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On the extremal graphs with respect to the variable sum exdeg index

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Abstract

The variable sum exdeg index of a graph G is defined as $\mathrm{SEI}_a(G) = \sum_{uv\in E(G)}(a^{d(u)} + a^{d(v)})$, where $d(u)$ is the degree of a vertex u and $a \neq 1$ is a positive real number. In [1], maximal trees, unicyclic and bicyclic graphs (i.e., graphs with cyclomatic number $0, 1$ and 2) and minimal trees and unicyclic graphs (i.e., graphs with cyclomatic number 0 and 1) with respect to variable sum exdeg index for $a > 1$ were determined. Here, we extend those results in two directions. Firstly, for $a > 1$, we characterize the extremal graphs with a cyclomatic number $k \leq n-2$, where n is the order of G. Secondly, for $0 < a < 1/e^2 \approx 0.135335$, we characterize the extremal graphs with $k \leq n-2$, and for $0 < a < 1/3$, we characterize the trees, unicyclic, bicyclic, tricyclic and tetracyclic graphs having maximal SEI_a value.

Keywords: chemical graph theory; topological index; variable sum exdeg index; extremal problem; cyclomatic number.

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1. Introduction and preliminaries

Chemical graphs have long been used to study molecules and macromolecules such as organic compounds, nucleic acids, and proteins. Vertices in a chemical graph correspond to the atoms while edges represent the covalent bonds between atoms [4, 10]. In theoretical chemistry, the physicochemical properties of chemical compounds are often modeled by the topological indices [3, 9]. Topological indices are numerical quantities of molecular graph, which are invariant under graph isomorphism [3]. In 2011, Vukičević [11] proposed the following topological index (and named it as the *variable sum exdeg index*) for predicting the octanol-water partition coefficient of certain chemical compounds:

$$\mathrm{SEI}_a(G) = \sum_{uv\in E(G)} (a^{d(u)} + a^{d(v)}),$$

where $a \neq 1$ is a positive real number, $E(G)$ is the edge set of the molecular graph G, $d(u)$ is degree of the vertex u. Among the set of 102 topological indices [8] proposed by the International Academy of Mathematical Chemistry [5] (respectively, among the discrete Adriatic indices [13]), the best topological index for predicting the octanol-water partition coefficient of octane isomers has 0.29 (respectively 0.36) coefficient of determination. While the variable sum exdeg index $\mathrm{SEI}_{0.37}$ has 0.99 coefficient of determination, for predicting the aforementioned property of octane isomers [11]. It is, therefore, interesting to study the mathematical properties of the variable sum exdeg index SEI_a, particularly the variable sum exdeg index $\mathrm{SEI}_{0.37}$. Vukičević [12] initiated the mathematical study of the variable sum exdeg index SEI_a. For $a > 1$, he found the extremal graphs with respect to the SEI_a among the classes of all n-vertex (i) connected graphs (ii) trees (iii) unicyclic graphs (iv) chemical graphs (v) chemical trees (vi) chemical unicyclic graphs (vii) graphs with given maximal degree (viii) graphs with given minimal degree (ix) trees with given number of pendant vertices (x) connected graphs with given number of pendant vertices. For $0 < a < 1$, the extremal graphs with respect to the SEI_a among the collections (iv), (v), (vi) were presented in [12] and characterizing the extremal graphs in the remaining seven collections was left as an open problem. Yarahmadi and Ashrafi [14] proposed a notion of the variable sum exdeg polynomial, studied the effects of this polynomial under some graph operations and investigated the behaviour of some nanotubes and nanotori under the aforementioned polynomial. Recently, Ghalavand and Ashrafi [1] found the extremal graphs with respect to the SEI_a (for $a > 1$) among the classes of all n-vertex trees and unicyclic graphs by using the majorization technique. The same authors also characterized the graphs having maximum SEI_a value (for $a > 1$) among the collections of all n-vertex bicyclic and tricyclic graphs. Recently Ali and Dimitrov [2] provided alternative proofs of four main results proved in [1] and extended the results

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from [1] for tetracyclic graphs. In [7], the problem of finding extremal graphs with respect variable sum exdeg index among the trees having vertices with prescribed degree was attempted.

