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On the Unified Extremal Results on Distance-Based Bond Additive Indices on Trees

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Abstract

Szeged-type bond additive indices are a class of distance-based topological indices defined by counting the vertices or edges that are closer to the end vertices of an edge. Important members of this family include the Szeged index, Mostar index, PI index, SPI index, and the Szeged–Sombor index, together with their corresponding edge versions. Although these indices have been extensively studied and extremal results have been obtained for various graph classes, a unified framework for their extremal analysis is still lacking.

In this paper, we introduce a unified approach for studying extremal problems of Szeged-type bond additive indices on trees. We show that, for 44 different Szedged type indices, the path and the star uniquely attain the extremal values of these indices. We also propose their exponential version of these indices and establish that the same graph attain the extrmal values for trees in these distance based bond additive indices.

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1 Introduction

The Szeged index is a classical bond-additive topological index proposed by Gutman [17] as an alternative to the Wiener index [30] for trees. Subsequently, several significant extensions of the Szeged index [19] have been introduced and extensively studied. Notable among these are the PI index [22], Mostar index [13], Szeged–Sombor index [3], SPI index [4], second geometric–arithmetic index [14], second atom–bond sum connectivity index [16], and second inverse sum indeg index [1], among others. In addition, the corresponding edge versions of these indices—such as the edge Szeged index, edge PI index [29], and edge Mostar index [2]—have also been proposed and investigated. For more works on these indices, refer [2, 6, 8, 9, 11–14, 19, 23, 24, 26–29, 31].

The study of extremal problems for topological indices has been a central topic in chemical graph theory, particularly for Szeged-type bond-additive indices. Numerous results concerning bounds and extremal structures for these indices have been established in the literature. However, despite being studied individually, there is no comprehensive and unified treatment of Szeged-type indices with respect to their extremal properties. While unified frameworks exist for analyzing extremal properties of degree-based topological indices, a similar framework for this class of distance-based indices is still lacking.

In this paper, we address this gap by proposing a unified framework for Szeged-type bond-additive indices. We classify these indices into three distinct categories and develop a systematic approach to study their extremal properties on trees. In particular, we establish that, for each of these classes of indices, the extremal trees are either paths or stars.

1.1 General framework for Szeged-type bond additive indices

Definition 1. Let $\phi(x, y)$ be a real-valued function defined on $\mathbb{N} \cup \{0\} \times \mathbb{N} \cup \{0\}$ (or $\mathbb{R} \times \mathbb{R}$) satisfying the following conditions:

1. $\phi(x, y) \geq 0$ for all $x, y \in \mathbb{N} \cup \{0\}$.

2. $\phi(x, y) = \phi(y, x)$ for all $x, y \in \mathbb{N} \cup \{0\}$.

In addition, ϕ may satisfy one of the following properties whenever $a > b$:

3.
$$\phi(a + 1, b - 1) > \phi(a, b).$$

4.
$$\phi(a + 1, b - 1) < \phi(a, b).$$

5.
$$\phi(a + 1, b - 1) = \phi(a, b).$$

Let G be a connected graph. The associated topological index TI_ϕ is defined as

$$TI_\phi(G) = \sum_{uv \in E(G)} \phi(f(u), f(v)).$$

When $f(u) = n_u$ and $f(v) = n_v$, where n_u and n_v denote the number of vertices closer to u and v, respectively, with respect to the edge uv, the resulting index is called a *Szeged-type distance-based bond-additive index*. Similarly, when $f(u) = m_u$ and $f(v) = m_v$, where m_u and m_v denote the number of edges closer to u and v, respectively, with respect to the edge uv, the index is called the *edge version of a Szeged-type distance-based bond-additive index*.

A vertex version of a Szeged-type topological index with associated function ϕ satisfying Properties 1, 2, and 3 is denoted by TI_M and is referred to as an M-class Szeged index (or M-Szeged index). If ϕ satisfies Properties 1, 2, and 4, then the index is denoted by TI_S and is called an S-class Szeged index (or S-Szeged index). Likewise, if ϕ satisfies Properties 1, 2, and 5, the index is denoted by TI_P and is called a P-class Szeged index (or P-Szeged index).

