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Research Article

On Variable Sum Exdeg Indices of Quasi-Tree Graphs and Unicyclic Graphs

Xiaoling Sun and Jianwei Du

School of Science, North University of China, Taiyuan 030051, China

Correspondence should be addressed to Xiaoling Sun; sunxiaoling@nuc.edu.cn

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In this work, by using the properties of the variable sum exdeg indices and analyzing the structure of the quasi-tree graphs and unicyclic graphs, the minimum and maximum variable sum exdeg indices of quasi-tree graphs and quasi-tree graphs with perfect matchings were presented; the minimum and maximum variable sum exdeg indices of unicyclic graphs with given pendant vertices and cycle length were determined.

1. Introduction

Topological indices are mathematical descriptors reflecting some structural characteristics of organic molecules on molecular graphs, and they play an important role in pharmacology, chemistry, etc. ([1–3]). For a graph G, the variable sum exdeg index (denoted by SEI_a) was proposed by Vukičević [4] and is defined as

$$\mathrm{SEI}_a(G) = \sum_{uv\in E(G)} \left(a^{d_G(u)} + a^{d_G(v)}\right) = \sum_{v\in V(G)} d_G(v)a^{d_G(v)}, \quad (1)$$

where $a \in (0,1) \cup (1,+\infty)$ and $d_G(v)$ is the degree of vertex v. This graph invariant has a good correlation with the octanol-water partition coefficient [4] and was used to study the octane isomers given by the International Academy of Mathematical Chemistry (IAMC) [5–7]. Yarahmadi and Ashrafi [8] proposed a polynomial form of this graph invariant which is applied in nanoscience. By using the technique of majorization, Ghalavand and Ashrafi [9] provided the maximal and minimal SEI_a (for $a > 1$) of trees, bicyclic graphs, unicyclic graphs, and tricyclic graphs.

All graphs considered in this work are simple connected graphs. Let $G = (V(G), E(G))$ be a graph with the vertex set $V(G)$ and the edge set $E(G)$. We denote by $\delta(G)$ the minimum degree of G. We use $N_G(v)$ to denote the neighbourhood of a vertex v and n_i to denote the number of vertices with degree i. Denoted by $G - uv$ and $G + uv$ the graphs arisen from G by deleting the edge $uv \in E(G)$ and by adding the edge $uv \notin E(G)\,(u, v \in V(G))$, respectively. We denote by $G - x$ the subgraph of G resulted by deleting the vertex $x\,(x \in V(G))$ with its incident edges. We call G a quasi-tree graph if there is a vertex x in G such that $G - x$ is a tree. A unicyclic graph is the graph with exactly one cycle. Let G_1 and G_2 be two vertex-disjoint graphs. We denote by $G_1 \vee G_2$ the graph having vertex set $V(G_1 \vee G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{xy \mid x \in V(G_1), y \in V(G_2)\}$. As usual, we use P_n, S_n, and C_n to denote the n-vertex path, the n-vertex star, and the n-vertex cycle, respectively. The readers should refer for other definitions to [10].

There are many papers on the mathematical properties of topological indices, such as [11–14], since these invariants can detect the desirable properties of chemical molecules. In this work, we studied the mathematical properties of SEI_a. This article is structured as follows. In Section 2, we present some useful lemmas. In Section 3, we obtain the maximal and minimal SEI_a (for $a > 1$) of quasi-tree graphs. In Section 4, we determine the maximal and minimal SEI_a (for $a > 1$) of quasi-tree graphs with perfect matchings. In Section 5, we derive the maximal and minimal SEI_a (for $a > 1$) of unicyclic graphs with given cycle length. In Section 6, we find the maximal and minimal SEI_a (for $a > 1$) of unicyclic graphs with given pendant vertex.

2. Preliminaries

Lemma 1 (see [6]). *Let $f_a(x) = xa^x$, where $x \geq 1, a > 1$. Then*

(i) $f_a(x)$ is strictly monotone increasing in x

(ii) $f_a''(x) > 0$ and $f_a(x)$ is strictly convex

By Lemma 1, we have Lemmas 2 and 3 immediately.