Let G be a simple connected graph with the vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$. For $v_i \in V(G)$, let $d(v_i)$ (or simply d_i) denote the degree of v_i, that is, the number of edges incident to v_i. The sequence $D(G) = (d_1, d_2, \ldots, d_n)$ is called degree sequence of the graph G. In the rest of paper, it will be assumed that $d_1 \geq d_2 \geq \cdots \geq d_n$.

The variable sum exdeg index of G can be expressed as

$$\mathrm{SEI}_a(G) = \sum_{u \in V(G)} d(u) a^{d(u)} = \sum_{u \in V(G)} f_a(u).$$

The last equality indicates that the variable sum exdeg index with a given a depends only on the degree sequence of G.

In the sequel we present some notation that will be used in the rest of the paper.

The *cyclomatic number* (or the *circuit rank*) of an undirected graph G is the minimum number of edges whose removal from G breaks all its cycles, making it into a tree or a forest. The cyclomatic number r can be expressed as $r = |E(G)| - |V(G)| + |C(G)|$, where $|C(G)|$ is the number of connected components of G. Since we are interested in connected graphs, we will assume that $|C(G)| = 1$. Connected graphs with $r = 0, 1, 2, 3$ are also called *trees, unicyclic, bicyclic* and *tricyclic* graphs. As usual, the n-vertex star graph is denoted by S_n. The unique n-vertex unicyclic graph obtained from S_n by adding an edge is denoted by S_n^+.

A function $f(x)$ is *convex* on an interval $[a, b]$ if for any x_1 and x_2 in $[a, b]$ and any λ, where $0 < \lambda < 1$, $f(\lambda x_1 + (1 - \lambda)x_2) \leq \lambda f(x_1) + (1 - \lambda) f(x_2)$. If the inequality above is strict for all x_1 and x_2, then $f(x)$ is called *strictly convex*. If the sign of the inequality is reversed, the function is called *(strictly) concave*.

Let $x = (x_1, x_2, ..., x_n)$ and $y = (y_1, y_2, ..., y_n)$ be non-increasing sequences of real numbers. Then x *majorizes* y if, for each $k = 1, 2, \ldots, n$, $\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{k} y_i$, with equality if $k = n$, and we write $x \succcurlyeq y$. If $x \neq y$, we write $x \succ y$.

The next inequality, known as Karamata's inequality [6], plays an important role in deriving the main result of this note.

Theorem 1.1. *Let $U \subseteq \mathbb{R}$ be an open interval and $f : U \to U$ a convex function. Let $x = (x_1, x_2, ..., x_n)$ and $y = (y_1, y_2, ..., y_n)$ be two non-increasing sequences in U. If $x \succcurlyeq y$ then $\sum_{i=1}^{n} f(x_i) \geq \sum_{i=1}^{n} f(y_i)$. Moreover, if f is a strictly convex function, then the above inequality holds with equality if and only if $x = y$, and the inequality is reversed if f is concave.*

In this work, firstly, we extend the work of Ghalavand and Ashrafi [1] by characterizing the extremal graphs with a cyclomatic number $k \leq n - 2$ with respect to the SEI_a, for $a > 1$. We obtain those characterizations also by applying the majorization technique and the Karamata's inequality.

Next, we characterize the extremal graphs with a cyclomatic number $k \leq n - 2$ with respect to the SEI_a, for $0 < a < 1/e^2 \approx 0.135335$. It turns out that for the case $1/e^2 \approx 0.135335 < a < 1$, the majorization technique is not applicable. Instead, here, we show a certain property of the graphs with maximal SEI_a, which significantly reduces the searching space within the considered family of graphs. With help of this property, we characterize trees, unicyclic, bicyclic, tricyclic and tetracyclic graphs with maximal SEI_a, for $0 < a < 1/3$. Thereby, we give (partial) solutions to some uncovered cases and open problems from [1, 12].

