# Research Article **Two general eccentricity-based topological indices**

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(Received: 9 June 2024. Received in revised form: 28 August 2024. Accepted: 4 October 2024. Published online: 14 October 2024.)

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#### Abstract

This paper is concerned with the general eccentric distance sum index and the general degree eccentricity index of graphs. Bounds on the difference between these indices are presented for graphs of diameter 2. A relation between the mentioned indices, in terms of the graph's order and minimum degree, is also established. Additionally, an upper bound on the general eccentric distance sum for graphs of order at least 2 is presented. Furthermore, all the graphs attaining the bounds are identified, which demonstrates that the obtained bounds are optimal.

Keywords: eccentricity; degree; maximum degree; extremal graph.

2020 Mathematics Subject Classification: 05C09, 05C12.

## 1. Introduction

In this paper, we focus on connected simple graphs. We examine certain topological indices of such graphs that are crucial in graph theory and its applications. The number of vertices and edges in a graph are referred to as the order and size of the graph, respectively. The degree of a vertex v in a graph G is denoted by deg(v). The minimum degree of G is defined as

$$\delta(G) = \min_{v \in V(G)} \deg(v),$$

and the maximum degree of G is defined as

$$\Delta(G) = \max_{v \in V(G)} \deg(v).$$

The eccentricity of a vertex v in G is defined as the maximum distance from v to any other vertex of G. The diameter of G is defined as

$$d(G) = \max_{v \in V(G)} \operatorname{ecc}(v).$$

For undefined terms from graph theory, we refer the reader to [18].

The present study focuses on the generalized versions of the following two eccentricity-based topological indices: the degree eccentricity index (DEI) and the eccentric distance sum (EDS) index. The DEI and EDS index of a graph G are defined as follows:

$$\mathrm{DEI}(G) = \sum_{v \in V(G)} \mathrm{ecc}(v) \deg(v) \quad \text{and} \quad \mathrm{EDS}(G) = \sum_{v \in V(G)} \mathrm{ecc}(v) D(v),$$

respectively, where

 $D(v) = \sum_{u \in V(G)} d(v, u)$ 

represents the sum of the distances from the vertex v to all other vertices of G.

There exists an excellent correlation between several physical/biological properties of chemical substances and certain eccentricity-based topological indices [8, 14]. These indices also have strong predictive power in determining pharmaceutical properties, such as the anti-HIV activity, of chemical compounds [5]. The mathematical properties of these indices have extensively been studied; for example, see [1-3, 9-11, 19, 22].

Bounds on the EDS index for various graph classes have been presented in [4, 7, 12, 13, 20]. Similarly, bounds on the ECI for different graph types have been provided in [6, 21-24]. The relationship between the EDS index and other distance-based indices has been explored in [7].



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The general degree-eccentricity index [11] is defined as

$$\mathrm{DEI}_{a,b}(G) = \sum_{v \in V(G)} \mathrm{ecc}(v)^a \deg(v)^b.$$

This general form allows us to obtain the general eccentric connectivity index [17] by setting a = 1, and the classical eccentric connectivity index by setting a = b = 1. By setting a = 0 and b = 1, we obtain the total degree, which is equal to twice the size of the graph. While, with the choice a = 1 and b = 0, we obtain the total eccentricity.

The general eccentric distance sum index [15] is defined as

$$EDS_{a,b}(G) = \sum_{v \in V(G)} ecc(v)^a D(v)^b$$

The topological index  $EDS_{a,b}$  encompasses several existing eccentricity-based topological indices, such as the ordinary EDS index and the total eccentricity index.

Sharp bounds on  $DEI_{a,b}(G)$  for different types of graphs and graph parameters have been provided in [1,9–11]. Sharp bounds on  $EDS_{a,b}(G)$  for various graph types and parameters have been reported in [2,3,15,16].

In this paper, we provide bounds on the difference between  $EDS_{a,b}$  and  $DEI_{a,b}$  for graphs of diameter 2. We also establish a relation between these indices in terms of the graph's order and minimum degree when b = 1. Additionally, we present an upper bound on  $EDS_{a,b}$  for a graph of order  $n \ge 2$  containing at least two vertices of degree n - 1 when b = 1. Furthermore, we identify all extremal graphs, demonstrating that our bounds are optimal.