Lemma 2. *Suppose $G = (V(G), E(G))$ is a connected graph, then*

(i) If $e \in E(G)$, $SEI_a(G) > SEI_a(G-e)$ for $a > 1$

(ii) If $e = uv \notin E(G), u, v \in V(G)$, $SEI_a(G) < SEI_a(G+e)$ for $a > 1$

Lemma 3. *Let x_1, y_1, x_2 and y_2 be positive integers with $x_1 + x_2 = y_1 + y_2$ and $|y_1 - y_2| > |x_1 - x_2|$. Then for $a > 1$, we have*

$$x_1 a^{x_1} + x_2 a^{x_2} < y_1 a^{y_1} + y_2 a^{y_2}. \quad (2)$$

By simple calculation, Lemma 4 is immediate.

Lemma 4. *Let*

$$l(x) = f_a(x) - f_a(x-1) = xa^x - (x-1)a^{x-1}, \quad (3)$$

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

Lemma 5. *Let*

$$g(k) = (k+1)a^{k+1} + 2(k-2)a^2 - 3(k-1)a^3, \quad (4)$$

where $k \geq 3$ and $a > 1$. Then $g(k) > 0$.

Proof. Note that

$$g'(k) = (k+1)a^{k+1}\ln a + a^{k+1} - 3a^3 + 2a^2. \quad (5)$$

$$g''(k) = \ln a\left[2a^{k+1} + (k+1)a^{k+1}\ln a\right] > 0. \quad (6)$$

So, $g'(k) \geq g'(3) = a^4 - 3a^3 + 2a^2 + 4a^4\ln a$. Let $h(a) = a^4 - 3a^3 + 2a^2 + 4a^4\ln a$, where $a \geq 1$. Then

$$h'(a) = a\left(8a^2 - 9a + 4\right) + 16a^3\ln a > 0. \quad (7)$$

Thus, $g'(k) \geq g'(3) = h(a) > h(1) = 0$. So, $g(k) \geq g(3) = 4a^4 - 6a^3 + 2a^2 = 2a^2(a-1)(2a-1) > 0$ for $a > 1$. □

3. Variable Sum Exdeg Indices of Quasi-Tree Graphs

Suppose G is a quasi-tree graph and x is a vertex in G such that $G - x$ is a tree. If $d_G(x) = 1$, then G is a tree with extremal variable sum exdeg index (for $a > 1$), that had been presented in [6, 9]. Thus, we always consider the case of $d_G(x) \geq 2$ in this section. Let.

$\mathrm{QT}(n) = \{H \mid H \text{ is a quasi} - \text{tree graph on } n \text{ vertices with } d_G(x) \geq 2\}$.

Let Q_n be the graph arisen from complete bipartite graph $K_{2,n-2}$ by adding one edge between the two non-adjacent vertices with degree $n-2$, as shown in Figure 1. We can easily obtain that $\mathrm{SEI}_a(Q_n) = 2(n-1)a^{n-1} + 2(n-2)a^2$.

Lemma 6. *Suppose $G \in QT(n)$ such that G has the maximal value of SEI_a for $a > 1$. Let $x \in V(G)$ such that $G - x$ is a tree. Then, $\delta(G) \geq 2$ and $d_G(x) = n - 1$.*

Proof. If $d_G(x) < n-1$, then there exists $z \in V(G)$ such that $xz \notin V(G)$. Clearly, $G + xz \in \mathrm{QT}(n)$. In view of Lemma 2, $\mathrm{SEI}_a(G + xz) > \mathrm{SEI}_a(G)$, a contradiction. Therefore $d_G(x) = n - 1$, and it can be concluded that $\delta(G) \geq 2$. □

Theorem 1. *Let $G \in QT(n)$, where $n \geq 3$. Then, for $a > 1$,*

$$2na^2 \leq \mathrm{SEI}_a(G) \leq 2(n-2)a^2 + 2(n-1)a^{n-1}, \quad (8)$$

with the left equality if and only if $G \cong C_n$ and with the right equality if and only if $G \cong Q_n$.

Proof. By induction on n. When $n = 3$, it follows that $G \cong C_3$ and (8) holds. Assume that $n \geq 4$ and (8) holds for $\mathrm{QT}(n-1)$.

First, we obtain the lower bound. If there is no pendant vertex in G, since $G \in \mathrm{QT}(n)$, then there exists $u \in V(G)$ such that $d_G(u) = 2$. Let $N_G(u) = \{v_1, v_2\}$. For $v_1v_2 \notin E(G)$, let $G' = G - u + v_1v_2 \in \mathrm{QT}(n-1)$. By (1) and induction hypothesis, for $a > 1$, we have

$$\begin{aligned}\mathrm{SEI}_a(G) &= \mathrm{SEI}_a(G') + 2a^2 \\ &\geq 2(n-1)a^2 + 2a^2 = 2na^2,\end{aligned} \quad (9)$$

with equality holding only if $G' \cong C_{n-1}$. This implies $G \cong C_n$.

