Heliyon 9 (2023) e15706

Contents lists available at ScienceDirect

Heliyon

journal homepage: www.cell.com/heliyon

Research article

Conjugated tricyclic graphs with maximum variable sum exdeg index

Muhammad Rizwan [a], Akhlaq Ahmad Bhatti [a], Muhammad Javaid [b,*], Yilun Shang [c]

[a] Department of Sciences and Humanities, National University of Computer & Emerging Sciences, Lahore campus, Pakistan
[b] Department of Mathematics, School of Science, University of Management and Technology, Lahore 54770, Pakistan
[c] Department of Computer and Information Sciences, Northumbria University, Newcastle NE1 8ST, UK

ARTICLE INFO

Keywords:
Variable sum exdeg index
Conjugated tricyclic graph
Molecular graph

ABSTRACT

The variable sum exdeg index, initially introduced by Vukicevic (2011) [20] for predicting the octanol water partition co-efficient of certain chemical compounds, is an invariant for a graph G and defined as $SEI_a(G) = \sum_{v \in V(G)} (d_v a^{d_v})$, where d_v is the degree of vertex $v \in V(G)$, a is a positive real number different from 1. In this paper, we defined sub-collections of tricyclic graphs say $T^3_{2m}, T^4_{2m}, T^6_{2m}$ and T^7_{2m}. The graph with maximum variable sum exdeg index is characterized from each collection given above with perfect matching. Consequently, through a comparison among these extremal graphs, we indicate the graph which contains maximum SEI_a-value from T_{2m}.

1. Introduction

Let $G = (V, E)$ be a graph which is finite, connected and simple such that V and E denote the set of vertices and set of edges respectively. Let $y \in V(G)$, d_y or $d_y(G)$ is defined as the degree of the vertex y. Let $M(G) \subset E(G)$, if the degree of each vertex in $M(G)$ is 1 or 0 then $M(G)$ is called m-matching in G where $|M(G)| = m$. In a graph G if each vertex is incident to exactly one edge of matching set then such matching is called perfect matching such that $n = 2m$. Let e be an edge such that $e \in M(G)$ and $u \in V(G)$, the vertex u is said to be saturated by $M(G)$ if u is incident with e. A simple and connected graph with $2m$ vertices and $2m+2$ edges is called conjugated tricyclic graph, where m is the matching number of the graph.

A vertex which possesses degree one is called pendent vertex. A path $P = x_0x_1...x_s$ is said to be pendent path if $d_{x_0} \geq 3$, $d_{x_i} = 2(i = 1, 2, ...(s-1))$ and $d_{x_s} = 1$. A path $P = x_0x_1...x_s$ is said to be an internal path of a graph if $d_{x_0} \geq 3$, $d_{x_i} = 2(i = 1, 2, ...(s-1))$ and $d_{x_s} \geq 3$ whereas P is the shortest path from x_0 to x_s. We denote the length of the path P by $|P|$. In a graph G, an induced cycle is an induced sub-graph which has no chords. Set of neighbouring vertices of a vertex x in G is denoted by $N_G(x)$ whereas $N_G[x] = N_G(x) \cup \{x\}$.

Set of all conjugated tricyclic graphs is denoted by T_{2m} where $2m$ is order of the graph T_{2m} with $m \geq 2$. Since $T_4 = K_4$ here K_4 denotes the complete graph with order 4. That is why we consider in the following $m \geq 3$. From [10] we know that tricyclic graph has minimum 3 and maximum 7 cycles; furthermore there does not exist a graph in G with five cycles. We define $T_{2m} = T^3_{2m} \cup T^4_{2m} \cup T^6_{2m} \cup T^7_{2m}$ where $T^k_{2m}(k = 3, 4, 6, 7)$ represents the collection of all tricyclic graphs having k cycles in T_{2m}. We organized the rest of the paper as follows. In section 2, we have given some lemmas which help us in proving main result. In section 3, we investigated maximum values of SEI_a in $T^j_{2m}(j = 3, 4, 6, 7)$ for $a > 1$. At the end of this section, we have investigated the graph which contains maximum SEI_a-value in T_{2m} for $a > 1$. To read about the expressions and definitions related to this paper, the readers can see [2,4].

* Corresponding author.
E-mail addresses: L165514@lhr.nu.edu.pk (M. Rizwan), akhlaq.ahmad@nu.edu.pk (A.A. Bhatti), muhammad.javaid@umt.edu.pk (M. Javaid), yilun.shang@northumbria.ac.uk (Y. Shang).

https://doi.org/10.1016/j.heliyon.2023.e15706
Received 7 November 2022; Received in revised form 24 January 2023; Accepted 19 April 2023

Available online 27 April 2023

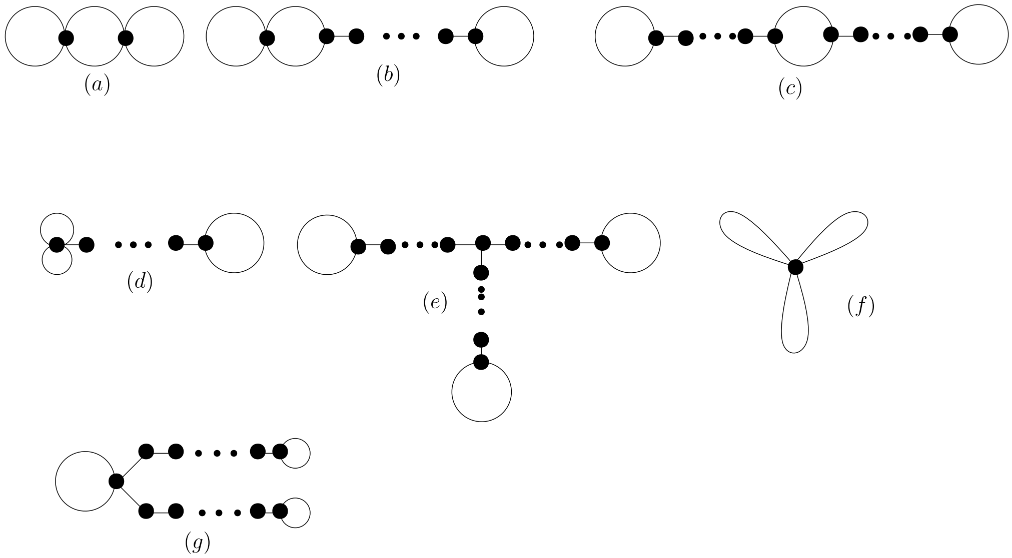

Fig. 1. Possible graphs in $G \in T^3_{2m}$.

Graphs help us design the chemical graph in which vertices and edges represent atoms and bonds respectively. Topological indices are used to investigate the physicochemical properties of a molecular graph. The graph invariants are called topological indices [22]. Actually, these topological indices give us the values which are the information about the physicochemical properties of a certain related chemical compound. In this way, we can spare ourselves from a heavy expense of chemical experiments.

