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A note on the variable sum exdeg index/coindex of trees

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Abstract

The variable sum exdeg index is a graph invariant introduced in 2011 for the purpose of predicting a particular physico-chemical property, namely the octanol-water partition coefficient, of certain molecules. The variable sum exdeg coindex has recently been devised by making some modifications in the definition of the variable sum exdeg index. The primary aim of this note is to establish several mathematical inequalities involving the aforementioned two graph invariants for the case of (chemical) trees.

Keywords: chemical graph theory; topological index; variable sum exdeg index; variable sum exdeg coindex; tree.

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1. Introduction

In graph theory, an invariant is a numerical quantity of graphs that depends only on their abstract structure, not on labeling of vertices or edges, or on the drawings of the graphs. In chemical graph theory, such quantities are usually referred to as topological indices [7, 17, 18]. Many of them are defined as simple functions of the degrees of the vertices of (chemical) graph. Most degree-based topological indices are viewed as the contributions of pairs of adjacent vertices. But, equally important are the degree-based topological indices that are defined over non-adjacent pairs of vertices for computing some topological properties of graphs, and such topological indices are named as coindices.

Let G be a graph with the vertex set $V = \{v_1, v_2, \dots, v_n\}$, edge set E and with the vertex-degree sequence $(d_1, d_2, \cdots, d_n)$ satisfying $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, where $n \geq 2$, $|E| = m$ and d_i is the degree of the vertex v_i for $i = 1, 2, \cdots, n$. If v_i and v_j are adjacent in G, we write $i \sim j$, otherwise we write $i \nsim j$. Denote by $\overline{G}$ the complement of G and $D = \mathrm{diag}(d_1, d_2, \dots, d_n)$ the diagonal degree matrix of G. The cyclomatic number of G is the minimum number of edges whose removal makes G as an acyclic graph (that is, a graph containing no cycle). Graphs having the cyclomatic numbers 0, 1, 2, 3, and 4 are known as the tree, unicyclic, bicyclic, tricyclic, and tetracyclic graphs, respectively.

One of the most popular and extensively studied topological indices is the first Zagreb index, appeared in the formula that was derived within a study of molecular modeling [9]. For the graph G, the first Zagreb index is denoted by $M_1(G)$ and is defined as

$$M_1(G) = \sum_{i=1}^{n} d_i^2 = \sum_{i\sim j}(d_i + d_j)\,.$$

The variable sum exdeg index is a degree-based topological index, introduced in [19] about a decade ago, for the purpose of predicting the octanol-water partition coefficient of certain molecules. The variable sum exdeg index of the graph G is denoted by $SEI_a(G)$ and is defined as

$$SEI_a(G) = \sum_{i=1}^{n} d_i a^{d_i} = \sum_{i\sim j}(a^{d_i} + a^{d_j}),$$

where 'a' is an arbitrary positive real number distinct from 1.

The primary motivation of analyzing the topological index SEI_a was its very good chemical applicability [19]. Due to its chemical applications, SEI_a attained a considerable attention from researchers, especially from mathematicians. The very first paper devoted to the mathematical aspects of SEI_a is [20], where several extremal results regarding SEI_a were obtained. Yarahmadi and Ashrafi [21] proposed and analyzed the variable sum exdeg polynomial. For $a > 1$, graphs attaining the extremum (maximum and minimum) values of SEI_a among all tree/unicyclic graphs of a fixed order were determined in [6]. For $a > 1$, graphs attaining the maximum values of SEI_a among all bicyclic/tricyclic graphs of a fixed

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order were also found in [6]. Ali and Dimitrov [1] gave alternative proofs of some of the main results of [6], and also they proved an extremal result regarding the variable sum exdeg index of tetracyclic graphs. For $a > 1$, the results of [1, 6] were generalized by Damitov and Ali [3] by considering the graphs of a fixed order and cyclomatic number; in [3], the case $0 < a < 1$ was also discussed but only the partial solutions to the considered problems for this certain case were obtained. The problem of finding graphs having the extremum values of the variable sum exdeg index of the trees of a fixed order and with the vertices having prescribed degrees was attacked in [12]. Further recent results about SEI_a can be found in the recent papers [2, 5, 10, 16].