For $v_1v_2 \in E(G)$, let $G'' = G - u \in \mathrm{QT}(n-1)$. By (i) of Lemma 1 and induction hypothesis, for $a > 1$, we have

$$\begin{aligned}\mathrm{SEI}_a(G) &= \mathrm{SEI}_a(G'') + 2a^2 + d_G(v_1)a^{d_G(v_1)} \\ &\quad - (d_G(v_1) - 1)a^{d_G(v_1)-1} \\ &\quad + d_G(v_2)a^{d_G(v_2)} \\ &\quad - (d_G(v_2) - 1)a^{d_G(v_2)-1} \\ &> 2(n-1)a^2 + 2a^2 = 2na^2.\end{aligned} \quad (10)$$

Otherwise, there is at least one pendant vertex in G. Let $y \in V(G)$ and $d_G(y) = 1$. Then, $G - y \in \mathrm{QT}(n-1)$. We

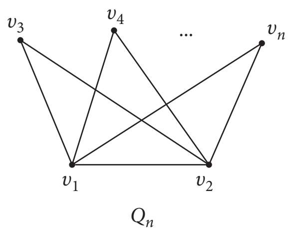

Figure 1: The graph Q_n.

denote by z the vertex with $yz \in E(G)$. It can be seen that $d_G(z) \geq 2$. If $d_G(z) = 2$, then $G - y \ncong C_n$. By (1) and induction hypothesis, for $a > 1$, we have

$$\mathrm{SEI}_a(G) = \mathrm{SEI}_a(G - y) + 2a^2 > 2(n-1)a^2 + 2a^2 = 2na^2. \tag{11}$$

If $d_G(z) > 2$, then by (1), (2), Lemma 4, and induction hypothesis, for $a > 1$, it follows that

$$\begin{aligned} \mathrm{SEI}_a(G) &= \mathrm{SEI}_a(G - y) + a + d_G(z)a^{d_G(z)} \\ &\quad - (d_G(z) - 1)a^{d_G(z)-1} \\ &\geq 2(n-1)a^2 + a + 3a^3 - 2a^2 \\ &= 2na^2 + 3a^3 + a - 2\cdot 2a^2 \\ &> 2na^2. \end{aligned} \tag{12}$$

Next, we obtain the upper bound. Choose $G \in \mathrm{QT}(n)$ such that G has the maximum SEI_a for $a > 1$. By Lemma 6, $\delta(G) \geq 2$. Then, there is a vertex v in G such that $d_G(v) = 2$ since G is a quasi-tree graph. By Lemma 6, it follows that $G - v \in \mathrm{QT}(n-1)$. Denote $N_G(v) = \{w_1, w_2\}$. If $d_G(w_1) = d_G(w_2) = n - 1$, then $G - \{w_1, w_2\}$ has no edges. This implies that $G \cong \mathcal{Q}_n$. If one of the vertices w_1, w_2, say w_1, satisfies $d_G(w_1) < n - 1$, then $G \ncong \mathcal{Q}_n$. By (1), Lemma 1, and induction hypothesis, we have

$$\begin{aligned} \mathrm{SEI}_a(G) &= SEI_a(G - v) + 2a^2 + d_G(w_1)a^{d_G(w_1)} - (d_G(w_1) - 1)a^{d_G(w_1)-1} \\ &\quad + d_G(w_2)a^{d_G(w_2)} - (d_G(w_2) - 1)a^{d_G(w_2)-1} \\ &\leq 2(n-3)a^2 + 2a^2 + 2(n-2)a^{n-2} + d_G(w_1)a^{d_G(w_1)} - (d_G(w_1) - 1)a^{d_G(w_1)-1} \\ &\quad + d_G(w_2)a^{d_G(w_2)} - (d_G(w_2) - 1)a^{d_G(w_2)-1} \\ &= 2(n-2)a^2 + 2(n-1)a^{n-1} - \Big\{2(n-1)a^{n-1} - 2(n-2)a^{n-2} - \Big[d_G(w_1)a^{d_G(w_1)} \\ &\quad - (d_G(w_1) - 1)a^{d_G(w_1)-1} + d_G(w_2)a^{d_G(w_2)} - (d_G(w_2) - 1)a^{d_G(w_2)-1}\Big]\Big\} \\ &= \mathrm{SEI}_a(\mathcal{Q}_n) - (2f_a'(\xi) - f_a'(\eta_1) - f_a'(\eta_2)) \\ &= \mathrm{SEI}_a(\mathcal{Q}_n) - [f_a'(\xi) - f_a'(\eta_1) + f_a'(\xi) - f_a'(\eta_2)] \\ &< \mathrm{SEI}_a(\mathcal{Q}_n), \end{aligned} \tag{13}$$