Similarly, for the edge versions, if the associated function ϕ satisfies Properties 1, 2, and 3, the index is denoted by $TI_{M'}$ and is called an

M'-class edge Szeged index (or M'-edge Szeged index). If ϕ satisfies Properties 1, 2, and 4, the index is denoted by $TI_{S'}$ and is called an S'-class edge Szeged index (or S'-edge Szeged index). Finally, if ϕ satisfies Properties 1, 2, and 5, the index is denoted by $TI_{P'}$ and is called a P'-class edge Szeged index (or P'-edge Szeged index). We also propose an exponential version of these topological indices, defined as

$$eTI_{\phi}(G) = \sum_{uv \in E(G)} e^{\phi(f(u),f(v))}.$$

These indices can also be classified into three different classes based on the previous definitions.

Note that the topological indices considered in this study correspond to the following choices of the function $\phi(x, y)$:

Although several studies have established unified extremal results for degree-based bond additive indices, such results are not yet available for Szeged-type bond additive indices. In this paper, we aim to fill this gap by proposing a unified approach to obtain extremal results for Szeged-type bond additive indices on trees. Using the same framework, we also determine the extremal graphs of fixed order for the exponential version of Szeged indices. Our primary focus is on investigating extremal properties of trees.

Although extremal studies for several of these indices and their edge versions on trees have been successfully completed, there still exist indices for which the corresponding extremal graphs have not been fully characterized. Let $\mathcal{T}_n$ denote the collection of all trees of order n. Among the members of this class, let P_n and S_n denote the path and star graphs on n vertices, respectively. The following table provides a comprehensive summary of the extremal trees [3, 4, 13, 14, 16, 19, 20, 22, 24, 28] obtained for these indices.

2 Main results

In this section, we determine the unified method to determine the extremal results of various szeged type indices on trees.

Function	Name of the Index
$\phi(x,y) = xy$	Szeged index(S_z) [17, 19]
$\phi(x,y) = \lvert x-y \rvert$	Mostar index(Mo) [6, 13, 24]
$\phi(x,y) = x+y$	PI index(PI) [22]
$\phi(x,y) = x^2+y^2$	SPI index(SPI) [4]
$\phi(x,y) = \sqrt{x^2+y^2}$	Szeged–Sombor index(SSz) [3]
$\phi(x,y) = \dfrac{xy}{x+y}$	Second Inverse Sum index(ISI_2) [1]
$\phi(x,y) = \dfrac{2\sqrt{xy}}{x+y}$	Second Geometric Arithmetic index(GA_2) [14]
$\phi(x,y) = \dfrac{x+y}{2\sqrt{xy}}$	Second Arithmetic Geometric index(AG_2) [15]
$\phi(x,y) = \sqrt{\dfrac{x+y-2}{xy}}$	Second Atom–Bond Connectivity index(ABC_2) [16]
$\phi(x,y) = \dfrac{1}{xy}$	Reverse Szeged index(RS_z) [15]
$\phi(x,y) = \dfrac{x}{y} + \dfrac{y}{x}$	Symmetric division Szeged index (SDZ) [15]

Table 1. Different functions $\phi(x,y)$ and their corresponding topological indices

TI	S_z	Mo	PI	SPI	SS_z	ISI_2	GA_2	AG_2	ABC_2	RS_z	SDZ
LB	S_n	P_n	$\mathcal{T}_n$	P_n	P_n	—	S_n	S_n	S_n	—	P_n
UB	P_n	S_n	$\mathcal{T}_n$	S_n	S_n	—	P_n	P_n	P_n	—	S_n
TI_e	S_{z_e}	Mo_e	PI_e	SPI_e	SS_{z_e}	ISI_{2e}	GA_{2e}	AG_{2e}	ABC_{2e}	RS_{z_e}	SDZ_e
LB	S_n	P_n	$\mathcal{T}_n$	—	—	—	—	—	—	—	—
UB	P_n	S_n	$\mathcal{T}_n$	—	—	—	—	—	—	—	—

Table 2. Summary of extremal trees for Szeged-type indices

We can classify the listed topological indices into three classes, as described in the following lemma.