Topological indices are used in quantitative structure-property relation (QSPR) and quantitative structure-activity relation (QSAR) studies to model the physicochemical characteristics of chemical compounds including total surface area, melting points, molar refraction, boiling points, acentric factor, octanol-water partition coefficient, motor octane number, and standard enthalpy of formation [5,11,19]. In addition to QSPR and QSAR the topological indices are also used in many fields of knowledge including chemistry, physics, biology, and the social sciences see for more detail [7–9,17,18]. There are a large number of topological indices in literature which have been used to investigate the above mentioned physicochemical properties for their related molecular structure. To investigate these properties researchers find extremal graphs from related class of molecular structures. For instance, in [13], extremal graphs have been characterized by using different graph parameters such as segments and vertices of degree two. Xiaoling Sun et al. [16] investigated extremal values of exdeg index for cuasi-tree graphs and unicyclic graphs by using some graph parameters. In [3], the first three maximum and minimum values of SEI_a have been undersought for n-vertex trees. Furthermore, n-vertex trees with given diameter d have first three largest values of SEI_a. In [12], lower bounds of some topological indices have been found for some family of graphs. In the following lines we will discuss the topological index related to our current work.

The variable sum exdeg index of a graph G is denoted by Vukicevic as,

$$SEI_a(G)=\sum_{uv\in E(G)}\left(a^{d_u}+a^{d_v}\right)=\sum_{u\in V(G)}(d_u a^{d_u}) \tag{1}$$

where $a > 0$ but $a \neq 1$. The above mentioned molecular structure descriptor/topological index having a good correlation with octane-water partition coefficient [19] and octane isomers is studied very well by this index, see [20]. The role of this index in nanoscience can be seen in [23]. Rizwan et al. investigated sharp lower and upper bounds on SEI_a for conjugated uni cyclic graphs with respect to the length of its cycle [15]. In [14], the author investigated sharp lower and upper bounds on SEI_a for conjugated bicyclic graphs. The author et al. investigated extremal values of SEI_a for cactus graphs with fixed number of cycles [6]. We refer the following papers to see mathematical properties and chemical application of this index [1,19,21]. In the below sections of this paper we apply some graph operations or transformation on a graph G and the resulting graph is depicted by G'. In such case whenever we discuss the degree of a vertex x say d_x, it means the degree of the vertex x in G i.e., $|V(G)| = |V(G')|$.

2. Some lemmas

Here we will put some lemmas for supporting our main goal. Let $G \in T^j_{2m}(j = 3,4,6,7)$ (with perfect matching) be a connected graph having minimal connected subgraph H with j cycles $(j = 3,4,6,7)$ and some trees. Let $G'_j(j = 3,4,6,7)$ contain maximum SEI_a which means for all $G \in T^j_{2m}(j = 3,4,6,7)$ we have $SEI_a(G'_j) \geq SEI_a(G)$ where $a > 1$. For a graph $G'_j(j = 3,4,6,7)$, minimal subgraph and perfect matching are depicted by H'_j and M'_j respectively. By [10], the arrangement of j cycles of the graph from $T^j_{2m}(j = 3,4,6,7)$ contains 7, 4, 3 and 1 possible cases respectively, as depicted in Fig. 1, Fig. 2, and Fig. 3, respectively.

Lemma 1. *For any pendent path P from $G'_j(j = 3,4,6,7)$ we have the following results:*

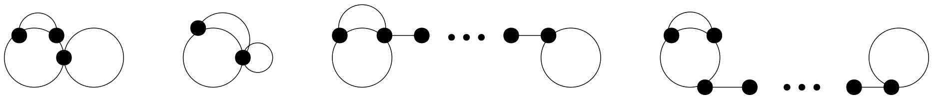

Fig. 2. Possible graphs in $G \in T_{2m}^{4}$.

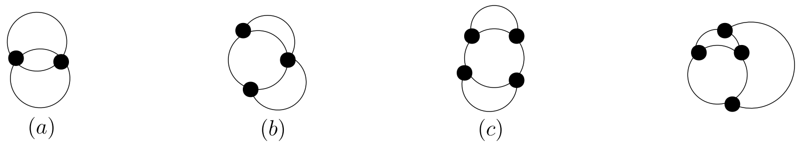

Fig. 3. Possible graphs in $G \in T_{2m}^{6}$ and one graph in $G \in T_{2m}^{7}$.

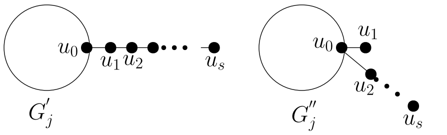

Fig. 4. G_j' and G_j'' in *(1)*.

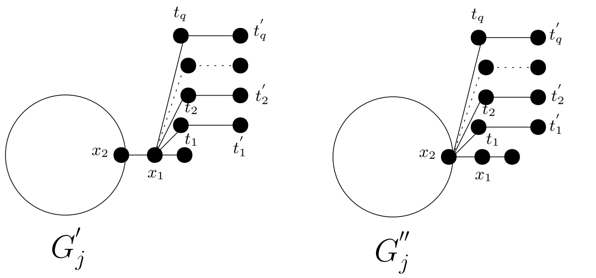

Fig. 5. G_j' and G_j'' in *(2)*.

1. *The length of the pendent path P is less or equal to two.*
2. *In G_j' every pendent path of length two (if there exists) is attached to the vertex u where the vertex u has maximum degree in H_j'.*

Proof. *(1)* We suppose on the contrary that $P = u_0 u_1 ... u_s$ where $s \geq 3$ be a pendent path where $d_{u_0} \geq 3$, $d_{u_s} = 1$ and $d_{u_i} = 2(i = 1, 2, ..., (s-1))$. We define $G_j'' = G_j' - u_{s-2}u_{s-1} + u_0 u_{s-1}$ clearly $G_j'' \in T_{2m}^{j}(j = 3, 4, 6, 7)$. For instance we show G_j'' in Fig. 4. So we have,

$$\begin{aligned} SEI_a(G_j'') - SEI_a(G_j') &= \left[(d_{u_0} + 1)a^{d_{u_0}+1} - (d_{u_0})a^{d_{u_0}}\right] - \left[\left(d_{u_{s-2}}\right)a^{d_{u_{s-2}}} - (d_{u_{s-2}} - 1)a^{d_{u_{s-2}}-1}\right] \\ &= \left[a^{\mu_2}(1 + \mu_2 lna) - a^{\mu_1}(1 + \mu_1 lna)\right], \end{aligned} \tag{2}$$

from $a > 1$, $\mu_1 \in (d_{u_{s-2}} - 1, d_{u_{s-2}})$, $\mu_2 \in (d_{u_0}, d_{u_0} + 1)$ and $\mu_2 > \mu_1$, we have $SEI_a(G_j'') > SEI_a(G_j')$, a contradiction.
(2) We suppose on the contrary there exist x_1 and x_2 vertices in H_j' such that $d_{x_2} \geq d_{x_1} \geq 2$. Let x_1 be the end vertex of some pendent paths of length two, say $P_1 = x_1 t_1 t_1'$, $P_2 = x_1 t_2 t_2'$, ... $P_q = x_1 t_q t_q'$. We define $G_j'' = G_j' - \sum_{l=1}^{q}(x_1 t_l) + \sum_{l=1}^{q}(x_2 t_l)$ clearly $G_j'' \in T_{2m}^{j}$. For instance, we show G_j'' in Fig. 5. From G_j' and G_j'' we have,

$$\begin{aligned} SEI_a(G_j'') - SEI_a(G_j') &= \left[(d_{x_2} + q)a^{d_{x_2}+q} - (d_{x_2})a^{d_{x_2}}\right] - \left[(d_{x_1})a^{d_{x_1}} - (d_{x_1} - q)a^{d_{x_1}-q}\right] \\ &= \left[a^{\mu_2}(1 + \mu_2 lna) - a^{\mu_1}(1 + \mu_1 lna)\right], \end{aligned} \tag{3}$$

from $a > 1$, $\mu_1 \in (d_{x_1} - q, d_{x_1})$, $\mu_2 \in (d_{x_2}, d_{x_2} + q)$ and $\mu_2 > \mu_1$, we have $SEI_a(G_j'') > SEI_a(G_j')$, a contradiction. □

