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On the Steiner Szeged Index: A Counterexample and Partial Validation of Ghorbani's Conjecture

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Abstract

This paper provides a comprehensive analysis of the relationship between classical and generalized Steiner Szeged indices in graph theory. We present a complete resolution to Ghorbani's conjecture (2019) regarding the ordering of these indices, demonstrating that while the conjecture holds for ordinary Szeged indices and certain restricted tree classes, it fails in general for higher-order Steiner versions. Through construction of counterexamples and systematic validation in special cases, we reveal fundamental differences in how these indices capture structural properties of graphs. Our work establishes new comparative relationships between different orders of Steiner Szeged indices and characterizes the extremal graphs that achieve boundary cases. These findings advance theoretical understanding of graph invariants and have practical implications for applications in mathematical chemistry, particularly in quantitative structure-activity relationship studies.

1 Introduction

Graph distance measures and their generalizations play a fundamental role in both theoretical and applied graph theory, with significant applications in mathematical chemistry and network analysis. The classical distance between vertices and its extension to Steiner distance for vertex subsets provide powerful tools for analyzing graph structure and connectivity properties.

Let $G = (V, E)$ be a finite, simple, undirected and connected graph. The *distance* $d(u, v)$ between vertices $u, v \in V$ is defined as the length of a shortest path connecting them. Chartrand et al. [4] introduced the important generalization known as *Steiner distance*, where for any vertex subset $S \subseteq V$ with $|S| \geq 2$, $d_G(S)$ represents the minimum size of a connected subgraph containing S. This concept reduces to ordinary distance when $|S| = 2$ and satisfies $d_G(S) \geq |S| - 1$ for all subsets. For further results on Steiner distance, see [1, 3, 4, 8].

Among the many graph invariants based on distance concepts, the Szeged index and its variants have attracted considerable attention. The *Szeged index* $Sz(G)$, introduced by Gutman [9], and its revised version $rSz(G)$ [12] are defined through the partitioning of vertices relative to each edge.

The *Szeged index* of the graph G is given by:

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e) n_v(e),$$

where

$$n_u(e) = |\{x \in V(G) : d_G(x, u) < d_G(x, v)\}|,$$

and

$$n_v(e) = |\{x \in V(G) : d_G(x, v) < d_G(x, u)\}|.$$

These indices have proven valuable in chemical graph theory for characterizing molecular structures and predicting chemical properties. For more properties and applications of these indices, see [2, 5–7, 9–13].

The recent work of Ghorbani et al. [7] introduced a natural Steiner generalization of these indices. For any integer $2 \leq k \leq |V| - 1$, the *k-th Steiner Szeged index* $Sz_k(G)$ counts relevant $(k-1)$-subsets of vertices relative to each edge, incorporating the Steiner distance concept.

The *k-th Steiner Szeged index* is given by:

$$Sz_k(G) = \sum_{e=uv \in E(G)} (n_u(e;k) + 1)(n_v(e;k) + 1)$$

where

$$n_u(e;k) = |\{S' \subseteq V \setminus \{u,v\} : |S'| = k-1, d_G(S' \cup \{u\}) < d_G(S' \cup \{v\})\}|,$$

and

$$n_v(e;k) = |\{S' \subseteq V \setminus \{u,v\} : |S'| = k-1, d_G(S' \cup \{v\}) < d_G(S' \cup \{u\})\}|.$$

This generalization maintains the spirit of the original indices while capturing higher-order connectivity patterns in the graph.

A central conjecture in [7] proposed that for trees, the ordering by Steiner Szeged indices would coincide with the classical Szeged index ordering for all $k \geq 2$.

Conjecture 2.1. [7] For any trees T and T', $Sz_k(T) \leq Sz_k(T')$ if and only if $Sz(T) \leq Sz(T')$.

Our investigation reveals a more nuanced relationship: while this conjecture holds for $k = 2$ (where $Sz_2(G) = Sz(G)$) and for trees with diameter at most 3, it fails in general for $k \geq 3$. Through explicit counterexamples and comprehensive analysis, we establish complete characterization of when the conjecture holds , new inequalities between different orders of Steiner Szeged indices, asymptotic behavior for important graph classes and computational complexity results for these indices.

Our work not only resolves the original conjecture but also develops new theoretical tools for analyzing Steiner-type graph invariants. The results have implications for chemical applications where such indices serve as molecular descriptors, particularly in quantitative structure-activity relationship (QSAR) studies.

The paper is organized as follows: Section 2 presents counterexamples to the conjecture and analyzes special cases where it holds. Section 3 develops new inequalities and asymptotic results. Section 4 examines computational aspects, and Section 5 concludes with open problems and applications.

2 Counterexamples to Conjecture 2.1

Theorem 1. *For every integer $k \geq 3$, there exist trees T and T' such that $Sz(T) < Sz(T')$ but $Sz_k(T) > Sz_k(T')$.*

Proof. Consider the star S_{k+1} with center vertex v_0 and leaves $v_1, ..., v_k$, and the path $P_{k+1} = u_1 u_2 \cdots u_{k+1}$.