Lemma 1. *Let $\phi : \mathbb{R}^2 \to \mathbb{R}$ be a symmetric function and let a, b be positive*

integers with $a > b$. Then, under the transformation $(a, b) \mapsto (a+1, b-1)$, the considered topological indices can be classified into the following three classes:

- *M, M'-class:*

$$\mathcal{M} = \{Mo,\ SPI,\ SSz,\ AG_2,\ ABC_2,\ RSz,\ SDSz\}.$$
$$\mathcal{M}' = \{Mo_e,\ SPI_e,\ SSz_e,\ AG_{2e},\ ABC_{2e},\ RSz_e,\ SDS_e\}.$$

- *S, S'-class:*

$$\mathcal{S} = \{Sz,\ ISI_2,\ GA_2\}.$$
$$\mathcal{S}' = \{Sz_e,\ ISI_{2e},\ GA_{2e}\}.$$

- *P, P'-class:*

$$\mathcal{P} = \{PI\} \quad \mathcal{P}' = \{PI_e\}.$$

The above classification is based on the behavior of ϕ under the transformation $(a, b) \mapsto (a + 1, b - 1)$.

Proof. All these indices satisfy the first two properties, which follow directly from the definition. Now, we analyze the behavior of $\phi(a, b)$ under the transformation $(a, b) \mapsto (a + 1, b - 1)$.

M, M'-class: $\phi(a + 1, b - 1) > \phi(a, b)$.

- Mo, Mo_e: $\phi(x, y) = |x - y|$. Since $a > b$,

$$\phi(a + 1, b - 1) = a - b + 2 > a - b = \phi(a, b).$$

- SPI, SPI_e: $\phi(x, y) = x^2 + y^2$.

$$\phi(a + 1, b - 1) = (a + 1)^2 + (b - 1)^2 = a^2 + b^2 + 2(a - b) + 2.$$

Thus,

$$\phi(a + 1, b - 1) - \phi(a, b) = 2(a - b) + 2 > 0.$$

- SSz, SSz_e: $\phi(x,y) = \sqrt{x^2+y^2}$. Since

$$(a+1)^2 + (b-1)^2 > a^2 + b^2,$$

and the square root function is increasing, we obtain

$$\phi(a+1, b-1) > \phi(a,b).$$

- AG_2, AG_{2e}: $\phi(x,y) = \dfrac{x+y}{2\sqrt{xy}}$. Since $x+y$ is fixed and

$$(a+1)(b-1) < ab,$$

we get

$$\phi(a+1, b-1) > \phi(a,b).$$

- ABC_2, ABC_{2e}: $\phi(x,y) = \sqrt{\dfrac{x+y-2}{xy}}$. Since $x+y$ is fixed and $(a+1)(b-1) < ab$, we obtain

$$\phi(a+1, b-1) > \phi(a,b).$$

- RSz, RSz_e: $\phi(x,y) = \dfrac{1}{xy}$. Since

$$(a+1)(b-1) < ab,$$

we obtain

$$\phi(a+1, b-1) > \phi(a,b).$$

- $SDSz, SDSz_e$: $\phi(x,y) = \dfrac{x}{y} + \dfrac{y}{x}$. Let

$$f(x,y) = \frac{x}{y} + \frac{y}{x}.$$

Then

$$f(a+1, b-1) - f(a,b) = \left(\frac{a+1}{b-1} - \frac{a}{b}\right) + \left(\frac{b-1}{a+1} - \frac{b}{a}\right).$$

Now,

$$\frac{a+1}{b-1} - \frac{a}{b} = \frac{a+b}{b(b-1)} > 0,$$

and

$$\frac{b-1}{a+1} - \frac{b}{a} = \frac{-a-b}{a(a+1)} < 0.$$

Since $a > b$, we have

$$b(b-1) < a(a+1),$$

and hence

$$\frac{a+b}{b(b-1)} > \frac{a+b}{a(a+1)}.$$

Thus, the positive term dominates, and therefore

$$\phi(a+1, b-1) > \phi(a, b).$$

S, S'-class: $\phi(a+1, b-1) < \phi(a, b)$.

- Sz, Sz_e: $\phi(x, y) = xy$.

  $$\phi(a+1, b-1) = (a+1)(b-1) = ab - a + b - 1.$$

  Hence,

  $$\phi(a+1, b-1) - \phi(a, b) = -a + b - 1 < 0 \quad (\text{since } a > b).$$

- ISI_2, ISI_{2e}: $\phi(x, y) = \dfrac{xy}{x+y}$. Since $x + y$ is fixed and

  $$(a+1)(b-1) < ab,$$

  we obtain

  $$\phi(a+1, b-1) < \phi(a, b).$$

- GA_2, GA_{2e}: $\phi(x, y) = \dfrac{2\sqrt{xy}}{x+y}$. Since $x + y$ is fixed and

$(a+1)(b-1) < ab$, we obtain

$$\phi(a+1, b-1) < \phi(a, b).$$

P-class: $\phi(a+1, b-1) = \phi(a, b)$.