2. Extremal graphs with cyclomatic number k

2.1 Extremal graphs for $a > 1$

The following theorem was presented in [1] and it will be used in the proofs in the rest of this paper.

Theorem 2.1. *Let G and G' be two simple connected graphs with degree sequences $D(G) = (d_1, d_2, \ldots, d_n)$ and $D(G') = (d'_1, d'_2, \ldots, d'_n)$. If $a > 1$ and $D(G) \succcurlyeq D(G')$ then $\mathrm{SEI}_a(G) \geq \mathrm{SEI}_a(G')$ with equality if and only if $D(G) = D(G')$.*

Next, we characterize the graphs with maximal variable sum exdeg index with an cyclomatic number k.

Theorem 2.2. *Among all graphs with n vertices and cyclomatic number k, $1 \leq k \leq n - 2$, a graph G_k with the degree sequence $D(G_k) = (n - 1, k + 1, \underbrace{2, \ldots, 2}_{k}, \underbrace{1, \ldots, 1}_{n-k-2})$ has the maximal variable sum exdeg index for $a > 1$.*

Proof. Let G an arbitrary connected simple graph with n vertices and with cyclomatic number k, which is different than G_k with $D(G) = (d'_1, d'_2, \ldots, d'_n)$. It holds that $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i = 2n + 2k - 2$ and that at least $k + 2$ vertices of G have degree at least 2.

We show that $D(G_k) \succ D(G)$, by considering few cases with respect to the value of the index j in the sums $\sum_{i=1}^{j} d_i$ and $\sum_{i=1}^{j} d'_i$.

For $j = 1$, it holds that $d_1 \geq d'_1$, since $d_1 = n - 1$.

For $j = 2$ we have that $d'_1 + d'_2 \leq 2n + 2k - 2 - 2k - (n - k - 2) = n + k$. It holds that $d_1 + d_2 = n + k$, and thus $d_1 + d_2 \geq d'_1 + d'_2$.

Consider now the case $3 \leq j \leq k+2$. Here we have that $\sum_{i=1}^{j} d'_i \leq 2n+2k-2-2(k+2-j)-(n-k-2) = n+k+2j-4$. On the other hand $\sum_{i=1}^{j} d_i = n-1+k+1+2(j-2) = n+k+2j-4$. Therefore, also in this case we have $\sum_{i=1}^{j} d_i \geq \sum_{i=1}^{j} d'_i$.

The last case is when $k + 3 \leq j \leq n$. Then, $\sum_{i=1}^{j} d'_i \leq 2n + 2k - 2 - (n - j) = n + 2k + j - 2$. We have that $\sum_{i=1}^{j} d_i = n - 1 + k + 1 + 2k + (j - k - 2) = n + 2k + j - 2$, and consequently also in this case holds $\sum_{i=1}^{j} d_i \geq \sum_{i=1}^{j} d'_i$.

Thus, we have shown that $\sum_{k=1}^{i} d_k \geq \sum_{k=1}^{i} d'_k$, for any $i \in [1, n]$, or that $D(G_k) \succ D(G)$. By Theorem 2.1 we have that $\mathrm{SEI}_a(G_k) > \mathrm{SEI}_a(G)$. □

As special instances of Theorem 2.2 we have the following corollaries.

Corollary 2.1. *Among all trees graphs, a star graph S_n with the degree sequence $(n-1, \underbrace{1, \ldots, 1}_{n-1})$ has the maximal variable sum exdeg index for $a > 1$.*

Corollary 2.2. *Among all unicyclic graphs, a graph U_n with the degree sequence $(n-1, 2, 2, \underbrace{1, \ldots, 1}_{n-3})$ has the maximal variable sum exdeg index for $a > 1$.*

Corollary 2.3. *Among all bicyclic graphs, a graph with the degree sequence $(n-1, 3, 2, 2, \underbrace{1, \ldots, 1}_{n-4})$ has the maximal variable sum exdeg index for $a > 1$.*