### 2. Results

For any graph of diameter 2, we establish bounds on the difference  $EDS_{a,1} - DEI_{a,1}$  in Theorems 2.1 and 2.2, by utilizing the following known result:

**Lemma 2.1** (see [22]). Let G be a graph with diameter 2 and n = |G|.

- (i). If  $\Delta(G) = n 2$ , then  $|E(G)| \ge 2n 4$ .
- (ii). If  $\Delta(G) = n 3$ , then  $|E(G)| \ge 2n 5$ .
- (iii). If  $\Delta(G) \leq n 4$  and  $\delta(G) \leq 3$ , then  $|E(G)| \geq 2n 5$ .

**Theorem 2.1.** Let G be a graph with diameter 2 and  $|G| = n \ge 3$ . For a > 0,

$$\mathrm{EDS}_{a,1}(G) - \mathrm{DEI}_{a,1}(G) \ge 2^{a+2}$$

with equality if and only if G is  $K_n - e$ , where  $e \in E(K_n)$ .

**Proof.** Let  $C = \{v \in V(G) : ecc(v) = 1\}$ . Since d(G) = 2, we have

$$D(v) = \deg(v) + 2(n - 1 - \deg(v)) = 2(n - 1) - \deg(v).$$
<sup>(1)</sup>

We complete the proof by discussing two possible cases.

**Case 1.**  $\Delta(G) = n - 1$ .

For  $v \in C$ , we have ecc(v) = 1 and D(v) = n - 1. For  $v \in V(G) \setminus C$ , we have ecc(v) = 2 and

$$D(v) = 2(n-1) - \deg(v)$$

Then,

$$EDS_{a,1}(G) = |C|(n-1) + \sum_{v \in V(G) \setminus C} 2^a (2(n-1) - \deg(v)), \text{ and}$$
$$DEI_{a,1}(G) = |C|(n-1) + \sum_{v \in V(G) \setminus C} 2^a \deg(v).$$

Thus,

$$EDS_{a,1}(G) - DEI_{a,1}(G) = \sum_{v \in V(G) \setminus C} 2^a (2(n-1) - \deg(v) - \deg(v))$$
$$= 2^{a+1} \left( \sum_{v \in V(G) \setminus C} (n-1 - \deg(v)) \right)$$
$$= 2^{a+1} \left( (n-1)(n-|C|) - \sum_{v \in V(G) \setminus C} \deg(v) \right).$$

Since

$$2|E(G)| = \sum_{v \in C} \deg(v) + \sum_{v \in V(G) \setminus C} \deg(v),$$

$$\sum_{v \in V(G) \setminus C} \deg(v) = 2|E(G)| - |C|(n-1).$$

Therefore,

$$EDS_{a,1}(G) - DEI_{a,1}(G) = 2^{a+1} \left( (n-1)(n-|C|) - (2|E(G)| - |C|(n-1)) \right) = 2^{a+1} \left( n(n-1) - 2|E(G)| \right)$$

Case 2.  $\Delta(G) \leq n-2$ .

Since d(G) = 2, we have ecc(v) = 2 and  $D(v) = 2(n-1) - \deg(v)$  for all  $v \in V(G)$ . Hence, we have

$$\begin{split} \text{EDS}_{a,1}(G) &= \sum_{v \in V(G)} 2^a [2(n-1) - \deg(v)] \\ &= 2^a \left( 2n(n-1) - \sum_{v \in V(G)} \deg(v) \right) \\ &= 2^a \left( 2n(n-1) - 2|E(G) \right) \\ &= 2^{a+1} \left( n(n-1) - |E(G)| \right), \quad \text{and} \\ \text{DEI}_{a,1}(G) &= \sum_{v \in V(G)} 2^a \deg(v) = 2^a (2|E(G)|) = 2^{a+1} |E(G)|. \end{split}$$

Therefore,

$$EDS_{a,1}(G) - DEI_{a,1}(G) = 2^{a+1} \left( n(n-1) - |E(G)| - 2^{a+1} |E(G)| = 2^{a+1} \left( n^2 - n - 2|E(G)| \right).$$

Since d(G) = 2, the size of *G* cannot be greater than  $\binom{n}{2} - 1$ , i.e.,

$$|E(G)| \le \binom{n}{2} - 1 = \frac{n^2 - n - 2}{2}$$

Consequently, we have

$$EDS_{a,1}(G) - DEI_{a,1}(G) \ge 2^{a+1} \left( n^2 - n - 2 \left( \frac{n^2 - n - 2}{2} \right) \right)$$

$$= 2^{a+2}.$$
(2)

The equality in (2) is achieved if and only if

 $|E(G)| = \binom{n}{2} - 1,$ 

that is, if and only if G is  $K_n - e$ .