Lemma 2. *If $P_1 \in G_j' \in T_{2m}^{j}(j = 3, 4, 6, 7)$ is an internal path and $P_2 \in G_j' \in T_{2m}^{j}(j = 3, 4, 6, 7)$ is the shortest path between the vertices w_1 and w_2 where w_1 and w_2 are the common vertices of any two cycles, then*

1. *Length of the path P_1 is exactly one and both the vertices of P_1 exist in the same cycle.*
2. *Length of the path P_2 is exactly one.*

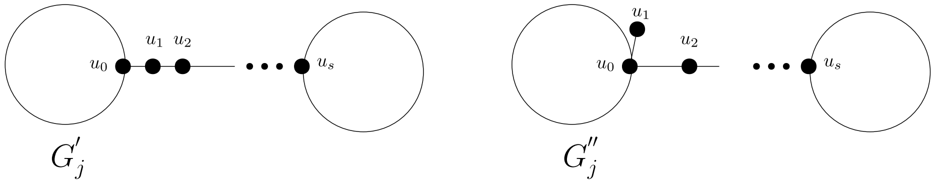

Fig. 6. G_j' and G_j'' in *(1)*.

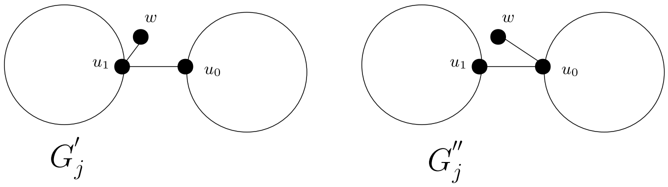

Fig. 7. G_j' and G_j'' in Lemma 2, Subcase-2.

Proof. *(1)* Let $P = u_0u_1...u_s$ where $s \geq 1$ be an internal path in $G_j'(j = 3,4,6,7)$ where $d_{u_0} \geq 3$, $d_{u_s} \geq 3$ and $d_{u_i} = 2(i = 1,2,...,(s-1))$.
Case-1: when $s \geq 2$
Subcase-1.1: if $u_0u_1 \in M_j'(j = 3,4,6,7)$.
We define $G_j'' = G_j' - u_1u_2 + u_0u_2$ clearly $G_j'' \in T_{2m}^j$, as G_j'' is shown in Fig. 6. We calculate,

$$SEI_a(G_j'') - SEI_a(G_j') = \left[(d_{u_0}+1)a^{d_{u_0}+1} - (d_{u_0})a^{d_{u_0}}\right] - \left[(d_{u_1})a^{d_{u_1}} - (d_{u_1}-1)a^{d_{u_1}-1}\right]$$
$$= \left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right], \tag{4}$$

from $a > 1$, $\mu_1 \in (d_{u_1}-1, d_{u_1})$, $\mu_2 \in (d_{u_0}, d_{u_0}+1)$ and $\mu_2 > \mu_1$, we conclude $SEI_a(G_j'') > SEI_a(G_j')$, a contradiction.
Subcase-1.2: if $u_0u_1 \notin M_j'(j = 3,4,6,7)$.
We define $G_j'' = G_j' - u_0u_1 + u_0u_k$ clearly $G_j'' \in T_{2m}^j$.

$$SEI_a(G_j'') - SEI_a(G_j') = \left[(d_{u_k}+1)a^{d_{u_k}+1} - (d_{u_k})a^{d_{u_k}}\right] - \left[(d_{u_1})a^{d_{u_1}} - (d_{u_1}-1)a^{d_{u_1}-1}\right]$$
$$= \left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right], \tag{5}$$

from $a > 1$, $\mu_1 \in (d_{u_1}-1, d_{u_1})$, $\mu_2 \in (d_{u_k}, d_{u_k}+1)$ and $\mu_2 > \mu_1$, we conclude $SEI_a(G_j'') > SEI_a(G_j')$, a contradiction.
Subcase-2: if $s = 1$ but u_0 and u_1 does not exist on same cycle.
As we know that $s = 1$, $d_{u_1} \geq 3$. Here we let $d_{u_0} \geq d_{u_1}$ then there must exist a vertex $w \in N_{G_j'}(u_1) - N_{G_j'}(u_0)$ such that $u_1w \notin M_j'(j = 3,4,6,7)$. We define $G_j'' = G_j' - u_1w + u_0w$ clearly $G_j'' \in T_{2m}^j$ as shown in Fig. 7.

$$SEI_a(G_j'') - SEI_a(G_j') = \left[(d_{u_0}+1)a^{d_{u_0}+1} - (d_{u_0})a^{d_{u_0}}\right] - \left[(d_{u_1})a^{d_{u_1}} - (d_{u_1}-1)a^{d_{u_1}-1}\right]$$
$$= \left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right], \tag{6}$$

from $a > 1$, $\mu_1 \in (d_{u_1}-1, d_{u_1})$, $\mu_2 \in (d_{u_0}, d_{u_0}+1)$ and $\mu_2 > \mu_1$, we have $SEI_a(G_j'') > SEI_a(G_j')$, a contradiction.
(2) We assume that $P_2 = u_0u_1...u_s$ where $s \geq 1$, $w_1 = u_0$ and $u_s = w_2$. Let P_2 be the shortest path between the vertices w_1 and w_2 with $d_{w_1} \geq 3$ and $d_{w_2} \geq 3$. We suppose on the contrary $|P_2| = s \geq 2$ then by proof *(1)* and Lemma 1 we can find a vertex of degree one adjacent to u_1 and $u_1u_2 \notin M_j'(j = 3,4,6,7)$, so it becomes clear that $d_{u_1} = 3$. We define $G_j'' = G_j' - u_1u_2 + u_2w_1$ clearly $G_j'' \in T_{2m}^j$.

$$SEI_a(G_j'') - SEI_a(G_j') = \left[(d_{w_1}+1)a^{d_{w_1}+1} - (d_{w_1})a^{d_{w_1}}\right] - \left[(d_{u_1})a^{d_{u_1}} - (d_{u_1}-1)a^{d_{u_1}-1}\right]$$
$$= \left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right], \tag{7}$$

from $a > 1$, $\mu_1 \in (d_{u_1}-1, d_{u_1})$, $\mu_2 \in (d_{w_1}, d_{w_1}+1)$ and $\mu_2 > \mu_1$, we derive the relation $SEI_a(G_j'') > SEI_a(G_j')$, a contradiction. □

Lemma 3. *For any induced cycle say C from $G_j' \in T_{2m}^j(j = 3,4,6,7)$ the length of this cycle is 3 such that $|C| = 3$.*

Proof. From Lemma 2 we are sure that all induced cycles which belong to $G_7' \in T_{2m}^7$ having exactly three vertices in it. That is why we discuss the graph $G_j' \in T_{2m}^j(j = 3,4,6)$ only. We suppose on the contrary, $|C| \geq 4$. Let x and y be the vertices in C where x has the maximum degree and y be at the farthest distance from x. Let $P : x = x_0x_1...x_s(= y)$, be the shortest path and the vertices $x_1, x_2, ...x_{s-1}$ are not common between any two cycles. Length of the path P can be greater or equal to 2 such that $|P| = s \geq 2$.
Case-1: when $s = 2$

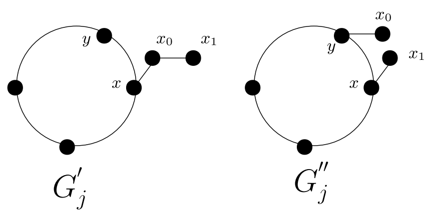

Fig. 8. G_j' and G_j'' in Lemma 4, Case-1.