- PI, PI_e: $\phi(x, y) = x + y$.

$$\phi(a+1, b-1) = (a+1) + (b-1) = a + b = \phi(a, b).$$

Thus, all the listed indices are classified into M-, S-, and P- as well as M'-, S'-, and P'- classes. ■

The following result is immediate from Lemma

Corollary. *Exponential versions of topological indices can be classified into the classes M, M', S, S', P, and P' according to the same criteria given in Lemma 1. Moreover, if a Szeged-type topological index belongs to a particular class, then its exponential counterpart also belongs to the same class.*

We now present a general classification for an arbitrary function $\phi(x, y)$ under suitable constraints.

Theorem 1. *Let a, b be positive integers such that $a > b$. Let $\phi(x, y)$ be a symmetric function of two positive variables. Suppose $\phi(x, y)$ is monotonic with respect to the difference $x - y$ when the sum $x + y$ is fixed. Then the following hold:*

(i) If $\phi(x, y)$ is non–decreasing in $x - y$ (for fixed $x + y$), then

$$\phi(a+1, b-1) \geq \phi(a, b).$$

(ii) If $\phi(x, y)$ is non–increasing in $x - y$ (for fixed $x + y$), then

$$\phi(a+1, b-1) \leq \phi(a, b).$$

(iii) If $\phi(x, y)$ is independent of $x - y$ (i.e., depends only on $x + y$), then

$$\phi(a + 1, b - 1) = \phi(a, b).$$

Proof. Consider the transformation

$$(a, b) \to (a + 1, b - 1).$$

Observe that the sum remains constant:

$$(a + 1) + (b - 1) = a + b.$$

However, the difference increases:

$$(a + 1) - (b - 1) = a - b + 2 > a - b.$$

Thus, the transformation increases the difference between the variables while keeping the sum fixed.

Let $s = x + y$ and define

$$f(d) = \phi\left(\frac{s + d}{2}, \frac{s - d}{2}\right),$$

where $d = x - y$.

Under the transformation $(a, b) \to (a + 1, b - 1)$, we have

$$d \to d + 2.$$

(i) If ϕ is non–decreasing in d, then

$$f(d + 2) \geq f(d),$$

which implies

$$\phi(a + 1, b - 1) \geq \phi(a, b).$$

(ii) If ϕ is non–increasing in d, then

$$f(d+2) \leq f(d),$$

and hence

$$\phi(a+1, b-1) \leq \phi(a, b).$$

(iii) If ϕ depends only on $s = x + y$, then $f(d)$ is constant in d, and therefore

$$f(d+2) = f(d),$$

which gives

$$\phi(a+1, b-1) = \phi(a, b).$$ ■

2.1 Extremal trees

Lemma 2. *Let G be a connected graph containing a non–pendant bridge $e = uv$. Let G' be the graph obtained from G by deleting the edge uv, identifying the vertices of one component into a new vertex u_e, and attaching a pendant edge $u_e v$ at u_e. Then*

$$TI_\phi(G') > TI_\phi(G), \text{ when } \phi \in \{M, M'\}$$
$$TI_\phi(G') < TI_\phi(G), \text{ when } \phi \in \{S, S'\}$$
$$TI_\phi(G') = TI_\phi(G), \text{ when } \phi \in \{P, P'\}.$$

Proof. Let G_u and G_v denote the components of $G - uv$ containing u and v, respectively.

Note that for every edge xy belonging to G_u or G_v, the values of $n_x(m_x)$ and $n_y(m_y)$ remain unchanged after the above transformation. Hence the contribution of all such edges to the index remains the same before and after the transformation. Therefore,

$$\phi_G(n_x, n_y) = \phi_{G'}(n_x, n_y), \text{ whenever } e = xy \in G_u \cup G_v.$$
$$\phi_G(m_x, m_y) = \phi_{G'}(m_x, m_y), \text{ whenever } e = xy \in G_u \cup G_v.$$