The concept of the topological indices defined over non-adjacent pairs of vertices was introduced in [4]. In this case, the sum runs over the edges of the complement of G. By analogy with $SEI_a(G)$, we define the corresponding variable sum exdeg coindex, $\overline{SEI}_a(G)$, as

$$\overline{SEI}_a(G) = \sum_{i \nsim j}(a^{d_i} + a^{d_j}) = \sum_{i=1}^{n}(n-1-d_i)a^{d_i}.$$

In the remaining part of this paper, we assume that $G \cong T$ is a tree. In this note, we determine several sharp bounds on the invariants $SEI_a(T)$ and $\overline{SEI}_a(T)$. Also, some relations between these invariants are established. Most of the obtained results are sharp also for the chemical trees.

2. Preliminaries

Let f be a convex function on the interval $I \subset \mathbb{R}$, $x = (x_1, x_2, \ldots, x_n) \in I^n$, $n \geq 2$, and $p = (p_1, p_2, \ldots, p_n)$ be a positive n-tuple. Then the following inequality holds [13]

$$\sum_{i=1}^{n} p_i f(x_i) \geq P_n f\left(\frac{\sum_{i=1}^{n} p_i x_i}{P_n}\right), \tag{1}$$

where $P_n = \sum_{i=1}^{n} p_i$. If f is concave, the opposite inequality in (1) is valid. Equality sign in (1) holds if and only if $x_1 = x_2 = \cdots = x_n$.

As a special case of (1) (see e.g. [13, 14]) the following result is obtained.

Let $p = (p_i)$, $i = 1, 2, \ldots, n$, be a sequence of non-negative real numbers, and let $a = (a_i)$, $i = 1, 2, \ldots, n$, be a sequence of positive real numbers. Then for any real number r satisfying $r \leq 0$ or $r \geq 1$, it holds that

$$\left(\sum_{i=1}^{n} p_i\right)^{r-1} \sum_{i=1}^{n} p_i a_i^r \geq \left(\sum_{i=1}^{n} p_i a_i\right)^r. \tag{2}$$

When $0 \leq r \leq 1$, the opposite inequality in (2) is valid. Equality sign in (2) holds if and only if $r = 0$, or $r = 1$, or $a_1 = a_2 = \cdots = a_n$, or $p_1 = p_2 = \cdots = p_t = 0$ and $a_{t+1} = \cdots = a_n$ for some t satisfying the inequality $1 \leq t \leq n-1$.

Note that inequalities (1) and (2) are the generalizations of Jensen's inequality, which was proven in [11].

3. Main results

Firstly, we establish a lower bound for $SEI_a(T)$ in terms of $\det D$, n and Δ, where T is a tree.

Theorem 3.1. *Let T be a tree with $n \geq 4$ vertices. Then for any $a > 0$, $a \neq 1$, it holds that*

$$SEI_a(T) \geq \Delta a^{\Delta} + 2a + (n-3)a^{\frac{2n-\Delta-4}{n-3}}\left(\frac{\det D}{\Delta}\right)^{\frac{1}{n-3}}, \tag{3}$$

where the equality sign holds if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$.

Proof. The arithmetic–geometric mean inequality, AM–GM (see e.g. [14]), can be considered as

$$\sum_{i=2}^{n-2} a_i \geq (n-3)\left(\prod_{i=2}^{n-2} a_i\right)^{\frac{1}{n-3}}.$$

Now, for $a_i := d_i a^{d_i}$, $i = 2, \ldots, n-2$, $a > 0$, $a \neq 1$, the above inequality gives

$$\sum_{i=2}^{n-2} d_i a^{d_i} \geq (n-3)\left(\prod_{i=2}^{n-2} d_i a^{d_i}\right)^{\frac{1}{n-3}} = (n-3)a^{\frac{d_2+\cdots+d_{n-2}}{n-3}}\left(\prod_{i=2}^{n-2} d_i\right)^{\frac{1}{n-3}},$$

that is

$$\sum_{i=1}^{n} d_i a^{d_i} \geq \Delta a^{\Delta} + d_{n-1} a^{d_{n-1}} + d_n a^{d_n} + (n-3) a^{\frac{2m-\Delta-d_{n-1}-d_n}{n-3}} \left(\frac{\det D}{\Delta d_{n-1} d_n} \right)^{\frac{1}{n-3}} . \tag{4}$$

Since T is a tree, it has at least two vertices of degree 1. Therefore $d_n = d_{n-1} = 1$ and $m = n-1$, and from (4) we obtain (3).