Subcase-1.1: if $x_1x_2 \notin M_j'(j=3,4,6)$.
We define $G_j''=G_j'-x_1x_2+xx_2$ clearly $G_j''\in T_{2m}^j(j=3,4,6)$.

$$\begin{aligned} SEI_a(G_j'')-SEI_a(G_j') &= \left[(d_x+1)a^{d_x+1}-(d_x)a^{d_x}\right]-\left[(d_{x_1})a^{d_{x_1}}-(d_{x_1}-1)a^{d_{x_1}-1}\right] \\ &= \left[a^{\mu_2}(1+\mu_2lna)-a^{\mu_1}(1+\mu_1lna)\right], \end{aligned} \tag{8}$$

from $a>1$, $\mu_1\in(d_{x_1}-1,d_{x_1})$, $\mu_2\in(d_x,d_x+1)$ and $\mu_2>\mu_1$, we conclude $SEI_a(G_j'')>SEI_a(G_j')$, a contradiction.
Subcase-1.2: if $x_1x_2\in M_j'(j=3,4,6)$.
As we know that $M_j'(j=3,4,6)$ so Lemma 1 and Lemma 2 ensure that $d_{x_1}=2$. Let $G_j''=G_j'-xx_1+xx_2$ clearly $G_j''\in T_{2m}^j(j=3,4,6)$.

$$\begin{aligned} SEI_a(G_j'')-SEI_a(G_j') &= \left[(d_{x_2}+1)a^{d_{x_2}+1}-(d_{x_2})a^{d_{x_2}}\right]-\left[(d_{x_1})a^{d_{x_1}}-(d_{x_1}-1)a^{d_{x_1}-1}\right] \\ &= \left[a^{\mu_2}(1+\mu_2lna)-a^{\mu_1}(1+\mu_1lna)\right], \end{aligned} \tag{9}$$

from $a>1$, $\mu_1\in(d_{x_1}-1,d_{x_1})$, $\mu_2\in(d_{x_2},d_{x_2}+1)$ and $\mu_2>\mu_1$, we get $SEI_a(G_j'')>SEI_a(G_j')$, a contradiction.
Subcase-2: if $s\geq 3$
Subcase-2.1: if $x_2x_3\in M_j'(j=3,4,6)$.
We define $G_j''=G_j'-x_1x_2+xx_2$ clearly $G_j''\in T_{2m}^j$. We have,

$$\begin{aligned} SEI_a(G_j'')-SEI_a(G_j') &= \left[(d_x+1)a^{d_x+1}-(d_x)a^{d_x}\right]-\left[(d_{x_1})a^{d_{x_1}}-(d_{x_1}-1)a^{d_{x_1}-1}\right] \\ &= \left[a^{\mu_2}(1+\mu_2lna)-a^{\mu_1}(1+\mu_1lna)\right], \end{aligned} \tag{10}$$

from $a>1$, $\mu_1\in(d_{x_1}-1,d_{x_1})$, $\mu_2\in(d_x,d_x+1)$ and $\mu_2>\mu_1$, we have $SEI_a(G_j'')>SEI_a(G_j')$, a contradiction.
Subcase-2.2: if $x_2x_3\notin M_j'(j=3,4,6)$.
Let $G_j''=G_j'-x_2x_3+xx_3$ clearly $G_j''\in T_{2m}^j$.

$$\begin{aligned} SEI_a(G_j'')-SEI_a(G_j') &= \left[(d_x+1)a^{d_x+1}-(d_x)a^{d_x}\right]-\left[(d_{x_2})a^{d_{x_2}}-(d_{x_2}-1)a^{d_{x_2}-1}\right] \\ &= \left[a^{\mu_2}(1+\mu_2lna)-a^{\mu_1}(1+\mu_1lna)\right], \end{aligned} \tag{11}$$

since $a>1$, $\mu_1\in(d_{x_2}-1,d_{x_2})$, $\mu_2\in(d_x,d_x+1)$ and $\mu_2>\mu_1$, and we get $SEI_a(G_j'')>SEI_a(G_j')$, a contradiction. □

Lemma 4. *Let $P_1,P_2,\ldots,P_r$ be the pendent paths of length two in G_j'. All these pendent paths are attached to the vertex $x\in V(H_j')$ where x be the vertex of maximum degree. Then the graph $G_j'\in T_{2m}^j(j=3,4,6,7)$ contains a unique vertex of degree one adjacent to x such that $m\geq 4$.*

Proof. We suppose on the contrary that vertex x has no pendent edge adjacent to it. According to Lemma 1, Lemma 2, and Lemma 3 there will be two cases below.
Case-1:
We suppose that $P=xx_0x_1$ is one of the pendent paths which are adjacent to the vertex x. Let $y\in N_{H_j'}(x)$ such that $(d_y\geq d_{x_0}=2)$ with $xy\in M_j'$. We define $G_j''=G_j'-x_0x_1+yx_1$ clearly $G_j''\in T_{2m}^j(j=3,4,6,7)$ for our convenience we show G_j'' in Fig. 8. Since $M_j''=M_j'-\{x_0x_1,xy\}+\{xx_0,yx_1\}$ is a perfect matching of $G_j''(j=3,4,6,7)$. We have,

$$\begin{aligned} SEI_a(G_j'')-SEI_a(G_j') &= \left[(d_y+1)a^{d_y+1}-(d_y)a^{d_y}\right]-\left[(d_{x_0})a^{d_{x_0}}-(d_{x_0}-1)a^{d_{x_0}-1}\right] \\ &= \left[a^{\mu_2}(1+\mu_2lna)-a^{\mu_1}(1+\mu_1lna)\right], \end{aligned} \tag{12}$$

from $a>1$, $\mu_1\in(d_{x_0}-1,d_{x_0})$, $\mu_2\in(d_y,d_y+1)$ and $\mu_2>\mu_1$, we have $SEI_a(G_j'')>SEI_a(G_j')$, a contradiction.
Case-2: if pendent path of length 2 does not exist.
Lemma 2 and Lemma 3 guarantee that the vertex x must be common in at least two induced cycles of length 3 in $G_j'(3,4,6,7)$. As we know that $m\geq 4$, so we consider w_1 is a pendent vertex adjacent to $w_2\in V(H_j')-x$ where $w_2\in N_{H_j'}(x)$. We consider the vertex $w_3\in H_j'$ with $xw_3\in M_j'(d_{w_3}\geq 2)$. Here we make two sub-cases.
Subcase-2.1: if $w_3\in N_{H_j'}(x)\cap N_{H_j'}(w_2)$

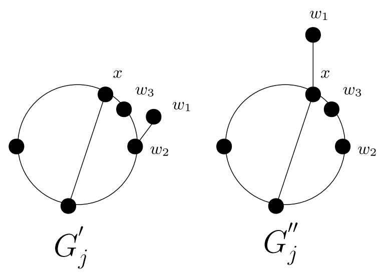

Fig. 9. G_j' and G_j'' in Lemma 4, Case-2.1.