Corollary 2.4. *Among all tricyclic graphs, a graph with the degree sequence $(n-1, 4, 2, 2, 2, \underbrace{1, \ldots, 1}_{n-5})$ has the maximal variable sum exdeg index for $a > 1$.*

We would like to note that Corollaries 2.1, 2.2 and 2.3 coincide with the main results from [1]. However, in [1] it was claimed that among tricyclic graphs, a graph with the degree sequence $(n-1, 3, 3, 2, 2, \underbrace{1, \ldots, 1}_{n-5})$ has the maximal variable sum exdeg index for $a > 1$. A direct calculation shows that a graph with the degree sequence $(n-1, 4, 2, 2, 2, \underbrace{1, \ldots, 1}_{n-5})$ has a larger maximal variable sum exdeg index.

Next, we characterize the graphs with minimal variable sum exdeg index with an cyclomatic number k.

Theorem 2.3. *Let G_k be a graph with n vertices, cyclomatic number k, $1 \leq k \leq n-2$, that has the minimal variable sum exdeg index for $a > 1$. Let $x = \lfloor \frac{2n+2k-2}{n} \rfloor$ and $y \equiv 2n + 2k - 2n$. Then, $D(G_k) = (\underbrace{x+1, \ldots, x+1}_{y}, \underbrace{x, \ldots, x}_{n-y})$.*

Proof. Let G an arbitrary connected simple graph with n vertices and with cyclomatic number k, which is different than G_k with $D(G) = (d'_1, d'_2, \ldots, d'_n)$. Let denote the degree sequence of G_k as $D(G_k) = (d_1, d_2, \ldots, d_n)$.

Observe that when the sum of degrees of G_k, $2n + 2k - 2$ is divisible by n then $y = 0$, and $D(G_k) = (\underbrace{x, \ldots, x}_{n})$.

Assume that there are l_1 degrees in G that have degree larger than $x + 1$ (or x, when $2n + 2k - 2$ is divisible by n), l_2 degrees in G are same as in G_k, and l_3 degrees in G are smaller than x. It holds that $x + 1$ (or x, when $2n + 2k - 2$ is divisible by n) is the smallest maximal degree that a graph with a cyclomatic number k can have. Thus, it follows that $l_1, l_3 > 0$. It holds that

$$\sum_{i=1}^{l_1} d'_i > \sum_{i=1}^{l_1} d_i, \qquad \sum_{i=l_1+l_2+1}^{n} d'_i < \sum_{i=l_1+l_2+1}^{n} d_i,$$
$$\sum_{i=l_1+1}^{l_1+l_2} d'_i = \sum_{i=l_1+1}^{l_1+l_2} d_i, \quad \text{and} \tag{1}$$
$$\sum_{i=1}^{l_1} d'_i + \sum_{i=l_1+l_2+1}^{n} d'_i = \sum_{i=1}^{l_1} d_i + \sum_{i=l_1+l_2+1}^{n} d_i. \tag{2}$$

Since $d_n = x$ and $d'_n < x$, we have from (2)

$$\sum_{i=1}^{l_1} d'_i + \sum_{i=l_1+l_2+1}^{n-1} d'_i > \sum_{i=1}^{l_1} d_i + \sum_{i=l_1+l_2+1}^{n-1} d_i. \tag{3}$$

From (1) and (3), it follows that

$$\sum_{i=1}^{n-1} d'_i \; > \; \sum_{i=1}^{n-1} d_i.$$

Together with $\sum_{i=1}^{n} d'_i = \sum_{i=1}^{n} d_i$, it follows that $D(G) \succ D(G_k)$, and thus, by Theorem 2.1 $\mathrm{SEI}_a(G) < \mathrm{SEI}_a(G_k)$. □

As special instances of Theorem 2.3, we have the following corollaries.