Let  $S_n^*$  (or  $S_n^{**}$ ) be a graph obtained by connecting two (or two pairs of) pendant vertices of  $S_n$  with an edge (or two edges), respectively.

**Theorem 2.2.** Let G be a graph with diameter 2 and  $n = |G| \ge 7$ . Then for a > 0,

$$EDS_{a,1}(G) - DEI_{a,1}(G) \le 2^{a+1} \left[ n^2 - 3n + 2 \right],$$

with equality obtained if and only if  $G \cong S_n$ .

**Proof.** First, we calculate  $EDS_{a,1}(G) - DEI_{a,1}(G)$  when  $G \in \{S_n^{**}, S_n^*, S_n\}$ . We recall that  $S_n^{**}$  is obtained from  $S_n$  by adding two edges. These two new edges may or may not share a vertex. If the two new edges of  $S_n^{**}$  share a vertex, then

$$EDS_{a,1}(S_n^{**}) = 2^a \left[ (2n-5) + 2(2n-4) + (n-4)(2n-3) \right] + (n-1)$$
$$DEI_{a,1}(S_n^{**}) = 2^a \left[ 3 + 2(2) + (n-4) \right] + (n-1),$$
$$EDS_{a,1}(S_n^{**}) - DEI_{a,1}(S_n^{**}) = 2^a \left[ 2n^2 - 6n - 4 \right] = 2^{a+1} \left[ n^2 - 3n - 2 \right].$$

If the two new edges of  $S_n^{\ast\ast}$  do not share a vertex, then

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$$EDS_{a,1}(S_n^{**}) = 2^a \left[4(2n-4) + (n-5)(2n-3)\right] + (n-1),$$
$$DEI_{a,1}(S_n^{**}) = 2^a \left[4(2) + (n-5)\right] + (n-1),$$
$$S_{a,1}(S_n^{**}) - DEI_{a,1}(S_n^{**}) = 2^a \left[2n^2 - 6n - 4\right] = 2^{a+1} \left[n^2 - 3n - 2\right].$$

Therefore, in either case, we have

$$EDS_{a,1}(S_n^{**}) - DEI_{a,1}(S_n^{**}) = 2^{a+1} \left[ n^2 - 3n - 2 \right].$$

For the graph  $S_n^*$ , we have

$$EDS_{a,1}(S_n^*) = 2^a \left[ 2(2n-4) + (n-3)(2n-3) \right] + (n-1),$$
$$DEI_{a,1}(S_n^*) = 2^a \left[ 2(2) + (n-3) \right] + (n-1),$$
$$EDS_{a,1}(S_n^*) - DEI_{a,1}(S_n^*) = 2^a \left[ 2n^2 - 6n \right] = 2^{a+1} \left[ n^2 - 3n \right].$$

Also, for the star  $S_n$ , we have

$$EDS_{a,1}(S_n) = 2^a(n-1)(2n-3) + (n-1),$$
$$DEI_{a,1}(S_n) = 2^a(n-1) + (n-1),$$
$$EDS_{a,1}(S_n) - DEI_{a,1}(S_n) = 2^{a+1} \left[ n^2 - 3n + 2 \right].$$

Since  $n^2 - 3n - 2 < n^2 - 3n < n^2 - 3n + 2$ , we have

$$EDS_{a,1}(S_n^{**}) - DEI_{a,1}(S_n^{**}) < EDS_{a,1}(S_n^{*}) - DEI_{a,1}(S_n^{*}) < EDS_{a,1}(S_n) - DEI_{a,1}(S_n).$$