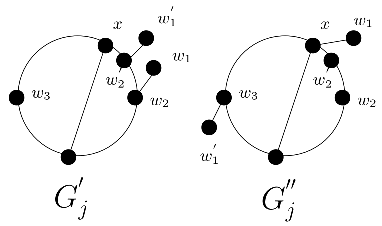

Fig. 10. G_j' and G_j'' in Lemma 4, Subcase-2.2.

We define $G_j'' = G_j' - w_1w_2 + w_1x$ clearly $G_j'' \in T_{2m}^j$ for our convenience we show G_j'' in Fig. 9. Since $M_j'' = M_j' - \{xw_3, w_1w_2\} + \{xw_1, w_2w_3\}$ is a perfect matching of $G_j''(j = 3,4,6,7)$. We have,

$$\begin{aligned} SEI_a(G_j'') - SEI_a(G_j') &= \left[(d_x+1)a^{d_x+1} - (d_x)a^{d_x}\right] - \left[(d_{w_2})a^{d_{w_2}} - (d_{w_2}-1)a^{d_{w_2}-1}\right] \\ &= \left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right], \end{aligned} \tag{13}$$

from $a > 1$, $\mu_1 \in (d_{w_2}-1, d_{w_2})$, $\mu_2 \in (d_x, d_x+1)$ and $\mu_2 > \mu_1$, we have $SEI_a(G_j'') > SEI_a(G_j')$, a contradiction.
Subcase-2.2: if $w_3 \notin N_{H_j'}(x) \cap N_{H_j'}(w_2)$
Lemma 2 and Lemma 3 guarantee that there exists a vertex w_1' adjacent to $w_2' \notin N_{H_j'}(x) \cap N_{H_j'}(w_2)$ such that $d_{w_1'=1}$ and one of $\{w_2, w_2'\}$ has degree 3. We assume that $d_{w_2'} = 3$. We define $G_j'' = G_j' - w_1w_2 - w_2'w_1' + xw_1 + w_3w_1'$ clearly $G_j'' \in T_{2m}^j$ because $M_j'' = M_j' - \{w_1w_2, w_2'w_1', xw_3\} + \{xw_1, w_2w_2', w_3w_1'\}$ is a perfect matching of $G_j''(j = 3,4,6,7)$. For instance we define G_j'' in Fig. 10. We have,

$$\begin{aligned} SEI_a(G_j'') - SEI_a(G_j') &= \left[(d_x+1)a^{d_x+1} - (d_x)a^{d_x}\right] - \left[(d_{w_2})a^{d_{w_2}} - (d_{w_2}-1)a^{d_{w_2}-1}\right] \\ &+ \left[(d_{w_3}+1)a^{d_{w_3}+1} - (d_{w_3})a^{d_{w_3}}\right] - \left[(d_{w_2'})a^{d_{w_2'}} - (d_{w_2'}-1)a^{d_{w_2'}-1}\right] \\ &= \left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right] \\ &+ \left[a^{\mu_4}(1+\mu_4 lna) - a^{\mu_3}(1+\mu_3 lna)\right], \end{aligned} \tag{14}$$

from $a > 1$, $\mu_1 \in (d_{w_2}-1, d_{w_2})$, $\mu_2 \in (d_x, d_x+1)$, $\mu_3 \in (d_{w_2'}-1, d_{w_2'})$, $\mu_4 \in (d_{w_3}, d_{w_3}+1)$ and $\mu_2 > \mu_1$, $\mu_4 > \mu_3$, we have $SEI_a(G_j'') > SEI_a(G_j')$, a contradiction. □

3. Main results

In the current section, we have investigated the graph from $T_{2m}^j (j = 3,4,6,7)$ which has maximum SEI_a where $a > 1$. Following this, we also described the unique graph in T_{2m} having the highest SEI_a-value.

Theorem 1. *Let $m \geq 4$, $a > 1$ and $G \in T_{2m}^3$ then $SEI_a(G) \leq SEI_a(F_3(2m))$ and the equality in the bound is attained if and only if $G \cong F_3(2m)$ where $F_3(2m)$ is depicted in Fig. 11.*

Proof. From Lemma 1, Lemma 2 and Lemma 3, it is easy to understand that $H_3' \cong F_3$ or $H_3' \cong F_3'$ (depicted in Fig. 11). Let M_3' be the perfect matching in G_3'. Here we claim that $H_3' \cong F_3$.
We suppose on the contrary that $H_3' \cong F_3'$. Let x, y, x_1 and x_2 be the vertices depicted in Fig. 11. In Fig. 11, x and y are the only vertices which have maximum degree. Lemma 4 and Lemma 1 ensure the existence of a pendent vertex which is adjacent to y where all the pendent paths of length two end at the vertex y. From above discussion we can say $xy \notin M_3'$.

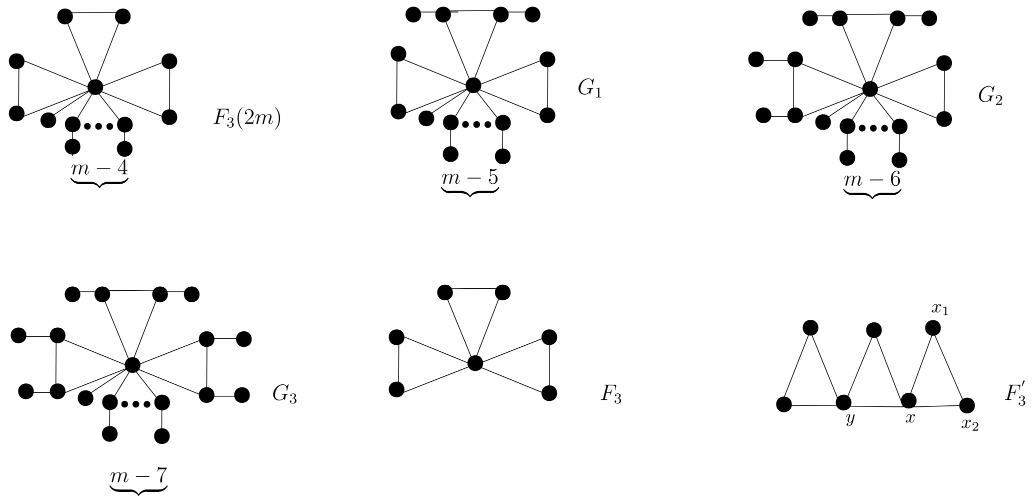

Fig. 11. $F_3(2m)$, F_3, F_3' and $G_i(i=1,2,3)$.