where $n - 2 < \xi < n - 1$, $d_G(w_1) - 1 < \eta_1 < d_G(w_1)$, $d_G(w_2) - 1 < \eta_2 < d_G(w_2)$, and $\xi > \eta_1$, $\xi \geq \eta_2$.

In [6], Vukičević obtained the minimal and maximal SEI_a of trees on n vertices for $a > 1$. The result is shown below. □

Theorem 2 (see [6]). *Suppose T is a tree on n vertices, then for $a > 1$,*

$$2(n-2)a^2 + 2a \leq \mathrm{SEI}_a(T) \leq (n-1)a^{n-1} + (n-1)a, \tag{14}$$

where the left equality holds only when $G \cong P_n$, and the right equality holds only when $G \cong S_n$.

Thus, by simple calculation, we can extend our result to the whole quasi-tree graphs, as follows.

Theorem 3. *Let G be an n-vertex quasi-tree graph. Then, for $a > 1$,*

$$2(n-2)a^2 + 2a \leq \mathrm{SEI}_a(G) \leq 2(n-2)a^2 + 2(n-1)a^{n-1}, \tag{15}$$

where the left equality holds if and only if $G \cong P_n$ and the right equality holds if and only if $G \cong \mathcal{Q}_n$.

4. Variable Sum Exdeg Indices of Quasi-Tree Graphs with a Perfect Matching

Let T_1 be the tree of order $2k-1$ arisen from S_{k+1} by adding a pendant edge to its $k-2$ pendant vertices, as shown in Figure 2. Let T_2 be the tree of order $2k-1$ arisen from S_k by adding a pendant edge to its every pendant vertex, as shown in Figure 2. Let $\mathbf{QT}_1(2k) = T_1 \vee K_1$ and $\mathbf{QT}_2(2k) = T_2 \vee K_1$.

Lemma 7. *Let $k \geq 3$ be positive integers. Then, for $a > 1$,*

$$\mathrm{SEI}_a(\mathbf{QT}_1(2k)) > \mathrm{SEI}_a(\mathbf{QT}_2(2k)). \quad (16)$$

Proof. By (1) (2) and Lemma 4, for $a > 1$, we have

$$\begin{aligned}\mathrm{SEI}_a(\mathbf{QT}_1(2k)) - \mathrm{SEI}_a(\mathbf{QT}_2(2k)) &= (2k-1)a^{2k-1} + (k+1)a^{k+1} + 2ka^2 + 3(k-2)a^3 \\ &\quad - (2k-1)a^{2k-1} - ka^k - 2(k-1)a^2 - 3(k-1)a^3 \\ &= (k+1)a^{k+1} - ka^k + 2a^2 - 3a^3 \\ &\geq 4a^4 + 2a^2 - 2\cdot 3a^3 > 0,\end{aligned} \quad (17)$$

since $k \geq 3$. □

Theorem 4. *Let G be a quasi-tree graph of order $2k$ with a perfect matching, where $k \geq 2$. Then, for $a > 1$,*

$$\mathrm{SEI}_a(G) \leq (2k-1)a^{2k-1} + (k+1)a^{k+1} + 3(k-2)a^3 + 2ka^2, \quad (18)$$

with equality only when $G \cong \mathbf{QT}_1(2k)$.

Proof. When $k = 2$, $G \in \{G_1, G_2, G_3, \mathbf{QT}_1(4)\}$ (as shown in Figure 3). By Lemma 2, we have $\mathrm{SEI}_a(\mathbf{QT}_1(4)) > \mathrm{SEI}_a(G_i)$, $i = 1, 2, 3$.

If $k \geq 3$, choose G such that G has the maximal value of SEI_a for $a > 1$. Assume that M is a perfect matching of G. We can suppose that $T = G - x$ is a tree since G are quasi-tree graphs. Choose $y \in V(T)$ such that $d_T(y) = \max\{d_T(u) \mid u \in V(T)\}$. □

Claim 1. For any vertex v of T, $xv \in E(G)$.

The proof is similar to Lemma 6 (thus omitted).

