertex graphs with maximum degree Δ.

Theorem 2.15. *Given integers $2 \le \Delta < n$.*

(1) *If $a > 1$ and Δn is even, then the unique graphs that maximize the SEI_a index in $\mathcal{I}_c(n,\Delta)$ are the connected Δ-regular graphs.*

(2) *If $a > 1$ and Δn is odd, then the unique graphs that maximize the SEI_a index in $\mathcal{I}_c(n,\Delta)$ are the connected $(\Delta, \Delta-1)$-quasi-regular graphs.*

(3) *If $a > 1$, then the unique graphs that minimize the SEI_a index in $\mathcal{I}_c(n,\Delta)$ are the trees in $\mathcal{S}_{n,\Delta}$.*

(4) *If $0 < a < 1/2$ and Δn is even, then the unique graphs that minimize the SEI_a index in $\mathcal{I}_c(n,\Delta)$ are the connected Δ-regular graphs.*

(5) *If $0 < a < 1/2$ and Δn is odd, then the unique graphs that minimize the SEI_a index in $\mathcal{I}_c(n,\Delta)$ are the connected $(\Delta, \Delta-1)$-quasi-regular graphs.*

(6) *If $0 < a < 1/2$ and a graph maximizes the SEI_a index in $\mathcal{I}_c(n,\Delta)$, then it is a tree.*

(6′) *If $0 < a < 1/3$, then the unique graphs that maximize the SEI_a index in $\mathcal{I}_c(n,\Delta)$ are the trees in $\mathcal{T}_{n,\Delta}$.*

Proof. Assume that $0 < a < 1/2$. Since $d_u \le \Delta$ for every $u \in V(G)$, Proposition 2.5 gives

$$SEI_a(G) = \sum_{u \in V(G)} d_u a^{d_u} \ge \sum_{u \in V(G)} \Delta a^{\Delta} = n\Delta a^{\Delta},$$

and the equality is attained if and only if $d_u = \Delta$ for every $u \in V(G)$.

If Δn is even, then Lemma 2.6 gives that there is a connected Δ-regular graph with n vertices. Hence, the unique graphs that minimize the SEI_a index in $\mathcal{I}_c(n,\Delta)$ are the connected Δ-regular graphs.

If Δn is odd, then handshaking lemma gives that there is no regular graph. Hence, there is a vertex v with $d_v \le \Delta - 1$ and

$$SEI_a(G) = d_v a^{d_u} + \sum_{u \in V(G) \setminus \{v\}} d_u a^{d_u} \ge (n-1)\Delta a^{\Delta} + (\Delta - 1) a^{\Delta - 1},$$

and the equality is attained if and only if $d_u = \Delta$ for every $u \in V(G) \setminus \{v\}$, and $d_v = \Delta - 1$. Lemma 2.6 gives that there is a connected $(\Delta, \Delta-1)$-quasi-regular graph with n vertices.

Therefore, the unique graphs that minimize the SEI_a index in $\mathcal{I}_c(n,\Delta)$ are the connected $(\Delta,\Delta-1)$-quasi-regular graphs.

Given any graph $G \in \mathcal{I}_c(n,\Delta)$ which is not a tree, then there is a cycle C in G and a vertex $u \in V(G)$ with $d_u = \Delta$. Since C has at least three edges, there exists $vw \in E(G) \cap C$ such that $u \notin \{v,w\}$. Thus, $G \setminus \{vw\} \in \mathcal{I}_c(n,\Delta)$ and Proposition 2.5 gives $SEI_a(G) < SEI_a(G \setminus \{vw\})$. By iterating this argument, we obtain that if a graph maximizes the SEI_a index in $\mathcal{I}_c(n,\Delta)$, then it is a tree.

If $0 < a < 1/3$, then Theorem 2.4 gives that there exists a strictly convex function F on $[1,\infty)$ with $F(k) = ka^k$ for every $k \in \mathbb{Z}^+$. Thus, Theorem 2.14 gives that the unique trees in $\mathcal{I}_c(n,\Delta)$ that maximize the SEI_a index (on the set of trees) are the trees in $\mathcal{T}_{n,\Delta}$. Hence, the unique graphs that maximize the SEI_a index in $\mathcal{I}_c(n,\Delta)$ are the trees in $\mathcal{T}_{n,\Delta}$.