Case-1: if $xx_1 \notin M_3'$ and $xx_2 \notin M_3'$.
We define $G_3'' = G_3' - xx_1 - xx_2 + yx_1 + yx_2$ clearly $G_3'' \in T_{2m}^3$. We have,

$$\begin{aligned} SEI_a(G_3'') - SEI_a(G_3') &= \left[(d_y+2)a^{d_y+2} - (d_y)a^{d_y}\right] - \left[(d_x)a^{d_x} - (d_x-2)a^{d_x-2}\right] \\ &= 2.\left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right], \end{aligned} \tag{15}$$

from $a>1$, $\mu_1 \in (d_x-2, d_x)$, $\mu_2 \in (d_y, d_y+2)$ and $\mu_2 > \mu_1$, we have $SEI_a(G_3'') > SEI_a(G_3')$, a contradiction.
Case-2: if $xx_1 \in M_3'$ or $xx_2 \in M_3'$.
If $xx_1 \in M_3'$ then there exists a vertex of degree one say x_3 adjacent to x_2 such that $x_2x_3 \in M_3'$. We define $G_3'' = G_3' - x_2x_3 + xx_3$ clearly $G_3'' \in T_{2m}^3$ because $M_3'' = M_3' - \{xx_1, x_2x_3\} + \{xx_3, x_1x_2\}$, and M_3'' belongs to the perfect matching in G_3''.

$$\begin{aligned} SEI_a(G_3'') - SEI_a(G_3') &= \left[(d_x+1)a^{d_x+1} - (d_x)a^{d_x}\right] - \left[(d_{x_2})a^{d_{x_2}} - (d_{x_2}-1)a^{d_{x_2}-1}\right] \\ &= \left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right], \end{aligned} \tag{16}$$

from $a>1$, $\mu_1 \in (d_{x_2}-1, d_{x_2})$, $\mu_2 \in (d_x, d_x+1)$ and $\mu_2 > \mu_1$, we obtain $SEI_a(G_3'') > SEI_a(G_3')$, a contradiction.
For $m \geq 4$ there exist some graphs (depicted in Fig. 11). These graphs fulfil (characterized by Lemma 1, Lemma 2, Lemma 3, and Lemma 4) the properties of the graph for maximum SEI_a. We calculate the difference,

$$\begin{aligned} SEI_a(F_3(2m)) - SEI_a(G_1) &= \left[(m+3)a^{m+3} - (m+2)a^{m+2} - 2.3a^3 + 3.2a^2 - a\right] \\ &> \left[4a^4 - 3a^3 - 2.3a^3 + 3.2a^2 - a\right] > 0 \end{aligned} \tag{17}$$

In the same way, we can show that $SEI_a(G_1) > SEI_a(G_2) > SEI_a(G_3)$. Hence the graph $F_3(2m)$ contains maximum SEI_a-value in T_{2m}^3. □

Theorem 2. *Let $m \geq 3$, $a > 1$ and $G \in T_{2m}^4$ then $SEI_a(G) \leq SEI_a(F_4(2m))$ and the equality in the bound is attained if and only if $G \cong F_4(2m)$. Particularly when $m = 3$ then F_4 contains maximum SEI_a where $F_4(2m)$ and F_4 are depicted in Fig. 12.*

Proof. From Lemma 1, Lemma 2, and Lemma 3, it is easy to understand that $H_4' \cong F_4$ or $H_4' \cong F_4'$ (depicted in Fig. 12). Let G_4' contain a perfect matching say M_4'. Here we claim that $H_4' \cong F_4$.
We suppose on the contrary that $H_4' \cong F_4'$. Let x, y be the vertices in F_4' depicted in Fig. 12. As we know that $d_x = 2$ in F_4' so there will exist a vertex $x_1 \in F_4'(d_{x_1} \geq 2)$ such that $yx_1 \notin M_4'$. We define $G_4'' = G_4' - yx_1 + xy$ clearly $G_4'' \in T_{2m}^4$.

$$\begin{aligned} SEI_a(G_4'') - SEI_a(G_4') &= \left[(d_y+1)a^{d_y+1} - (d_y)a^{d_y}\right] - \left[(d_{x_1})a^{d_{x_1}} - (d_{x_1}-1)a^{d_{x_1}-1}\right] \\ &= \left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right], \end{aligned} \tag{18}$$

from $a>1$, $\mu_1 \in (d_{x_1}-1, d_{x_1})$, $\mu_2 \in (d_y, d_y+1)$ and $\mu_2 > \mu_1$, we have $SEI_a(G_4'') > SEI_a(G_4')$, a contradiction.
It is easy to calculate that (F_4) contains maximum SEI_a-value for $m = 3$. For $m \geq 4$ there are only four possible graphs (depicted in Fig. 12). These graphs fulfil the properties of the graph for maximum SEI_a. We calculate the difference,

$$SEI_a(F_4(2m)) - SEI_a(G_1) = \left[(m+2)a^{m+2} - (m+1)a^{m+1} - 4a^4 + 2.2a^2 - a\right]$$

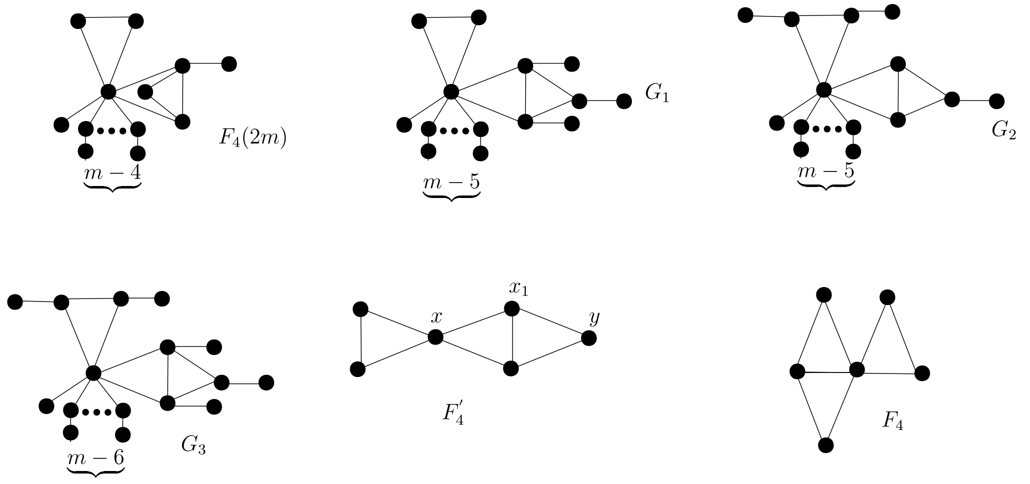

Fig. 12. $F_4(2m)$, F_4, F_4' and $G_i (i = 1, 2, 3)$.