Claim 2. For any vertex u of T except y, $d_T(u) \leq 2$.

To the contrary, assume that there is $y' \in (V(T)\backslash\{y\})$ such that $d_T(y') \geq 3$. Let $N_T(y) = \{u_1, u_2, \ldots, u_r\}$ and $N_T(y') = \{v_1, v_2, \ldots, v_s\}$, where $r \geq s \geq 3$. By Claim 1, $d_G(y) = r+1$ and $d_G(y') = s+1$. Since T is a tree, we suppose that P is the unique path P from y to y' in T. Assume without loss of generality that $u_1, v_1 \in V(P)$ (maybe $u_1 = y'$ or $v_1 = y$). Notice that $|M \cap \{v_2y', v_3y', \ldots, v_sy'\}| \leq 1$. Without loss of generality, assume that $v_3y', \ldots, v_sy' \notin M$. Let $G' = G - \{v_3y', \ldots, v_sy'\} + \{v_3y, \ldots, v_sy\}$. Clearly, G' is also a quasi-tree graph of order $2k$ with a perfect matching. By (1) and (2),

$$\begin{aligned}\mathrm{SEI}_a(G') - \mathrm{SEI}_a(G) &= (r+s-1)a^{r+s-1} + 3a^3 - (s+1)a^{s+1} - (r+1)a^{r+1} > 0,\end{aligned} \quad (19)$$

a contradiction with the choice of the graph G.

By Claim 2, T is a tree with some pendant paths attached to y.

Claim 3. $d_T(y) \geq 3$.

On the contrary, assume that $d_T(y) \leq 2$. By the choice of y, $d_T(y) \geq 2$, thus $d_T(y) = 2$ and T is a path on $2k-1$ vertices. Denote $T = x_1x_2 \ldots x_{2k-1}$. By Claim 1, $xx_i \in E(G)$, $i = \{1, 2, \ldots, 2k-1\}$. It is not difficult to get that $\mathrm{SEI}_a(G) = (2k-1)a^{2k-1} + 3(2k-3)a^3 + 4a^2$. By Lemma 5, for $a > 1$ and $k \geq 3$, we have

$$\begin{aligned}\mathrm{SEI}_a(\mathbf{QT}_1(2k)) - \mathrm{SEI}_a(G) &= (k+1)a^{k+1} + (2k-1)a^{2k-1} + 3(k-2)a^3 + 2ka^2 \\ &\quad - (2k-1)a^{2k-1} - 3(2k-3)a^3 - 4a^2 \\ &= (k+1)a^{k+1} - 3(k-1)a^3 + 2(k-2)a^2 > 0,\end{aligned} \quad (20)$$

a contradiction with the choice of the graph G.

We denote by $P_1, P_2, \ldots, P_t$ $(t \geq 3)$ the paths attached to y in T.

Claim 4. $|E(P_i)| \leq 2$ for $1 \leq i \leq t$ in T.

To the contrary, suppose without loss of generality that $|E(P_1)| \geq 3$ in T. Denote $P_1 = y_1y_2 \ldots y_r$, where $y_1 = y$ and $r \geq 4$. Then, there is at least one edge y_jy_{j+1} satisfying $y_jy_{j+1} \notin M$ and $j \in \{2, 3, \ldots, r-1\}$. Let $G'' = G - y_jy_{j+1} + yy_{j+1}$. Obviously, G'' is also a quasi-tree graph of order $2k$ with a perfect matching. By (1) and (2),

$$\begin{aligned}\mathrm{SEI}_a(G'') - \mathrm{SEI}_a(G) &= (d_G(y)+1)a^{d_G(y)+1} + 2a^2 - d_G(y)a^{d_G(y)} - 3a^3 \\ &= (t+2)a^{t+2} + 2a^2 - (t+1)a^{t+1} - 3a^3 > 0,\end{aligned} \quad (21)$$

a contradiction with the choice of the graph G.

Denote $V_1 = \{u \in V(T) \mid d_T(u) = 1, uy \in E(G)\}$. Since G has a perfect matching, by Claim 4, it follows that $|V_1| = 0$ or $|V_1| = 2$.

If $|V_1| = 0$, then $G \cong \mathbf{QT}_2(2k)$. If $|V_1| = 2$, then $G \cong \mathbf{QT}_1(2k)$. By (16), for $k \geq 3$, $\mathrm{SEI}_a(\mathbf{QT}_1(2k)) > \mathrm{SEI}_a(\mathbf{QT}_2(2k))$. Therefore, $G \cong \mathbf{QT}_1(2k)$.