Next, we show that

$$EDS_{a,1}(G) - DEI_{a,1}(G) < EDS_{a,1}(S_n^{**}) - DEI_{a,1}(S_n^{**})$$

for any graph G with diameter 2 such that  $n \ge 7$  and  $G \notin \{S_n, S_n^*, S_n^{**}\}$ . Let  $C = \{v \in V(G) : \deg(v) = n - 1\}$ . Since G has  $n \ge 7$  vertices and diameter 2, from Theorem 2.1, we get

$$EDS_{a,1}(G) - DEI_{a,1}(G) = 2^{a+1} \left[ n^2 - n - 2|E(G)| \right].$$

**Case 1.**  $\Delta(G) = n - 1$ .

If 
$$|C| = 1$$
, then

$$2|E(G)| \ge n - 1 + 2(n - 1) \ge 2(n - 1) + 6 = 2(n + 2)$$

i.e.,  $|E(G)| \ge n + 2$ . If  $|C| \ge 2$ , then  $\deg(v) = n - 1$  for  $v \in C$  and  $\deg(v) \ge |C|$  for  $v \in V(G) \setminus C$ .

$$\begin{split} 2|E(G)| &= \sum_{v \in C} \deg(v) + \sum_{v \in V(G) \setminus C} \deg(v) \\ &\geq |C|(n-1) + |C|(n-|C|) \\ &= (2n-1)|C| - |C|^2 \\ &\geq 2(2n-1) - 4 \quad \text{(because } |C| \geq 2) \\ &= 4n - 6 = 2n + 2n - 6 \\ &> 2n + 4 = 2(n+2), \quad \text{because } 2n - 6 > 4 \text{ for } n \geq 7. \end{split}$$

Thus, in general, it holds that  $|E(G)| \ge n+2$ . Hence, we have

$$EDS_{a,1}(G) - DEI_{a,1}(G) = 2^{a+1} [n^2 - n - 2|E(G)|]$$
  
$$\leq 2^{a+1} [n^2 - n - 2(n+2)]$$
  
$$= 2^{a+1} [n^2 - 3n - 4]$$
  
$$< 2^{a+1} [n^2 - 3n - 2]$$
  
$$= EDS_{a,1}(S_n^{**}) - DEI_{a,1}(S_n^{**})$$

**Case 2.**  $\Delta(G) \le n - 2$ .

Case 2.1.  $\Delta(G) = n - 2$  or  $\Delta(G) = n - 3$ 

Using the first two parts of Lemma 2.1, we have  $|E(G)| \ge 2n - 5$ .

**Case 2.2.** 
$$\Delta(G) \le n - 4$$
.

In this case, we discuss two further possibilities.

- If  $\delta(G) \leq 3$ , the by Lemma 2.1(iii) we have  $|E(G)| \geq 2n 5$ .
- If  $\delta(G) \ge 4$ , then  $2|E(G)| \ge n\delta \ge 4n$ , i.e.,  $|E(G)| \ge 2n > 2n 5$ .

In either of the cases Case 2.1 and Case 2.2, we have  $|E(G)| \ge 2n - 5$ . Thus,

$$\begin{split} \text{EDS}_{a,1}(G) - \text{DEI}_{a,1}(G) &= 2^{a+1} \left[ n^2 - n - 2|E(G)| \right] \\ &\leq 2^{a+1} \left[ n^2 - n - 2(2n-5) \right] \\ &= 2^{a+1} \left[ n^2 - 5n + 10 \right] = 2^{a+1} \left[ n^2 - 3n - 2 + 12 - 2n \right] \\ &< 2^{a+1} \left[ n^2 - 3n - 2 \right], \quad \text{because } 12 - 2n < 0 \text{ for } n \geq 7 \end{split}$$

Thus, we have

$$EDS_{a,1}(G) - DEI_{a,1}(G) < EDS_{a,1}(S_n^{**}) - DEI_{a,1}(S_n^{**}).$$

Therefore, for a > 0 and for any graph *G* with diameter 2, we have

$$EDS_{a,1}(G) - DEI_{a,1}(G) \le EDS_{a,1}(S_n) - DEI_{a,1}(S_n) = 2^{a+1} [n^2 - 3n + 2].$$

**Theorem 2.3.** Let G be a graph on  $n \ge 2$  vertices. For  $a, b \in \mathbb{R}$  where b > 0, we have

$$EDS_{a,b}(G) \le (n-1)^b DEI_{a+b,0}(G).$$

Equality holds if and only if  $G \cong K_n$ .