Equality in (4) is attained if and only if $\Delta a^{\Delta} \geq d_2 a^{d_2} = \cdots = d_{n-2} a^{d_{n-2}} \geq a$. If $d_{n-2} \neq 1$, then $T \cong P_n$, since P_n is the only tree with exactly two vertices of degree 1. If $d_2 = \cdots = d_{n-2} = 1$, then $\Delta = n-1$, i.e. $T \cong K_{1,n-1}$. □

In the next theorem, we determine lower bound for $SEI_a(T)$ in terms of $M_1(T)$ and parameter n.

Theorem 3.2. *Let T be a tree with $n \geq 3$ vertices. Then for any $a > 1$, the following inequality holds*

$$SEI_a(T) \geq 2a + 2(n-2) a^{\frac{M_1(T)-2}{2n-4}} . \tag{5}$$

Equality holds if and only if $T \cong P_n$.

Proof. For $a > 1$ the function $f(x) = a^x$ is convex for $x \geq 0$. Therefore, for $p_i = x_i = d_i$, $i = 1, 2, \ldots, n-2$, according to (1) we have

$$\sum_{i=1}^{n-2} d_i a^{d_i} \geq \left(\sum_{i=1}^{n-2} d_i \right) a^{\frac{d_1^2 + \cdots + d_{n-2}^2}{d_1 + \cdots + d_{n-2}}} ,$$

that is

$$\sum_{i=1}^{n} d_i a^{d_i} - d_{n-1} a^{d_{n-1}} - d_n a^{d_n} \geq (2m - d_{n-1} - d_n)\, a^{\frac{M_1(G) - d_{n-1}^2 - d_n^2}{2m - d_{n-1} - d_n}} . \tag{6}$$

Since T is a tree, it has at least two vertices of degree 1, $d_n = d_{n-1} = 1$. Since $m = n-1$, from (6) we obtain

$$SEI_a(T) - 2a \geq 2(n-2) a^{\frac{M_1(T)-2}{2n-4}} ,$$

from which we arrive at (5).

Equality in (6) is attained if and only if $d_1 = d_2 = \cdots = d_{n-2}$, therefore equality in (5) holds if and only if $T \cong P_n$. □

Corollary 3.1. *If T is a tree with $n \geq 2$ vertices then for any $a > 1$, it holds that*

$$SEI_a(T) \geq 2a + 2(n-2) a^2 . \tag{7}$$

Equality holds if and only if $T \cong P_n$.

Proof. In [8] it was proven

$$M_1(T) \geq 4n - 6 = M_1(P_n).$$

From the above and (5) we obtain (7). □

The inequality (7) was proven in [20].

By a similar arguments as in Theorem 3.2 the following result can be proven.

Theorem 3.3. *Let T be a tree with $n \geq 4$ vertices. Then for any $a > 1$, it holds that*

$$SEI_a(T) \geq \Delta a^{\Delta} + 2a + (2n - \Delta - 4) a^{\frac{M_1(T) - \Delta^2 - 2}{2n - \Delta - 4}} .$$

Equality holds if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$.

In the next theorem, we prove the Nordhaus–Gaddum type inequality [15] for the topological index $SEI_a(T)$ and coindex $\overline{SEI}_a(T)$.

Theorem 3.4. *Let T be a tree with $n \geq 4$ vertices. Then for any $a > 0$, $a \neq 1$, the following inequality holds*

$$SEI_a(T) + \overline{SEI}_a(T) \geq (n-1) \left(a^{\Delta} + 2a + (n-3) a^{\frac{2n-4-\Delta}{n-3}} \right) . \tag{8}$$

Equality holds if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$.