Corollary 2.5. *Among all unicyclic graphs the cyclic graph C_n has the minimal variable sum exdeg index for $a > 1$.*

Corollary 2.6. *Among all bicyclic graphs a graph with the degree sequence $(3, 3, \underbrace{2, \ldots, 2}_{n-2})$ has the minimal variable sum exdeg index for $a > 1$.*

Corollary 2.7. *Among all tricyclic graphs a graph with the degree sequence $(3, 3, 3, 3, \underbrace{2, \ldots, 2}_{n-4})$ has the minimal variable sum exdeg index for $a > 1$.*

We would like to note that Corollaries 2.5 and 2.6 coincide with the main results from [1].

In the next section, we consider the extremal graphs with respect to the variable sum exdeg index for $0 < a < 1$, the interval that was not considered before. Here, we characterize the extremal trees, unicyclic, bicyclic, tricyclic and tetracyclic graphs.

2.2 Extremal graphs for $0 < a < 1$

The first and the second derivative of the function $f_a(x) = xa^x$ are

$$\frac{d\,f_a(x)}{d\,x} = a^x + a^x x \ln a \qquad \text{and} \qquad \frac{d^2\,f_a(x)}{d\,x^2} = 2a^x \ln a + a^x x (\ln a)^2.$$

The maximum of $f_a(x)$ is reached at $x = -1/\ln a$ and it has one inflection point at $x = -2/\ln a$. Thus, the function is increasing for $0 < x < -1/\ln a$ decreasing for $x > -1/\ln a$, for $0 < x < -2/\ln a$ it si concave, while for $x > -2/\ln a$ it is convex. Thus, for $0 < a < 1$ is in general neither concave nor convex. As consequence, we cannot apply the above used majorization technique for all $a \in (0, 1)$. Instead, we consider subintervals of $(0, 1)$. First, we consider when $a \in (0, 1/e^2) \approx (0, 0.135335)$.

Theorem 2.4. *Among all graphs with n vertices and cyclomatic number k, $1 \le k \le n-2$, a graph G_k with the degree sequence $D(G_k) = (n-1, k+1, \underbrace{2, \ldots, 2}_{k}, \underbrace{1, \ldots, 1}_{n-k-2})$ has the maximal variable sum exdeg index for $0 < a < 1/e^2 \approx 0.135335$.*

Proof. For $a < 1/e^2$ the inflection point of $f_a(x)$ is smaller than 1, and thus, for $x > 1$ the function $f_{a<0.135335}(x)$ is convex. The rest of the proof is identical with the proof of Theorem 2.2. □

The proof of the following result follows also from the fact that $f_{a<0.135335}(x)$ is convex and from the proof of Theorem 2.3, and therefore, it will be omitted.

Theorem 2.5. *Let G_k be a graph with n vertices, cyclomatic number k, $1 \le k \le n-2$, that has the minimal variable sum exdeg index for $0 < a < 1/e^2 \approx 0.135335$. Let $x = \lfloor \frac{2n+2k-2}{n} \rfloor$ and $y \equiv 2n + 2k - 2n$. Then, $D(G_k) = (\underbrace{x+1, \ldots, x+1}_{y}, \underbrace{x, \ldots, x}_{n-y})$.*

Next, we show the following property of the extremal graphs in this case $0 < a < 1/3$, which significantly reduces the searching space within the family of trees, unicyclic, bicyclic, tricyclic and tetracyclic graphs.

Lemma 2.1. *Let G be a graph with n vertices and cyclomatic number k, $1 \le k \le \binom{n}{2} - n + 1$ a graph G_k. If G has maximal variable sum exdeg index for $0 < a < 1/3$, then maximal degree in G is n-1.*

Proof. For $a < 1/e \approx 0.367879$, $f_a(x)$, $x > 1$ is decreasing. For $a < 1/3$, $f(x)$ has its maximum for $x_m < 0.91024$ and the inflection point $x_i < 1.82048$. The function $f_a(x)$ for $0 < x < x_m$ is concave, while for $x > x_m$ is convex. For $a < 1/3$, it holds

$$f_a(1) - f_a(2) > f_a(2) - f_a(3) \qquad \text{and} \qquad f_a(2) - f_a(3) > f_a(3) - f_a(4). \tag{4}$$