If $a > 1$, then similar arguments as above give the result. ■

Note that items (1) and (3) in Theorem 2.15 are known [18, Propositions 4 and 14].

Given integers $2 \le \Delta < n$ such that $n-\Delta$ is even, let $\mathcal{U}_{n,\Delta}$ be the family of all n-vertex graphs with degree sequence $\mathbf{w} = (\Delta, 2, 1, \dots, 1)$. Note that a graph has degree sequence $\mathbf{w}$ if and only if it is either the union of the star graph $S_{\Delta+1}$, $(n-\Delta-4)/2$ path graphs P_2 and a path graph P_3, or the union of the $(n-\Delta-2)/2$ path graphs P_2 and the tree obtained from the star graph $S_{\Delta+1}$ by replacing an edge by path graph P_2. Let us define by $\mathcal{I}(n,\Delta)$ the family of all n-vertex graphs with maximum degree Δ.

Theorem 2.16. *Given integers $2 \le \Delta < n$.*

(1) If $a > 1$ and $n-\Delta$ is odd, then the unique graph that minimizes the SEI_a index in $\mathcal{I}(n,\Delta)$ is the union of the star graph $S_{\Delta+1}$ and $(n-\Delta-1)/2$ path graphs P_2.

If $a > 1$ and $n-\Delta$ is even, then the unique graphs that minimize the SEI_a index in $\mathcal{I}(n,\Delta)$ are the forests in $\mathcal{U}_{n,\Delta}$.

(2) If $0 < a < 1/2$ and $n-\Delta$ is odd, then the unique graph that maximizes the SEI_a index in $\mathcal{I}(n,\Delta)$ is the union of the star graph $S_{\Delta+1}$ and $(n-\Delta-1)/2$ path graphs P_2.

If $0 < a < 1/2$ and $n-\Delta$ is even, then the unique graphs that maximize the SEI_a index in $\mathcal{I}(n,\Delta)$ are the forests in $\mathcal{U}_{n,\Delta}$.

Proof. Consider $G \in \mathcal{I}(n,\Delta)$. Thus, there is $v \in V(G)$ with $d_v = \Delta$

Assume that $0 < a < 1/2$. Since $d_u \ge 1$ for every $u \in V(G)$, Proposition 2.2 gives

$$SEI_a(G) = \sum_{u \in V(G)} d_u a^{d_u} \le \Delta a^{\Delta} + (n-1)a,$$

and the equality is attained if and only if $d_u = 1$ for every $u \in V(G) \setminus \{v\}$. If $n - \Delta$ is odd, then this happens if and only if G is disjoint union of the star graph $S_{\Delta+1}$ and $(n - \Delta - 1)/2$ path graphs P_2.

Assume now that $n - \Delta$ is even. Since $1 \cdot \Delta + (n-1) \cdot 1 = n + \Delta - 1 = n - \Delta + 2\Delta - 1$ is odd, handshaking lemma gives that there is $w \in V(G) \setminus \{v\}$ with $d_w \geq 2$. Hence, Proposition 2.2 gives

$$SEI_a(G) = \sum_{u \in V(G)} d_u a^{d_u} \leq \Delta a^{\Delta} + 2a^2 + (n-2)a,$$

and the equality in is attained if and only if G has degree sequence **w**, i.e., G is a forest in $\mathcal{U}_{n,\Delta}$.

If $a > 1$, then a similar argument as above gives the result. ∎

Remark 2.17. *If we replace $\mathcal{I}_c(n, \Delta)$ with $\mathcal{I}(n, \Delta)$ in the statement of the items* (1), (2), (4) *and* (5) *in Theorem 2.15, then the arguments in their proofs give that the same conclusions hold in these items if we remove everywhere the word "connected".*

The following result is consequence of Theorems 2.15 and 2.16, and Remark 2.17.

Theorem 2.18. *Let G be a graph with order n, maximum degree $\Delta \geq 2$ and $j_0 = \left\lfloor \frac{n-2}{\Delta-1} \right\rfloor$.*

(1) *If $a > 1$ and Δn is even, then*

$$SEI_a(G) \leq n\Delta a^{\Delta},$$

and the equality is attained if and only if G is Δ-regular.

(2) *If $a > 1$ and Δn is odd, then*

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

and the equality is attained if and only if G is $(\Delta, \Delta - 1)$-quasi-regular.