By Theorem 3, Theorem 5 is obtained immediately.

Theorem 5. *Suppose G is a quasi-tree graph of order $2k$ with a perfect matching, where $k \geq 2$, then for $a > 1$,*

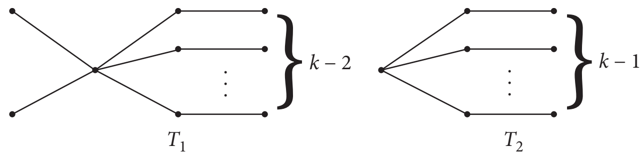

FIGURE 2: The graph T_1 and T_2.

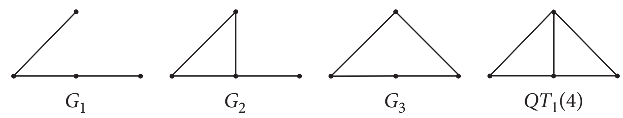

FIGURE 3: The graph G_1, G_2, G_3 and $\boldsymbol{QT}_1(4)$.

$$\mathrm{SEI}_a(G) \geq 4(k-1)a^2 + 2a, \tag{22}$$

with equality if and only if $G \cong P_{2k}$.

5. Variable Sum Exdeg Indices of Unicyclic Graphs with Given Cycle Length

Let $C^1_{n,l}$ and $C^2_{n,l}$ (as shown in Figure 4) denote the graph obtained from C_l by identifying its one vertex with the center vertex of S_{n-l+1} and the graph obtained from C_l by identifying its one vertex with a pendant vertex of P_{n-l+1}, respectively.

Theorem 6. *Let U be an n-vertex unicyclic graph with cycle length $l \leq n-1$. Then, for $a > 1$,*

$$\mathrm{SEI}_a(U) \leq (n-l+2)a^{n-l+2} + (n-l)a + 2(l-1)a^2, \tag{23}$$

with equality only when $U \cong C^1_{n,l}$.

Proof. Choose U such that U has the maximum SEI_a for $a > 1$. Suppose C is the only cycle in U. □

Claim 1. There is at most one vertex $u \in V(C)$ with $d_U(u) \geq 3$ in U.

To the contrary, suppose that there exist two vertices $x, y \in V(C)$ such that $d_U(x) \geq d_U(y) \geq 3$. Thus, there exists one vertex $z \in N_U(y)$, but $z \notin V(C)$. It is evident that $z \notin N_U(x)$. Let $U' = U - yz + xz$. Then, C has no change and U' is also an n-vertex unicyclic graph with cycle length l. By (1) and (2), it follows that

$$\begin{aligned}\mathrm{SEI}_a(U') - \mathrm{SEI}_a(U) &= (d_U(y)-1)a^{d_U(y)-1} + (d_U(x)+1)a^{d_U(x)+1} \\ &\quad - d_U(y)a^{d_U(y)} - d_U(x)a^{d_U(x)} > 0.\end{aligned} \tag{24}$$

a contradiction with the choice of the graph U.

Claim 2. For $v \notin V(C)$, $d_U(v) = 1$.

Assume, to the contrary, that there exists one vertex $v \notin V(C)$ with $d_U(v) = d \geq 2$. Denoted by $P = x_1x_2 \ldots x_r$ (where $v = x_1$ and $x_r \in V(C)$) the path from v to C. Then $N_U(v) \cap P = \{x_2\}$. Since $v \notin V(C)$ and $d_U(v) = d \geq 2$, it follows that $(N_U(v)\backslash\{x_2\}) \neq \varnothing$ and $(N_U(v)\backslash\{x_2\}) \cap N_U(x_r) = \varnothing$. Denote $(N_U(v)\backslash\{x_2\}) = \{y_1, y_2, \ldots y_s\}$, where $s \geq 1$. Let $U'' = U - \{vy_1, vy_2, \ldots, vy_s\} + \{x_ry_1, x_ry_2, \ldots, x_ry_s\}$. Then, C has no change and U'' is also an n-vertex unicyclic graph with cycle length l. By (1) and (2), it follows that

$$\begin{aligned}\mathrm{SEI}_a(U'') - \mathrm{SEI}_a(U) &= (d_U(x_r)+s)a^{d_U(x_r)+s} + a - d_U(x_r)a^{d_U(x_r)} \\ &\quad - (s+1)a^{s+1} > 0,\end{aligned} \tag{25}$$

a contradiction again.