The slope of $f_a(x)$, $f_a'(x)$ is maximal for $x_i = 1.82048$ and it is decreasing function for $x > x_i$. This together with (4) implies

$$\begin{aligned} f_a(k-1) - f_a(k) &> f_a(l) - f_a(l+1), \quad \text{for } l \geq k \geq 2, \\ f_a(k-s) - f_a(k) &> f_a(l) - f_a(l+s), \quad \text{for } l \geq k \geq s+1. \end{aligned} \tag{5}$$

Suppose that the statement of the theorem is false and G has maximal degree at most $n-2$. Let u be a vertex of G with maximum degree. The assumption $d(u) \leq n-2$ implies that there exists a vertex $v_1 \in V(G)$, which is not adjacent with u. Let v be a non-pendent neighbor of v_1. Then, $N(v) \setminus N(u)$ is not-empty. Here, $N(x)$ denotes the neighbors of a vertex x. Let $N(v) \setminus N(u) = \{v_1, v_2, \ldots, v_s\}$. Suppose that G' is the graph obtained from G by removing the edges $vv_1, vv_2, \ldots, vv_s$ and adding the edges $uv_1, uv_2, \ldots, uv_s$. Then,

$$\begin{aligned} \mathrm{SEI}_a(G') - \mathrm{SEI}_a(G) &= f(d(v)-s) + f(d(u)+s) - f(d(v)) - f(d(u) \\ &= f(d(v)-s) - f(d(v)) - (f(d(u)) - f(d(u)+s)). \end{aligned} \tag{6}$$

From (5) it follows that (6) is larger than 0, and thus $\mathrm{SEI}_a(G') > \mathrm{SEI}_a(G)$, which is a contradiction to the initial assumption that G is a graph maximal variable sum exdeg index. □

Now, we can obtain trees, unicyclic, bicyclic, tricyclic and tetracyclic graphs with maximum value of the SEI_a, $0 < a < 1/3$. Recall that by S_n^+, we denote the unique n-vertex unicyclic graph obtained from S_n by adding an edge.

Theorem 2.6. *For $0 < a < 1/3$, the graphs S_n, S_n^+, B_1 (depicted in Figure 1) have the maximum SEI_a values among trees, unicyclic, and bicyclic graphs, respectively. For $\frac{1}{4} \leq a < \frac{1}{3}$ and for $0 < a \leq \frac{1}{4}$ the graphs G_4 and G_5 (depicted in Figure 2), respectively, have the maximum SEI_a values among tricyclic graphs. For $0.22042795720542145 < a < \frac{1}{3}$ and for $0 < a < 0.22042795720542144$ the graphs H_4 and H_5 (depicted in Figure 3), respectively, have the maximum SEI_a values among tetracyclic graphs.*

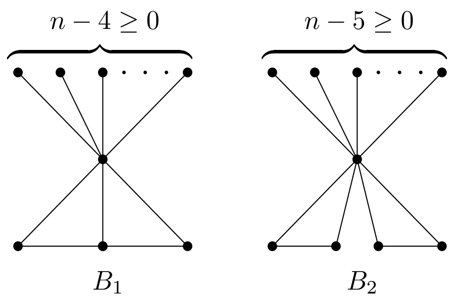

Figure 1: All non-isomorphic n-vertex bicyclic graphs with maximum degree $n-1$.