(3) *If $a > 1$ and G is connected, then*

$$SEI_a(G) \geq \Delta a^{\Delta} + 2(n - \Delta - 1)a^2 + \Delta a,$$

and the equality is attained if and only if G is a tree in $\mathcal{S}_{n,\Delta}$.

(4) *If $a > 1$ and $n - \Delta$ is odd, then*

$$SEI_a(G) \geq \Delta a^{\Delta} + (n-1)a,$$

and the equality is attained if and only if G *is the disjoint union of the star graph* $S_{\Delta+1}$ *and* $(n-\Delta-1)/2$ *path graphs* P_2.

If $a>1$ *and* $n-\Delta$ *is even, then*

$$SEI_a(G) \geq \Delta a^{\Delta} + 2a^2 + (n-2)a,$$

and the equality is attained if and only if G *is a forest in* $\mathcal{U}_{n,\Delta}$.

(5) *If* $0<a<1/2$ *and* Δn *is even, then*

$$SEI_a(G) \geq n\Delta a^{\Delta},$$

and the equality is attained if and only if G *is* Δ*-regular.*

(6) *If* $0<a<1/2$ *and* Δn *is odd, then*

$$SEI_a(G) \geq (n-1)\Delta a^{\Delta} + (\Delta-1)a^{\Delta-1},$$

and the equality is attained if and only if G *is* $(\Delta,\Delta-1)$*-quasi-regular.*

(7) *If* $0<a<1/3$ *and* G *is connected, then*

$$SEI_a(G) \leq j_0\Delta a^{\Delta} + (n-1-j_0(\Delta-1))a^{n-1-j_0(\Delta-1)} + (n-j_0-1)a,$$

and the equality is attained if and only if G *is a tree in* $\mathcal{T}_{n,\Delta}$.

(8) *If* $0<a<1/2$ *and* $n-\Delta$ *is odd, then*

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

and the equality is attained if and only if G *is the union of the star graph* $S_{\Delta+1}$ *and* $(n-\Delta-1)/2$ *path graphs* P_2.

If $0<a<1/2$ *and* $n-\Delta$ *is even, then*

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

and the equality is attained if and only if G *is a forest in* $\mathcal{U}_{n,\Delta}$.

Note that items (1) and (3) in Theorem 2.16 are known [18, Propositions 4 and 14].

Corollary 2.19. *Let* G *be a graph with order* n, *maximum degree* $\Delta \geq 2$ *and* $j_0 = \left\lfloor \frac{n-2}{\Delta-1} \right\rfloor$.

(1) *If* Δn *is even, then*

$$SEI_{1/2}(G) \geq \frac{n\Delta}{2^{\Delta}},$$

and the equality is attained if G is Δ-regular.

(2) *If Δn is odd, then*

$$SEI_{1/2}(G) \geq \frac{(n-1)\Delta}{2^\Delta} + \frac{\Delta-1}{2^{\Delta-1}},$$

and the equality is attained if G is $(\Delta, \Delta-1)$-quasi-regular.

(3) *If G is connected, then*

$$SEI_{1/3}(G) \leq \frac{j_0\Delta}{3^\Delta} + \frac{n-1-j_0(\Delta-1)}{3^{n-1-j_0(\Delta-1)}} + \frac{n-j_0-1}{3},$$

and the equality is attained if G is a tree in $\mathcal{T}_{n,\Delta}$.

(4) *Then*

$$SEI_{1/2}(G) \leq \frac{\Delta}{2^\Delta} + \frac{n-1}{2},$$

and the equality is attained for each odd $n-\Delta$ if G is the union of the star graph $S_{\Delta+1}$ and $(n-\Delta-1)/2$ path graphs P_2, and for each even $n-\Delta$ if G is a forest in $\mathcal{U}_{n,\Delta}$.

Proof. If we take limits as $a \to (1/2)^-$ (respectively, $a \to (1/3)^-$) in the items (4), (5) and (6′) (respectively, (6)) in Theorem 2.18, then we obtain the desired inequalities.

Since the equality in (1) is attained if G is Δ-regular for every $0 < a < 1/2$, then continuity extends the result up to $a = 1/2$ if G is Δ-regular.

A similar argument gives the statements on equality in (2), (3) and (4). ■

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