By Claims 1 and 2, we have $U \cong C^1_{n,l}$.

Theorem 7. *Let U be a unicyclic graph of order n with cycle length $l \leq n-1$. Then, for $a > 1$,*

$$\mathrm{SEI}_a(U) \geq 2(n-2)a^2 + 3a^3 + a, \tag{26}$$

with equality only when $U \cong C^2_{n,l}$.

Proof. Choose U such that U has the minimum SEI_a for $a > 1$. Suppose C is the only cycle in U. □

Claim 3. U contains at most one pendant vertex.

Suppose that U contains at least two pendant vertices. Let $x, y \in V(U)$ be two pendant vertices. We denote by $P = z_1z_2 \ldots z_t$ (where $x = z_1$, $y = z_t$ and $t \geq 3$) the path from x to y with minimum length. Then, there is $1 < i < t$, $j \in \{1, 2, \ldots, i-1\}$ such that $d_U(z_i) \geq 3$ and $d_U(z_j) \leq 2$. Obviously, $z_{i-1} \notin N_U(y)$.

Let $U' = U - z_{i-1}z_i + z_{i-1}y$. Since $x \notin V(C)$ and $d_U(z_{i-1}) \leq 2$, then $z_{i-1} \notin V(C)$. Thus C has no change and U' is also an n-vertex unicyclic graph with cycle length l. By (1) and (2), it follows that

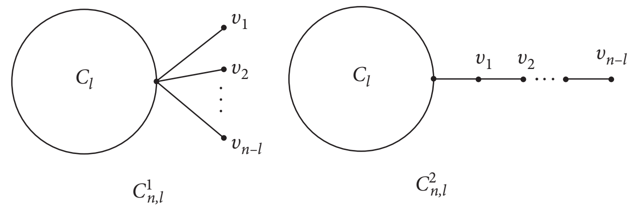

FIGURE 4: The graphs $C^1_{n,l}$ and $C^2_{n,l}$.

$$\begin{aligned}&\mathrm{SEI}_a(U') - \mathrm{SEI}_a(U)\\&\quad = (d_U(z_i) - 1)a^{d_U(z_i)-1} + 2a^2 - d_U(z_i)a^{d_U(z_i)} - a < 0,\end{aligned} \tag{27}$$

a contradiction with the choice of the graph U.

Since $l \le n-1$, by Claim 3, U has exactly one pendant vertex. This implies $U \cong C^2_{n,l}$.

6. Variable Sum Exdeg Index of Unicyclic Graphs with Given Pendant Vertex

Let $\mathscr{U}^1_{n,p}$ (as shown in Figure 5) be the graph obtained from C_{n-p} by identifying its one vertex with the center vertex of S_{p+1}.

Let $\mathscr{U}^2_{n,p}$ be the n-vertex unicyclic graphs having p pendant vertices and degree sequence $(\underbrace{b+2,\ldots,b+2}_{n-b(n-p)}, \underbrace{b+1,\ldots,b+1}_{b(n-p)-p}, \underbrace{1,\ldots,1}_{p})$, where $b = \lfloor n/(n-p) \rfloor$.

Theorem 8. *Let U be an n-vertex unicyclic graph with $p \ge 1$ pendant vertices. Then, for $a > 1$,*

$$\mathrm{SEI}_a(U) \le (p+2)a^{p+2} + 2(n-p-1)a^2 + pa, \tag{28}$$

the equality holds only when $U \cong \mathscr{U}^1_{n,p}$.

Proof. Choose U such that U has the maximum SEI_a for $a > 1$. □

Claim 1. There is at most one vertex u with $d_U(u) \ge 3$ in U.

Assume that there exist two vertices $x, y \in V(U)$ with $d_U(y) \ge d_U(x) \ge 3$. Let $P = x_1x_2,\ldots,x_r$ (where $x = x_1$, $y = x_r$) be the path from x to y with minimum length. Since $d_U(x) \ge 3$, there exists a vertex $z \in (N_U(x)\backslash(\{x_2\})) \cup N_U(y)$. Let $U' = U - xz + yz$. Clearly, U' is also an n-vertex unicyclic graph with p pendant vertices. In view of (1) and (2), it follows that

$$\begin{aligned}&\mathrm{SEI}_a(U') - \mathrm{SEI}_a(U)\\&\quad = (d_U(x) - 1)a^{d_U(x)-1}(d_U(y) + 1)a^{d_U(y)+1}\\&\qquad - d_U(x)a^{d_U(x)} - d_U(y)a^{d_U(y)} > 0,\end{aligned} \tag{29}$$

a contradiction with the choice of the graph U.