Proof. Due to Lemma 2.1, we need to consider only those graphs, which have at least one vertex of degree $n-1$. There is only one n-vertex tree, unicyclic graph, namely S_n, S_n^+ respectively, having maximum vertex degree $n-1$. Also, there are only two non-isomorphic n-vertex bicyclic graphs B_1 and B_2, depicted in Figure 1. Moreover, all the non-isomorphic n-vertex tricyclic graphs $G_1, G_2, ..., G_5$ and all the non-isomorphic n-vertex tetracyclic graphs $H_1, H_2, ..., H_{11}$ are shown in Figure 2 and Figure 3, respectively. Routine calculations yield: $\mathrm{SEI}_a(B_1) - \mathrm{SEI}_a(B_2) = a(1-4a+3a^2)$, $\mathrm{SEI}_a(G_4) - \mathrm{SEI}_a(G_1) = 2a(1-3a+2a^3)$, $\mathrm{SEI}_a(G_4) - \mathrm{SEI}_a(G_2) = a(1-2a-3a^2+4a^3)$, $\mathrm{SEI}_a(G_4) - \mathrm{SEI}_a(G_3) = 2a^2(1-3a+2a^2)$, which are all positive for $a < 1/3$. Also,

$$\mathrm{SEI}_a(G_4) - \mathrm{SEI}_a(G_5) = a(-1+6a-9a^2+4a^3) \begin{cases} > 0 & \text{for } \frac{1}{4} < a < \frac{1}{3}, \\ < 0 & \text{for } 0 < a < \frac{1}{4}, \\ = 0 & \text{for } a = \frac{1}{4}. \end{cases}$$

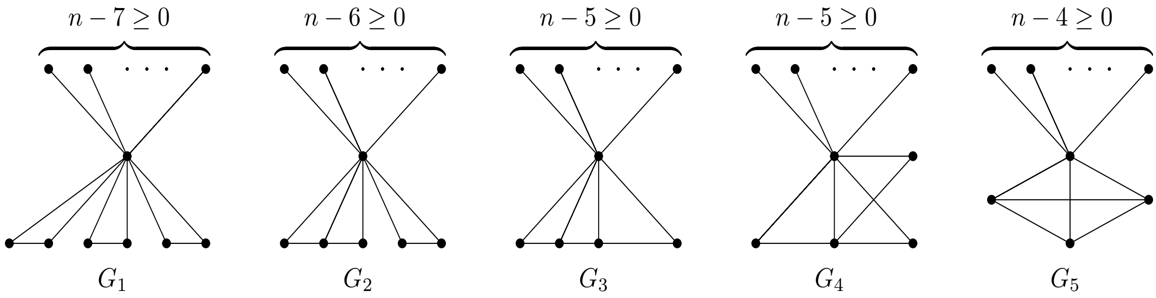

Figure 2: All non-isomorphic n-vertex tricyclic graphs with maximum degree $n-1$.