The only edge whose contribution changes is the bridge $e = uv$. Suppose

$n_x = a(m_x = a)$ and $n_y = b(m_y = b)$, where $a + b = n(a + b = n - 1)$. Then after the transformation the new values become $n_{u_e} = n - 1, n_v = 1$ or $m_{u_e} = n - 2, m_v = 0$. Now, by the definition,

$$\phi(a,b) < \phi(a+1,b-1) < \cdots < \phi(n-1,1), \text{ when } \phi \in M - \text{class}.$$
$$\phi(a,b) > \phi(a+1,b-1) > \cdots > \phi(n-1,1), \text{ when } \phi \in S - \text{class}.$$
$$\phi(a,b) = \phi(a+1,b-1) = \cdots = \phi(n-1,1), \text{ when } \phi \in P - \text{class}.$$

Similarly for the edge versions as well. Hence the contribution of the modified edge changes. Therefore the result follows. ■

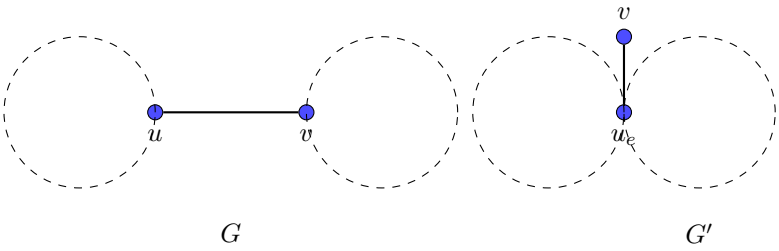

Figure 1. Transformation of graph G to G' described in Lemma 2.

Theorem 2. *Among all trees of fixed order n, the star graph S_n uniquely maximizes all M- and M'-class Szeged indices and uniquely minimizes all S- and S'-class Szeged indices.*

Proof. We prove the result by establishing the Lemma 2. By repeated applications transformation in Lemma 2, we eventually obtain the star S_n. Hence for every tree T of order n with $T \neq S_n$,

$$TI_M(S_n) > TI_M(T), \quad TI_{M'}(S_n) > TI_{M'}(T).$$
$$TI_S(S_n) < TI_S(T), \quad TI_{S'}(S_n) < TI_{S'}(T)$$

This completes the proof. ■

Corollary. *Among all trees of fixed order n, the star graph S_n uniquely maximizes all M- and M'-class exponential Szeged indices and uniquely minimizes all S- and S'-class exponential Szeged indices.*

Proof. The result directly follows from Lemma 2 and the fact that e^x is an inceasing function. ■

Remark. In the case of P-class indices, for which

$$\phi(a+1, b-1) = \phi(a, b),$$

the following holds.

For vertex-based Szeged indices of any tree $T \in \mathcal{T}_n$,

$$TI_P(T) = (n-1)\,\phi(a, b), \quad \text{where } a + b = n.$$

For edge-based Szeged indices of any tree $T \in \mathcal{T}_n$,

$$TI_P(T) = (n-1)\,\phi(a, b), \quad \text{where } a + b = n - 2.$$

Now, we study the lower bounds of these classes of indices for trees of fixed order. We consider several transformations to obtain the results.

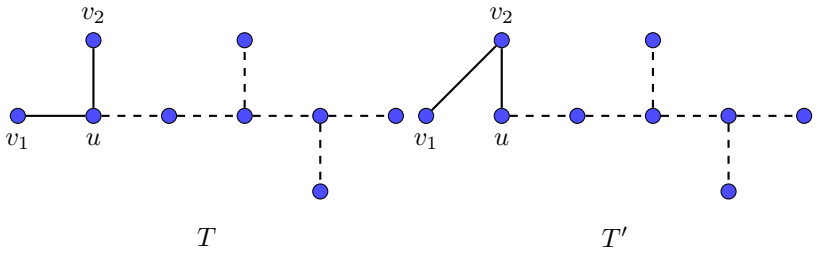

Figure 2. Transformation of tree T into T' described in Lemma 3.

Lemma 3. *Let T be a tree of order n containing a vertex u that is incident with at least two pendant edges. Let*

$$P = \{v \in V(T) : uv \in E(T), d(v) = 1\},$$

with $|P| \geq 2$. Let $v_1, v_2 \in P$ and construct

$$T' = T - uv_1 + v_1v_2.$$

Then

$$TI_\phi(T') < TI_\phi(T), \text{ when } \phi \in \{M, M'\}$$
$$TI_\phi(T') > TI_\phi(T), \text{ when } \phi \in \{S, S'\}$$

Proof. Let T_u denote the component containing u after deleting the edges uv_1 and uv_2.