Proof. Since

$$\overline{SEI}_a(T) = \sum_{i=1}^{n}(n-1-d_i)a^{d_i} = (n-1)\sum_{i=1}^{n} a^{d_i} - \sum_{i=1}^{n} d_i a^{d_i},$$

we have that

$$SEI_a(T) + \overline{SEI}_a(T) = (n-1)\sum_{i=1}^{n} a^{d_i}. \tag{9}$$

On the other hand, by arithmetic–geometric mean inequality, we get

$$\sum_{i=2}^{n-2} a^{d_i} \geq (n-3)\left(\prod_{i=2}^{n-2} a^{d_i}\right)^{\frac{1}{n-3}},$$

i.e.

$$\sum_{i=1}^{n} a^{d_i} \geq a^{d_1} + a^{d_{n-1}} + a^{d_n} + (n-3)a^{\frac{2m-d_1-d_{n-1}-d_n}{n-3}}.$$

For $m = n-1$, $d_1 = \Delta$, $d_{n-1} = d_n = 1$, the above inequality gives

$$\sum_{i=1}^{n} a^{d_i} \geq a^{\Delta} + 2a + (n-3)a^{\frac{2n-\Delta-4}{n-3}}. \tag{10}$$

According to (10) and (9) we arrive at (8).

Equality in (10) holds if and only if $\Delta = d_1 \geq d_2 = \cdots = d_{n-2} \geq 1$, therefore equality in (8) holds if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$ (see the proof for the equality case in (3)). □

The proofs of the following theorems are analogous to that of Theorem 3.4, thus omitted.

Theorem 3.5. *Let T be a tree with $n \geq 3$ vertices. Then for any $a > 0$, $a \neq 1$, it holds that*

$$SEI_a(T) + \overline{SEI}_a(T) \geq (n-1)\left(2a + (n-2)a^2\right).$$

Equality holds if and only if $T \cong P_n$.

Theorem 3.6. *Let T be a tree with $n \geq 4$ vertices. Then for any $a > 0$, $a \neq 1$, the following inequality holds*

$$SEI_a(\overline{T}) + \overline{SEI}_a(\overline{T}) \geq (n-1)a^{n-1}\left(a^{-\Delta} + 2a^{-1} + (n-3)a^{\frac{\Delta+4-2n}{n-3}}\right).$$

Equality holds if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$.

Theorem 3.7. *Let T be a tree with $n \geq 3$ vertices. Then for any $a > 0$, $a \neq 1$, it holds that*

$$SEI_a(\overline{T}) + \overline{SEI}_a(\overline{T}) \geq (n-1)a^{n-3}\left(2a + n - 2\right).$$

Equality holds if and only if $T \cong P_n$.

Theorem 3.8. *Let T be a tree with $n \geq 3$ vertices. Then for any $a > 0$, $a \neq 1$, it holds that*

$$SEI_a(\overline{T})\overline{SEI}_a(T) \geq a^{n-1}(n-1)^2(n-2)^2. \tag{11}$$

Equality holds if and only if $T \cong K_{1,n-1}$.

Proof. For $r = -1$, $p_i := n-1-d_i$, $a_i := a^{d_i}$, $i = 1, 2, \ldots, n$, the inequality (2) transforms into

$$\left(\sum_{i=1}^{n}(n-1-d_i)\right)^{-2}\sum_{i=1}^{n}(n-1-d_i)a^{-d_i} \geq \left(\sum_{i=1}^{n}(n-1-d_i)a^{d_i}\right)^{-1},$$

that is

$$\sum_{i=1}^{n}(n-1-d_i)a^{-d_i} \geq \frac{(n(n-1)-2(n-1))^2}{\overline{SEI}_a(T)},$$

i.e.

$$a^{n-1}\sum_{i=1}^{n}(n-1-d_i)a^{-d_i} \geq \frac{a^{n-1}(n-1)^2(n-2)^2}{\overline{SEI}_a(T)}, \tag{12}$$

from which (11) is obtained.

Equality in (12) is attained if and only if $n-1 = \Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta = 1$, therefore equality in (11) holds if and only if $t = 1$, that is $T \cong K_{1,n-1}$. □

The proof of the next result is similar to that of Theorem 3.8, and hence we omit it.

Theorem 3.9. *Let T be a tree with $n \geq 2$ vertices. Then for any $a > 0$, $a \neq 1$, the following inequality holds*

$$(SEI_a(T) - 2a)(\overline{SEI}_a(\overline{T}) - 2a^{n-2}) \geq 4a^{n-1}(n-2)^2.$$

Equality holds if and only if $T \cong P_n$.

Remark 3.1. *Note that the path graph attains the equality sign in the inequalities, involving SEI_a or $\overline{SEI}_a$, given in all the results established in this section, except for Theorem 3.8. Thus, these results give sharp inequalities involving SEI_a or $\overline{SEI}_a$ also for the chemical trees.*

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