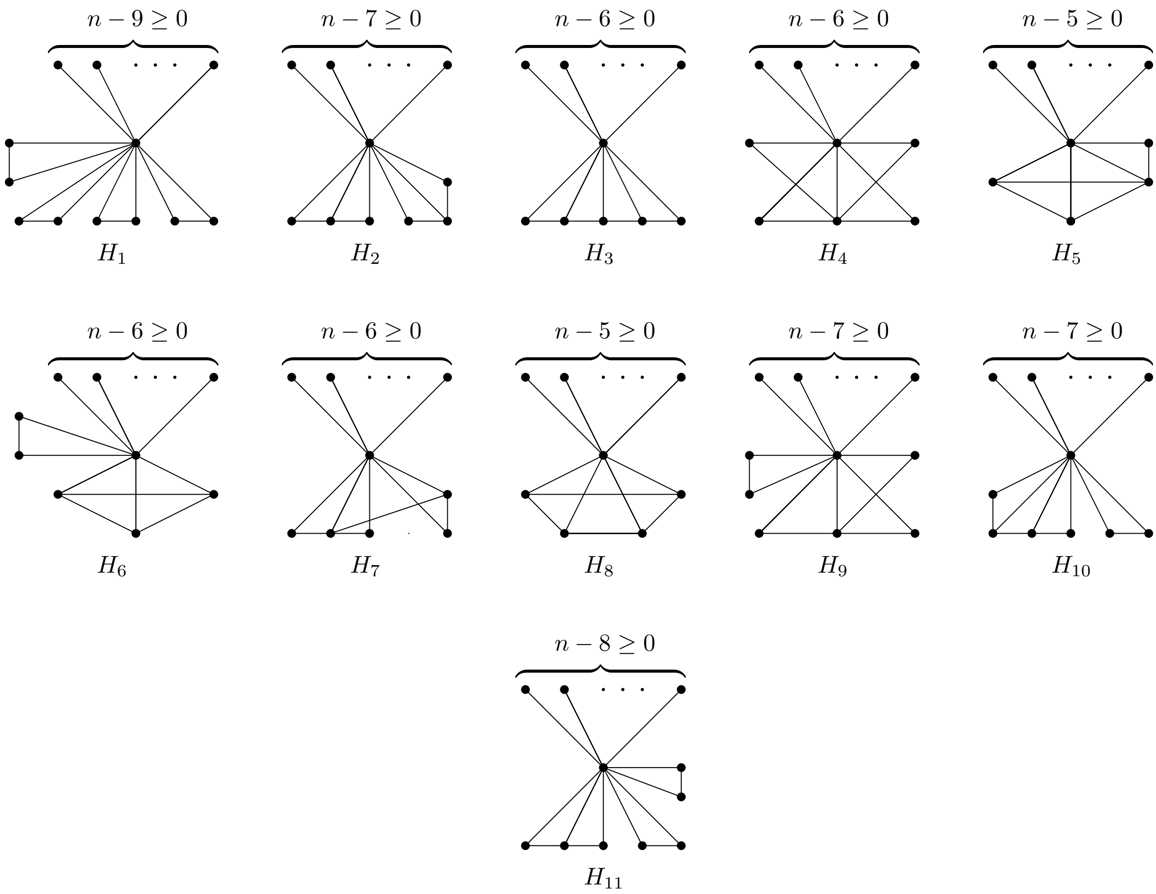

Figure 3: All non-isomorphic n-vertex tetracyclic graphs with maximum degree $n-1$.

After similar calculations, we obtain $\mathrm{SEI}_a(H_5)-\mathrm{SEI}_a(H_8)>0$ and $\mathrm{SEI}_a(H_4)-\mathrm{SEI}_a(H_i)>0$, where $i\in\{1,2,3,...,11\}\setminus\{5,8\}$ and $0<a<1/3$. Furthermore,

$$\mathrm{SEI}_a(H_4)-\mathrm{SEI}_a(H_5)=a(-1+6a-6a^2-4a^3+5a^4)\begin{cases}>0 & \text{for } 0.22042795720542145<a<\frac{1}{3},\\ <0 & \text{for } 0<a<0.22042795720542144.\end{cases}$$

Observe that the exact solution of the equality $-1+6a-6a^2-4a^3+5a^4=0$ (the case when $\mathrm{SEI}_a(G_4)=\mathrm{SEI}_a(G_5)$), for $a\in(0,1/3]$, has infinite decimal representations and it lies in the interval $(0.22042795720542144, 0.22042795720542145)$. $\square$

3. Concluding comments

By using the majorization technique, we have determined the graphs having maximal and minimal variable sum exdeg index SEI_a from the class of graphs with n vertices and k cyclomatic number for $0<a<1/e^2\approx 0.135335$ and $a>1$. It turns out that for the case $1/e^2\approx 0.135335<a<1$, the majorization technique is not applicable. Instead, here, we show a certain property of the graphs with maximal SEI_a, which significantly reduces the searching space within the considered family of graphs. With help of this property, we characterize trees, unicyclic, bicyclic, tricyclic and tetracyclic graphs with maximal SEI_a, for $0<a<1/3$. Consequently, we give (partial) solutions to some uncovered cases and open problems from [1, 12].

We would like to mention that the problem of finding the extremal graphs with respect to the variable sum exdeg index SEI_a, $1/e^2<a<1$, having a fixed cyclomatic number is open. Theorem 2.6 provides a step towards its solution.

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