For every edge xy in T_u, the values of $n_x(m_x)$ and $n_y(m_y)$ remain unchanged in both T and T'. Hence their contributions to the index remain the same.

Only the edges uv_1 and uv_2 change their contributions.

Thus for vertex version of Szeged indices,

$$\begin{aligned} TI_\phi(T') - TI_\phi(T) &= \phi_{T'}(n_{v_1}, n_{v_2}) + \phi_{T'}(n_u, n_{v_1}) \\ &\quad - \phi_T(n_u, n_{v_1}) - \phi_T(n_u, n_{v_2}) \\ &= \phi(n-1,1) + \phi(n-2,2) - 2\phi(n-1,1) \\ &= \phi(n-2,2) - \phi(n-1,1) \\ &= \begin{cases} < 0, & \text{if } \phi \in M \\ > 0, & \text{if } \phi \in S \end{cases} \end{aligned}$$

Now, in the case of edge based Szeged indices,

$$\begin{aligned} TI_\phi(T') - TI_\phi(T) &= \phi_{T'}(m_{v_1}, m_{v_2}) + \phi_{T'}(m_u, m_{v_1}) \\ &\quad - \phi_T(m_u, m_{v_1}) - \phi_T(m_u, m_{v_2}) \\ &= \phi(n-2,0) + \phi(n-3,1) - 2\phi(n-2,0) \\ &= \phi(n-3,1) - \phi(n-2,0) \\ &= \begin{cases} < 0, & \text{if } \phi \in M' \\ > 0, & \text{if } \phi \in S' \end{cases} \end{aligned}$$

Thus, the result holds. ■

Using the increasing property of the exponential function, we can directly obtain the following from the Lemma 3.

Corollary. *Let T and T' be the trees obtained as in Lemma 3, then*

$$eTI_\phi(T') < eTI_\phi(T), \text{ when } \phi \in \{M, M'\}$$
$$eTI_\phi(T') > eTI_\phi(T), \text{ when } \phi \in \{S, S'\}$$

Lemma 4. *Let T be a tree with a pendant edge $e = uv_1$ at the vertex u with $d(v_1) = 1$. Suppose there exist vertices w_1, w_2 such that $d(w_1) = 1$, $d(w_2) = 1$, $d(u, w_1) \geq 2$ and $d(w_2, u) \geq 2$. Let uu_1 be an edge of T with $d(u_1) \neq 1$. Define the tree*

$$T' = T - uu_1 + u_1v_1.$$

Then

$$TI_\phi(T') < TI_\phi(T), \text{ when } X \in \{M, M'\}$$
$$TI_\phi(T') > TI_\phi(T), \text{ when } X \in \{S, S'\}$$

Proof. Note that except for the edges uu_1 and uv_1 in T, for all other edges xy of T we have

$$n_x|_T = n_x|_{T'}, \qquad n_y|_T = n_y|_{T'}$$
$$m_x|_T = m_x|_{T'}, \qquad m_y|_T = m_y|_{T'}$$

Thus

$$\phi_T(n_x, n_y) = \phi_{T'}(n_x, n_y).$$
$$\phi_T(m_x, m_y) = \phi_{T'}(m_x, m_y).$$

Also note that

$$\phi_T(n_{u_1}, n_u) = \phi_{T'}(n_{u_1}, n_{v_1})$$
$$\phi_T(m_{u_1}, m_u) = \phi_{T'}(m_{u_1}, m_{v_1})$$

Let T_{u_1} and T_u (respectively, T'_{u_1} and T'_u) denote the components containing u_1 and u in T (respectively, T'), obtained by deleting the edge uu_1.