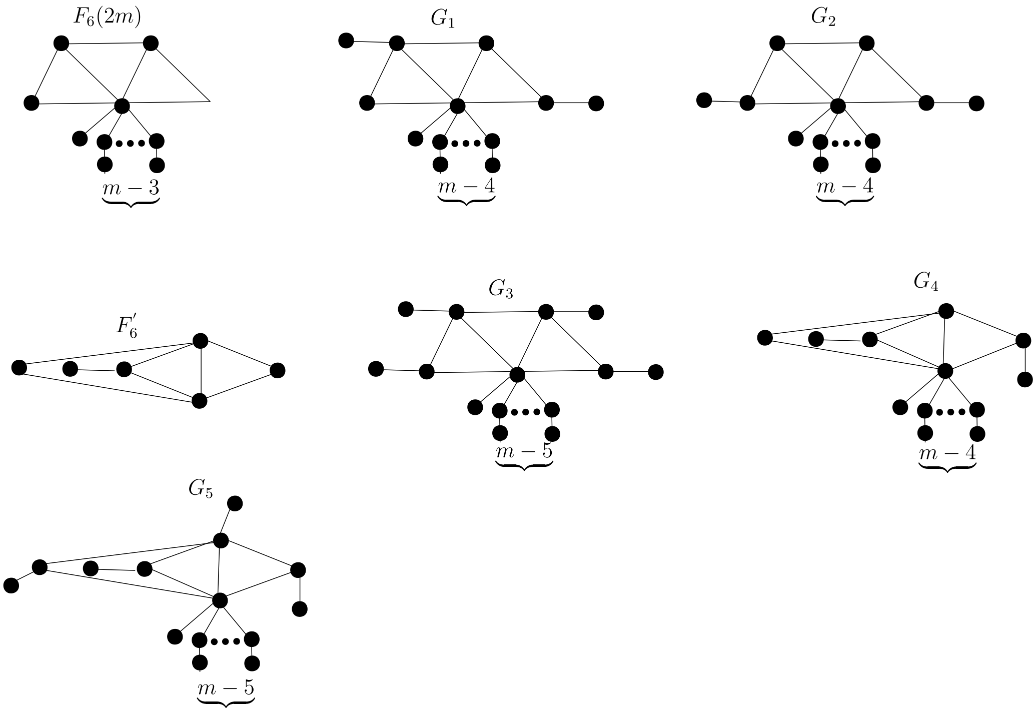

Fig. 13. $F_6(2m)$, F_6' and $G_i (i = 1, 2, 3, 4, 5)$.

$$> \left[5a^5 - 2.4a^4 + 2.2a^2 - a\right] > 0 \tag{19}$$

Similarly, we may demonstrate that $SEI_a(G_1) > SEI_a(G_2) > SEI_a(G_3)$. Hence the graph $F_4(2m)$ contains maximum SEI_a-value in T^4_{2m}. □

Theorem 3. *Let $m \geq 3$, $a > 1$ and $G \in T^6_{2m}$ then $SEI_a(G) \leq SEI_a(F_6(2m))$ and the equality in the bound is attained if and only if $G \cong F_6(2m)$ where $F_6(2m)$ is depicted in Fig. 13.*

Proof. For $m = 3$ from Lemma 1, Lemma 2, and Lemma 3, it becomes easy to understand that $G_6' \cong F_6(6)$ or $G_6' \cong F_6'$ (depicted in Fig. 13).

$$SEI_a(F_6(6)) - SEI_a(F_6') = \left[5a^5 - 4a^4\right] - \left[4a^4 - 3a^3\right]$$

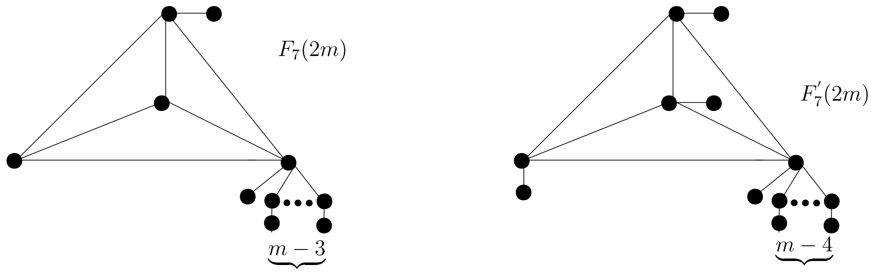

Fig. 14. $F_7(2m)$ and $F_7'(2m)$.

$$= \left[a^{\mu_2}(1+\mu_2 lna) - a^{\mu_1}(1+\mu_1 lna)\right], \tag{20}$$

from $a>1$, $\mu_1 \in (3,4)$, $\mu_2 \in (4,5)$ and $\mu_2 > \mu_1$, we get $SEI_a(F_6(6)) > SEI_a(F_6')$, a contradiction.
For $m \geq 4$ there are only six possible graphs (depicted in Fig. 13). These graphs fulfil (characterized by Lemma 1 to Lemma 4) the properties of the graph for maximum SEI_a. We calculate the difference,

$$\begin{aligned} SEI_a(F_6(2m)) - SEI_a(G_1) &= \left[(m+2)a^{m+2} - (m+1)a^{m+1} - 4a^4 + 2.2a^2 - a\right] \\ &> \left[5a^5 - 2.4a^4 + 2.2a^2 - a\right] > 0. \end{aligned} \tag{21}$$

Hence, $SEI_a(F_6(2m)) > SEI_a(G_1)$. In the same way, we can show that $SEI_a(G_1) > SEI_a(G_2) > SEI_a(G_3)$ and $SEI_a(G_4) > SEI_a(G_5)$. We also notice that $SEI_a(G_1) = SEI_a(G_4)$ because G_1 and G_4 have the same degree sequence. Hence the graph $F_6(2m)$ contains maximum SEI_a-value in T^6_{2m}. □

Theorem 4. *Let $m \geq 3$, $m \neq 4$, $a>1$ and $G \in T^7_{2m}$ then $SEI_a(G) \leq SEI_a(F_7(2m))$ and the equality in the bound is attained if and only if $G \cong F_7(2m)$ where $F_7(2m)$ is depicted in Fig. 14.*

Proof. For $m=3$, Lemma 4 ensures that $F_7(6)$ contains maximum SEI_a-value.
For $m \geq 5$ there exist some graphs (depicted in Fig. 14). These graphs fulfil the properties (characterized by Lemma 1 to Lemma 4) of the graph for maximum SEI_a-value in T^7_{2m}. We calculate the difference,

$$\begin{aligned} SEI_a(F_7(2m)) - SEI_a(F_7'(2m)) &= \left[(m+1)a^{m+1} - (m)a^m - 2.4a^4 + 2.3a^3 + 2a^2 - a\right] \\ &\geq \left[6a^6 - 5a^5 - 2.4a^4 + 2.3a^3 + 2a^2 - a\right] > 0 \end{aligned} \tag{22}$$

Finally, we conclude $F_7(2m)$ has maximum SEI_a-value in T^7_{2m}. □

Theorem 5. *For $a>1$, $F_6(6)$ and $F_3(2m)$ maximize SEI_a in T_{2m} when $m=3$ and $m \geq 4$ respectively.*

Proof. For $m=3$, we have the graphs $F_6(6)$, F_4 and $F_7(6)$. We calculate the following difference.

$$SEI_a(F_6(6)) - SEI_a(F_4) = \left[3a^3 + a - 2a + 2a^2\right] > 0, \tag{23}$$

and

$$SEI_a(F_6(6)) - SEI_a(F_7(6)) = \left[5a^5 + 2.2a^2 - 2.4a^4 - a\right] > 0. \tag{24}$$

This implies that $F_6(6)$ has the maximum SEI_a-value.
For $m=4$ we have the graphs $F_3(8)$, $F_4(8)$ and $F_6(8)$, $F_7(8)$ and $F_7'(8)$. We calculate the following difference.