**Proof.** From the definition of the eccentricity of a vertex, we have  $d(v, u) \leq ecc(v)$ . Thus,

$$D(v) = \sum_{u \in V(G)} d(v, u) \le \sum_{u \in V(G)} ecc(v) = (n - 1)ecc(v).$$
(3)

Equality in (3) holds when the vertex u is one of the vertices furthest from v in G, i.e., ecc(v) = d(v, u). For b > 0, we have

$$(D(v))^b \le ((n-1)ecc(v))^b.$$

Thus, we have

$$EDS_{a,b}(G) = \sum_{v \in V(G)} (ecc(v))^a (D(v))^b$$
$$\leq \sum_{v \in V(G)} (ecc(v))^a ((n-1)ecc(v))^b$$
$$= (n-1)^b \sum_{v \in V(G)} (ecc(v))^{a+b}.$$

Consequently, we have

$$EDS_{a,b}(G) \le (n-1)^b DEI_{a+b,0}(G)$$

where

$$DEI_{a+b,0}(G) = \sum_{v \in V(G)} (ecc(v))^{a+b}$$

We note that the equality in (3) holds if and only if  $G \cong K_n$ .

**Theorem 2.4.** Let G be a graph of order  $n \ge 3$ . For  $a, b \in \mathbb{R}$  with b > 0, the following inequality holds:

$$\operatorname{EDS}_{a,b}(G) \ge (n-1)^b \operatorname{DEI}_{a,0}(G),$$

with equality if and only if  $G \cong K_n$ .

**Proof.** For any  $v \in V(G)$  and b > 0, we have  $D_G(v) \ge n - 1$ . Thus,

$$(D_G(v))^b \ge (n-1)^b$$

and hence,

$$(ecc_G(v))^a (D_G(v))^b \ge (ecc_G(v))^a (n-1)^b$$

Summing over all vertices of G, we obtain

$$\sum_{v \in V(G)} (ecc_G(v))^a (D_G(v))^b \ge \sum_{v \in V(G)} (ecc_G(v))^a (n-1)^b.$$

Therefore,

$$EDS_{a,b}(G) \ge (n-1)^b \sum_{v \in V(G)} (ecc_G(v))^a = (n-1)^b DEI_{a+b,0}(G).$$

Equality follows from  $D_G(v) \ge n-1$  and ecc(v) = 1 for all  $v \in V(G)$ , i.e.,  $G \cong K_n$ .

From the proof of Theorem 4.2 in [7], we have Lemma 2.2, which we use to prove our next result (that is, Theorem 2.5).

**Lemma 2.2** (see [7]). Let G be a graph with order  $n \ge 5$ . For any vertex v in G, it holds that  $ecc_G(v) \le n - deg(v)$ , with equality if and only if G is obtained by deleting k pairwise independent edges from  $K_n$ , where  $k = 0, 1, 2, ..., \lfloor \frac{n}{2} \rfloor$ .

**Theorem 2.5.** Let G be a graph with order  $n \ge 2$  with minimum degree  $\delta$ . For  $a, b \in \mathbb{R}$  with b > 0, we have

$$EDS_{a,b}(G) \le n(n-1)^b(n-\delta)^{a+b}$$

where the equality holds if and only if  $G \cong K_n$ .

**Proof.** Let  $(d_1, d_2, \ldots, d_n)$  be the degree sequence of G such that  $d_n = \delta$ . From (3), for any  $v \in V(G)$ , we have

$$D(v) \le (n-1)ecc(v).$$

Hence, for b > 0, it holds that

$$(D(v))^b \le ((n-1)ecc(v))^b$$

Therefore, we have

$$\begin{split} \mathrm{EDS}_{a,b}(G) &\leq \sum_{v \in V(G)} (ecc(v))^a ((n-1)ecc(v))^b \\ &= (n-1)^b \sum_{v \in V(G)} (ecc(v))^{a+b} \\ &\leq (n-1)^b \sum_{v \in V(G)} (n-deg(v))^{a+b}, \quad \text{by Lemma 2.2.} \end{split}$$

If  $G \cong K_n$ , then  $d_i = n - 1$  for each i = 1, 2, ..., n. Thus,  $n - d_i = 1$ , ecc(v) = 1, and D(v) = n - 1. We have

$$EDS_{a,b}(K_n) = n(n-1)^b.$$

For any  $v \in V(G)$ , the inequality  $\delta \leq deg(v)$  holds and hence  $n - deg(v) \leq n - \delta$ . Hence, we have

$$EDS_{a,b}(G) \le (n-1)^b \sum_{i=1}^n (n - \deg(v))^{a+b}$$
$$\le (n-1)^b \sum_{i=1}^n (n-\delta)^{a+b} = n(n-1)^b (n-\delta)^{a+b}$$

Equality holds if and only if  $G \cong K_n$ .