Now,

$$n_{u_1}|_T = |T_{u_1}| = 1 \quad n_{u_1}|_{T'} = |T'_{u_1}| > 1$$
$$n_u|_T = |T_u| = n-1 \quad n_u|_{T'} = |T'_u| < n-1$$

and

$$m_{u_1}|_T = |T_{u_1}| - 1 = 0 \quad m_{u_1}|_{T'} = |T'_{u_1}| - 1 > 0$$
$$m_u|_T = |T_u| - 1 = n-2 \quad n_u|_{T'} = |T'_u| - 1 < n-2$$

Hence, for vertex version of Szeged index, we have

$$\begin{aligned} TI_\phi(T') - TI_\phi(T) &= \phi_{T'}(n_{v_1}, n_u) - \phi_T(n_{v_1}, n_u) \\ &= \phi_{T'}(n_{v_1}, n_u) - \phi_T(n-1, 1) \\ &= \begin{cases} < 0, & \text{for } \phi \in M \\ > 0, & \text{for } \phi \in S \end{cases} \end{aligned}$$

and for the edge version of Szged index, we have

$$\begin{aligned} TI_\phi(T') - TI_\phi(T) &= \phi_{T'}(m_{v_1}, m_u) - \phi_T(m_{v_1}, m_u) \\ &= \phi_{T'}(m_{v_1}, m_u) - \phi_T(n-2, 0) \\ &= \begin{cases} < 0, & \text{for } \phi \in M' \\ > 0, & \text{for } \phi \in S' \end{cases} \end{aligned}$$

Therefore,

$$TI_\phi(T') < TI_\phi(T), \text{ when } \phi \in \{M, M'\}$$
$$TI_\phi(T') > TI_\phi(T), \text{ when } \phi \in \{S, S'\}.$$ ■

Corollary. *Let T and T' be the trees obtained as in Lemma 4, then*

$$eTI_\phi(T') < eTI_\phi(T), \text{ when } \phi \in \{M, M'\}$$
$$eTI_\phi(T') > eTI_\phi(T), \text{ when } \phi \in \{S, S'\}.$$

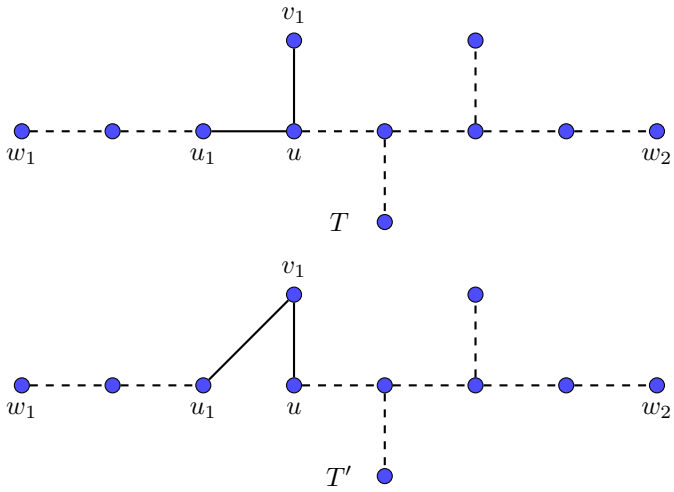

Figure 3. Transformation of tree T to T' described in Lemma 4.

Lemma 5. *Let T be a tree such that there exists a vertex u on T having at least two paths say P_1 and P_2 of lengths t and s attached to u respectively, where $t, s \leq \frac{n}{2}$. Denote*

$$P_1 : uu_1u_2 \dots u_t \qquad P_2 : uv_1v_2 \dots v_s$$

with $s \leq t$. Let T' be the tree obtained from T by

$$T' = T - uv_1 + u_1v_1.$$

Then

$$TI_\phi(T') < TI_\phi(T), \text{ when } \phi \in \{M, M'\}$$
$$TI_\phi(T') > TI_\phi(T), \text{ when } \phi \in \{S, S'\}.$$

Proof. It is clear that except for the edges uu_1, uv_1, u_1v_1 and v_1v, all the other edges have the same contribution of values of

$$\phi(f(u), f(v))$$

in T and T'. The only changes occur in these edges. Therefore, for vertex based Szeged indices,

$$\begin{aligned} TI_\phi(T') - TI_\phi(T) &= \phi_{T'}(n_{u_1}, n_{v_1}) + \phi_{T'}(n_{u_1}, n_u) \\ &\quad - \phi_T(n_u, n_{u_1}) - \phi_T(n_u, n_{v_1}) \\ &= \phi(n-(t+s), t+s) + \phi(n-t, t) \\ &\quad - \phi(n-t, t) - \phi(n-s, s) \\ &= \phi(n-(t+s), t+s) - \phi(n-s, s) \end{aligned}$$