Since $p \ge 1$, by Claim 1, we have $U \cong \mathscr{U}^1_{n,p}$.

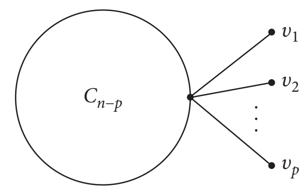

FIGURE 5: The graph $\mathscr{U}^1_{n,p}$.

Theorem 9. *Let U be an n-vertex unicyclic graph with $p \ge 1$ pendant vertices. Then, for $a > 1$,*

$$\begin{aligned}\mathrm{SEI}_a(U) \ge{}& [n - (n-p)b](b+2)a^{b+2}\\&+ [(n-p)b - p](b+1)a^{b+1} + pa,\end{aligned} \tag{30}$$

where $b = \lfloor n/(n-p) \rfloor$, with equality if and only if $U \cong \mathscr{U}^2_{n,p}$.

Proof. Choose U such that U has the minimum SEI_a for $a > 1$. Suppose C is the only cycle in U. □

Claim 2. If x and y are two nonpendant vertices of U, then $|d_U(x) - d_U(y)| \le 1$.

Assume that there are two vertices $x, y \in V(U)$ with $|d_U(x) - d_U(y)| \ge 2$. Suppose without loss of generality that $d_U(x) - 2 \ge d_U(y) \ge 2$. Since $d_U(x) \ge 4$, then there exist at least two vertices $z_1, z_2 \in (N_U(x)/V(C))$. Furthermore, since U is a unicyclic graph, $N_U(y) \cup \{y\}$ contains at most one of z_1, z_2. Set $z \in \{z_1, z_2\}$ and $z \notin (N_U(y) \cup \{y\})$. Let $U' = U - xz + yz$. Note that $d_{U'}(y) = d_U(y) + 1 \ge 3$ and $d_{U'}(x) = d_U(x) - 1 \ge 3$, so U is also a unicyclic graph with p pendant vertices. In view of (1) and (2), it follows that

$$\begin{aligned}&\mathrm{SEI}_a(U') - \mathrm{SEI}_a(U)\\&\quad = (d_U(y) + 1)a^{d_U(y)+1} + (d_U(x) - 1)a^{d_U(x)-1}\\&\qquad - d_U(y)a^{d_U(y)} - d_U(x)a^{d_U(x)} < 0,\end{aligned} \tag{31}$$

a contradiction with the choice of the graph U.

By Claim 2, we can find that U has degree 1, k, or $k+1$, where $k \ge 2$. Hence

$$p + n_k + n_{k+1} = n. \tag{32}$$

Since U is a unicyclic graph, then $p \le n-3$ and

$$p + kn_k + (k+1)n_{k+1} = 2n. \tag{33}$$

By (32) and (33), we have $k = n/(n-p) + n_k/(n-p)$. By (32), $n_k \leq n-p$, hence $k = \lfloor n/(n-p) \rfloor + 1$.

We also can get that $n_k = \lfloor n/(n-p) \rfloor (n-p) - p, n_{k+1} = n - \lfloor n/(n-p) \rfloor (n-p)$.

So, U has the degree sequence

$$\left(\underbrace{k+1,\ldots,k+1}_{n_{k+1}}, \underbrace{k,\ldots,k}_{n_k}, \underbrace{1,\ldots,1}_{p} \right) = \left(\underbrace{b+2,\ldots,b+2}_{n-b(n-p)}, \underbrace{b+1,\ldots,b+1}_{b(n-p)-p}, \underbrace{1,\ldots,1}_{p} \right), \quad (34)$$

where $b = \lfloor n/(n-p) \rfloor$.

7. Results and Discussion

As one of the 148 topological indices that turned out good predictive properties, SEI_a has a good correlation with the octanol-water partition coefficient. The mathematical properties of SEI_a are worth studying [6] since this invariant can detect the desirable properties of chemical molecules. Therefore, our results may be used to predict the extremal properties of organic molecules.

8. Conclusions

In this work, we present the minimum and maximum SEI_a $(a>1)$ of quasi-tree graphs and quasi-tree graphs with perfect matchings and determine the minimum and maximum SEI_a $(a>1)$ of unicyclic graphs with given pendant vertices and cycle length. We will consider the bicyclic graphs with some graph parameters for further study.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

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