**Theorem 2.6.** Let G be a graph of order  $n \ge 2$  containing at least two vertices of degree n - 1. For a > 0, we have

$$EDS_{a,1}(G) \le 2(n-1) + 2^{a+1}(n-2)^2,$$

with equality if and only if G is  $K_2 + (n-2)K_1$ .

**Proof.** Let  $\Phi = \{v \in V(G) : d_G(v) = n-1\}$ . Then  $|\Phi| \ge 2$  and d(G) = 2. For  $v \in \Phi$ , we have  $ecc_G(v) = 1$  and  $D_G(v) = n-1$ . However, for  $v \in V(G) \setminus \Phi$ , we have  $ecc_G(v) = 2$  and  $D_G(v) = 2(n-1) - d_G(v)$ . Hence, we have

$$\begin{aligned} \text{EDS}_{a,1}(G) &= \sum_{v \in \Phi} (ecc_G(v))^a D_G(v) + \sum_{v \in V(G) \setminus \Phi} (ecc_G(v))^a D_G(v) \\ &= |\Phi|(n-1) + \sum_{v \in V(G) \setminus \Phi} 2^a D_G(v) \\ &= |\Phi|(n-1) + \sum_{[} 2mm] v \in V(G) \setminus \Phi 2^a (2(n-1) - d_G(v)) \\ &= |\Phi|(n-1) + (n - |\Phi|) 2^a (2(n-1)) - 2^a \sum_{v \in V(G) \setminus \Phi} d_G(v) \\ &= |\Phi|(n-1) + (n - |\Phi|) 2^a (2(n-1)) - 2^a [2|E(G)| - (n-1)|\Phi|] \\ &= |\Phi|(n-1)(1+2^a) + (n - |\Phi|)(n-1) 2^{a+1} - 2^a (2|E(G)|). \end{aligned}$$

Note that  $deg_G(v) \ge |\Phi|$  for  $v \in V(G) \setminus \Phi$ . By the Handshaking lemma, we have

$$2|E(G)| \ge (n-1)|\Phi| + (n-|\Phi|)|\Phi|.$$
(5)

Therefore, from (4) and (5), it follows that

$$EDS_{a,1}(G) \le |\Phi|(n-1)(1+2^{a}) + (n-|\Phi|)(n-1)2^{a+1} - 2^{a}[(n-1)|\Phi| + (n-|\Phi|)|\Phi|]$$

$$= |\Phi|(n-1) + (n-|\Phi|)(n-1)2^{a+1} - 2^{a}|\Phi|(n-|\Phi|)$$
(6)

Equality in (5) holds if and only if  $deg_G(v) = |\Phi|$  for all  $v \in V(G) \setminus \Phi$ . Thus,

$$G \cong K_{|\Phi|} + (n - |\Phi|)K_1$$

Consequently, we have

$$EDS_{a,1}(G) \leq |\Phi|(n-1) + (n-|\Phi|)(n-1)2^{a+1} - 2^{a}|\Phi|(n-|\Phi|)$$
  
=  $|\Phi|(n-1) + 2^{a}(n-|\Phi|)[2(n-1) - |\Phi|]$   
 $\leq 2(n-1) + 2^{a}(n-2)[2(n-1) - 2]$   
=  $2(n-1) + 2^{a+1}(n-2)^{2}$ . (7)

Equality in (7) holds if and only if  $|\Phi| = 2$ . Therefore, equality  $EDS_{a,1}(G) = 2(n-1) + 2^{a+1}(n-2)^2$  is achieved whenever G is  $K_2 + (n-2)K_1$ .

## 3. Open problems

Some open problems related to the present study are listed below:

- 1. Find graphs with the largest and smallest  $EDS_{a,b}$  among trees of a given order and number of branching vertices.
- 2. Find bounds on  $EDS_{a,b}$  for trees of a given order and number of segments.
- 3. Establish relations between  $EDS_{a,b}$  and other general topological indices for general graphs.

We suggest studying the above three problems for either both general values of *a* and *b*, or one general value and the other equal to 1.

### Acknowledgment

The authors would like to thank the anonymous referees for their insightful feedback, which has greatly improved the quality and presentation of the submitted version of this paper.

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