$$SEI_a(F_3(8)) - SEI_a(F_4(8)) = \left[7a^7 - 6a^6 - 2.3a^3 + 3.2a^2 - a\right] > 0, \tag{25}$$

and

$$SEI_a(F_6(8)) - SEI_a(F_7(8)) = \left[6a^6 - 5a^5 - 4a^4 + 2.2a^2 - a\right] > 0, \tag{26}$$

and

$$SEI_a(F_6(8)) - SEI_a(F_7'(8)) = \left[6a^6 - 4.4a^4 + 2.3a^3 + 3.2a^2 - 2a\right] > 0. \tag{27}$$

As we know that $SEI_a(F_4(8)) = SEI_a(F_6(8))$, $F_3(8)$ contains maximum SEI_a-value.
For $m \geq 5$

$$\begin{aligned} SEI_a(F_3(2m)) - SEI_a(F_4(2m)) &= \left[(m+3)a^{m+3} - (m+2)a^{m+2} - 2.3a^3 + 3.2a^2 - a\right] \\ &> \left[4a^4 - 3a^3 - 2.3a^3 + 3.2a^2 - a\right] > 0, \end{aligned} \tag{28}$$

and

$$\begin{aligned} SEI_a(F_6(2m)) - SEI_a(F_7(2m)) &= \left[(m+2)a^{m+2} - (m+1)a^{m+1} - 4a^4 + 2.2a^2 - a\right] \\ &> \left[5a^5 - 2.4a^4 + 2.2a^2 - a\right] > 0. \end{aligned} \tag{29}$$

Since $SEI_a(F_4(2m)) = SEI_a(F_6(2m))$, we conclude that $F_3(2m)$ contains maximum SEI_a-value in T_{2m}. □

4. Conclusion

In this paper, the extremal values of variable sum exdeg index SEI_a have been investigated for the class of tricyclic graphs. Therefore, the extremal values of variable sum exdeg index for multicyclic graphs are still an open problem for different values of a.

CRediT authorship contribution statement

Muhammad Rizwan: Conceived and designed the experiments; Performed the experiments; Wrote the paper. Akhlaq Ahmad Bhatti, Muhammad Javaid, Yilun Shang: Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data.

Declaration of competing interest

The authors declare the following conflict of interests: We declare that Yilun Shang is a Section Editor of Heliyon.

Data availability

No data was used for the research described in the article.

Funding statement

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Acknowledgements

All authors of the manuscript had been informed of their inclusion and approved this. The authors thank anonymous referees for valuable suggestions which leads to a considerably improved presentation.

References

[1] A. Ali, D. Dimitrov, On the extremal graphs with respect to bond incident degree indices, Discrete Appl. Math. 238 (2018) 32–40, https://doi.org/10.1016/j.dam.2017.12.007.
[2] J.A. Bondy, Murty Graph Theory, Springer, London, 2008.
[3] S.B. Chen, S.S. Asghar, M.A. Binyamin, Z. Iqbal, T. Mahmood, A. Aslam, On the first three extremum values of variable sum exdeg index of trees, Complexity (2021), https://doi.org/10.1155/2021/6491886.
[4] R. Diestel, Graph Theory, Springer, Berlin, 2005.
[5] J. Devillers, A.T. Balaban, Topological indices and related descriptors in QSAR and QSPR, Gordon & Breach, Amsterdam, Netherlands, 1999, pp. 5055–5056.
[6] M. Javaid, A. Ali, I. Milovanovic, E. Milovanovic, On the extremal cactus graphs for variable sum exdeg index with a fixed number of cycles, AKCE Int. J. Graphs Comb. 17 (2020), https://doi.org/10.1016/j.akcej.2019.08.007.
[7] Y.C. Jun, D.H. Won, S.H. Lee, D.S. Kong, S.J. Hwang, A multimetric benthic macroinvertebrate index for the assessment of stream biotic integrity in Korea, Int. J. Environ. Res. Public Health 9 (2012) 3599–3628, https://doi.org/10.3390/ijerph9103599.
[8] P. Lucena-Moya, I. Pardo, An invertebrate multimetric index to classify the ecological status of small coastal lagoons in the Mediterranean ecoregion (MIBIIN), Mar. Freshw. Res. 63 (2012) 801–814, https://doi.org/10.1071/MF12104.
[9] F.D. Malliaros, V. Megalooikonomou, C. Faloutsos, Estimating robustness in large social graphs, Knowl. Inf. Syst. 45 (2015) 645–678, https://doi.org/10.1007/s10115-014-0810-7.
[10] S.C. Li, X.C. Li, Z.X. Zhu, On tricyclic graphs with minimal energy, MATCH Commun. Math. Comput. Chem. 59 (2008) 397–419.
[11] L.A.J. Muller, K.G. Kugler, A. Graber Dehmer, A network-base approach to classify the three domains of life, Biol. Direct 6 (2011) 140–141, https://doi.org/10.1186/1745-6150-6-53.
[12] A. Martinez-Perez, J.M. Rodriguez, New lower bounds for the first variable Zagreb index, Discrete Appl. Math. 306 (2022) 166–173, https://doi.org/10.1016/j.dam.2021.09.030.
[13] S. Noureen, A.A. Bhatti, A. Ali, Extremal trees for the modified first Zagreb connection index with fixed number of segments or vertices of degree 2, J. Taibah Univ. Sci. 14 (2020) 31–37, https://doi.org/10.1080/16583655.2019.1699227.
[14] M. Rizwan, A.A. Bhatti, M. Javaid, F. Jarad, Some bounds on bond incident degree indices with some parameters, Math. Probl. Eng. (2021), https://doi.org/10.1155/2021/8417486.
[15] M. Rizwan, A.A. Bhatti, M. Javaid, E. Bonyah, Extremal values of variable sum exdeg index for conjugated bicyclic graphs, J. Chem. (2021), https://doi.org/10.1155/2021/4272208.
[16] X. Sun, J. Du, On variable sum exdeg indices of quasi-tree graphs and unicyclic graphs, Discrete Dyn. Nat. Soc. (2020), https://doi.org/10.1155/2020/1317295.

[17] J.M. Sigarreta, Extremal problems on exponential vertex-degree-based topological indices, Math. Biosci. Eng. (2022), https://doi.org/10.3934/mbe.2022329.
[18] J.M. Sigarreta, Mathematical properties of variable topological indices, Symmetry (2020), https://doi.org/10.3390/sym13010043.
[19] D. Vukicevic, Bond additive modelling 4. QSPR and QSAR studies of the variable Adriatic indices, Croat. Chem. Acta 41 (2011) 87–91, https://doi.org/10.5562/cca1666.
[20] D. Vukicevic, Bond additive modelling 5. Mathematical properties of the variable sum exdeg index, Croat. Chem. Acta 84 (2011) 93–101, https://doi.org/10.5562/cca1667.
[21] D. Vukicevic, Bond additive modelling 1. Mathematical properties of the variable sum exdeg index, Croat. Chem. Acta 83 (2010) 243–260, https://doi.org/10.5562/cca1667.
[22] H.V.D. Waterbeemd, R.E. Carter, G. Grassy, H. Kubiny, Y.C. Martin, M.S. Tutte, P. Willet, Glossary of terms used in computational drug design, Pure Appl. Chem. 69 (1997) 1137–1152, https://doi.org/10.1351/pac199769051137.
[23] Z. Yarahmadi, A.R. Ashrafi, The exdeg polynomial of some graph operations and applications in nanoscience, J. Comput. Theor. Nanosci. 12 (2015) 45–51, https://doi.org/10.1166/jctn.2015.3696.