Now choose, $a = n-(s+t), b = (s+t), c = t$. Thus

$$\begin{aligned} \phi(n-(t+s), t+s) - \phi(n-s, s) &= \phi(a, b) - \phi(a+c, b-c) \\ &= \begin{cases} < 0, & \text{for } \phi \in M \\ > 0, & \text{for } \phi \in S \end{cases} \end{aligned}$$

Since

$$n - s > n - (t+s), n - (t+s) > t + s \text{ and } \phi(a+1, b-1) > \phi(a.b)$$

$$TI_\phi(T') - TI_\phi(T) = \begin{cases} < 0, & \text{for } \phi \in M \\ > 0, & \text{for } \phi \in S \end{cases}$$

Now, in the case of edge based Szeged indices,

$$\begin{aligned} TI_\phi(T') - TI_\phi(T) &= \phi_{T'}(m_{u_1}, m_{v_1}) + \phi_{T'}(m_{u_1}, m_u) \\ &\quad - \phi_T(m_u, m_{u_1}) - \phi_T(m_u, m_{v_1}) \\ &= \phi(n-(t+s)-1, t+s-1) + \phi(n-t-1, t-1) \\ &\quad - \phi(n-t-1, t-1) - \phi(n-s-1, s-1) \\ &= \phi(n-(t+s)-1, t+s-1) - \phi(n-s-1, s-1) \end{aligned}$$

Now choose, $a = n - (s+t) - 1, b = (s+t) - 1, c = t$. Thus

$$\begin{aligned}\phi(n-(t+s)-1, t+s-1) - \phi(n-s-1, s-1) \\ &= \phi(a,b) - \phi(a+c, b-c) \\ &= \begin{cases} < 0, & \text{for } \phi \in M' \\ > 0, & \text{for } \phi \in S' \end{cases}\end{aligned}$$

Thus, the result follows. ■

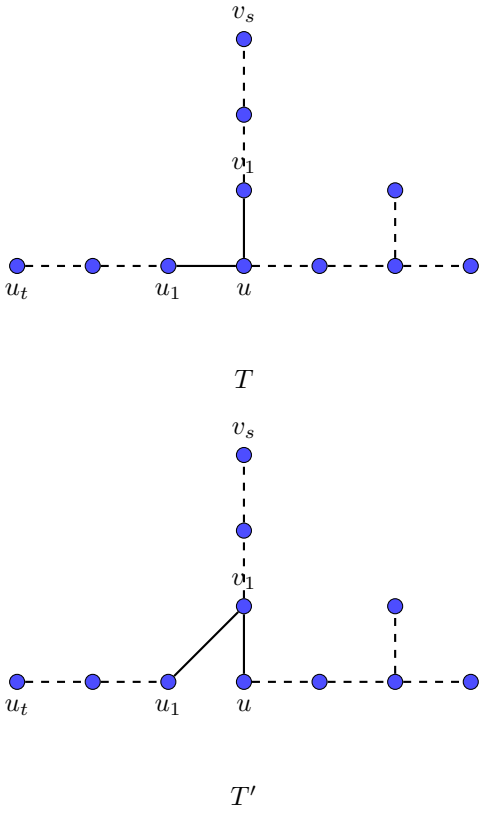

Figure 4. Transformation of tree T into T' described in Lemma 5.

Corollary. *Let T and T' be the trees obtained as in Lemma 4, then*

$$eTI_\phi(T') < eTI_\phi(T), \text{ when } \phi \in \{M, M'\}$$
$$eTI_\phi(T') > eTI_\phi(T), \text{ when } \phi \in \{S, S'\}.$$

Theorem 3. *Among all trees of fixed order n, the path graph P_n uniquely maximizes all S- and S'-class Szeged indices and uniquely minimizes all M- and M'-class Szeged indices.*

Proof. The result directly follows from the transformations described in Lemma 3, Lemma 4 and Lemma 5. ■

Theorem 4. *Among all trees of fixed order n, the path graph P_n uniquely maximizes all S- and S'-class exponential Szeged indices and uniquely minimizes all M- and M'-class exponential Szeged indices.*

Proof. The result follows directly from the transformations described in Lemmas 3–5 and their corresponding corollaries. ■

Remark. For the P, P'-class indices, the function ϕ satisfies

$$\phi(a+1, b-1) = \phi(a, b).$$

Hence, the value of the corresponding topological index remains invariant under the above transformation. Consequently, all trees of a fixed order attain the same value of the index.

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