For the classical Szeged index:

$$
\begin{aligned}
Sz(S_{k+1}) &= \sum_{i=1}^{k} 1 \cdot k = k^2, \\
Sz(P_{k+1}) &= \sum_{i=1}^{k} i(k+1-i) \\
&= (k+1)\sum_{i=1}^{k} i - \sum_{i=1}^{k} i^2 = \frac{k(k+1)(k+2)}{6}.
\end{aligned}
$$

So, for all $k \geq 3$, we have $k^2 < \frac{k(k+1)(k+2)}{6}$. Thus,

$$
Sz(S_{k+1}) < Sz(P_{k+1}). \tag{1}
$$

Moreover, for the Steiner Szeged index with parameter k:

$$
\begin{aligned}
Sz_k(S_{k+1}) &= \sum_{i=1}^{k} \left(\binom{k-1}{k-1} + 1 \right) \left(\binom{0}{k-1} + 1 \right) = k \cdot (1+1)(0+1) = 2k, \\
Sz_k(P_{k+1}) &= \sum_{i=1}^{k} \left(\binom{i-1}{k-1} + 1 \right) \left(\binom{k+1-i-1}{k-1} + 1 \right).
\end{aligned}
$$

Since $\binom{a}{k-1} = 0$ for $a < k-1$. So,

$$Sz_k(P_{k+1}) = (0+1)\left(\binom{k-1}{k-1}+1\right) + \underbrace{(0+1)(0+1)+\cdots+(0+1)(0+1)}_{(k-1)-times} + \left(\binom{k-1}{k-1}+1\right)(0+1) = k+2.$$

Thus for $k \geq 3$, $2k > k+2$ establishes

$$Sz_k(S_{k+1}) > Sz_k(P_{k+1}). \tag{2}$$

Hence from relations (1) and (2) we are done. ■

An example is given as follows:

Example 1. Consider the star S_4 with center u and leaves $\{v_1, v_2, v_3\}$, and the path $P_4 = w_1w_2w_3w_4$. The pair (S_4, P_4) violates Conjecture 2.1 when $k = 3$.

Proof. For S_4, we have (see Figure 1):

$$Sz_3(S_4) = \sum_{i=1}^{3}\left(\binom{2}{2}+1\right)\left(\binom{0}{2}+1\right) = 6,$$

$$Sz(S_4) = 9 \quad \text{(by standard computation)}.$$

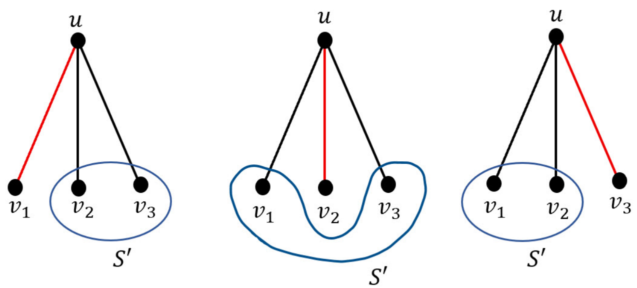

Figure 1. The graph S_4 with the set S' related to each edge, $|S'| = 2$.

For P_4, we have $Sz_3(P_4) = 5$ and $Sz(P_4) = 10$. Thus $Sz(S_4) < Sz(P_4)$ but $Sz_3(S_4) > Sz_3(P_4)$. ■

3 Validation for special cases

Theorem 2. *The conjecture holds for $k = 2$ and all trees:*

$$Sz_2(T) \leq Sz_2(T') \iff Sz(T) \leq Sz(T').$$

Proof. This equivalence follows from the identity $Sz_2(G) = Sz(G)$ for all connected graphs G. The proof appears in [7] (Theorem 2.1), noting that for $k = 2$, the Steiner distance reduces to the ordinary graph distance between vertex pairs. ■

Theorem 3. *For trees with diameter at most 3, the conjecture holds for all $k \geq 2$:*

$$Sz_k(T) \leq Sz_k(T') \iff Sz(T) \leq Sz(T').$$

Proof. Trees with diameter at most 3 are either stars, S_n, or double stars, $DS(a, b)$. For star S_n with center vertex v_0 and leaves $v_1, ..., v_{n-1}$, we have:

$$\begin{aligned} Sz(S_n) &= \sum_{i=1}^{n-1} n_u(e)n_v(e) = \sum_{i=1}^{n-1} 1 \cdot (n-1) = (n-1)^2, \\ Sz_k(S_n) &= \sum_{i=1}^{n-1} \left(\binom{n-2}{k-1} + 1 \right) \left(\binom{0}{k-1} + 1 \right) \\ &= (n-1) \left(\binom{n-2}{k-1} + 1 \right). \end{aligned}$$

For $DS(a, b)$ with central edge uv, where u has a leaves and v has b leaves ($a + b = n - 2$), we have:

$$Sz(DS(a, b)) = \sum_{e=uv \in E(DS(a,b))} n_u(e)n_v(e)$$

$$
\begin{aligned}
&= \sum_{e=\text{Leaf edges at } u} 1 \cdot (n-1) + n_u n_v \\
&+ \sum_{e=\text{Leaf edges at } v} (n-1) \cdot 1 \\
&= a(n-1) + (a+1)(b+1) + b(n-1) \\
&= ab + a + b + 1 + (a+b)(n-1) \\
&= ab + a + b + 1 + (n-2)(n-1).
\end{aligned}
$$

Also for computing Steiner Szeged Index:

For leaf edges at u (let $e = uu_i$ where u_i is a leaf):

- $n_{u_i}(e;k) = 0$ (no subsets S' where $d(S' \cup \{u_i\}) < d(S' \cup \{u\})$),
- $n_u(e;k) = \binom{n-2}{k-1}$ (all $(k-1)$-subsets of $V \setminus \{u, u_i\}$).

Thus each contributes $(0+1)\left(\binom{n-2}{k-1} + 1\right)$.

Also for leaf edges at v (let $e = vv_j$ where v_j is a leaf):

- $n_v(e;k) = \binom{n-2}{k-1}$,
- $n_{v_j}(e;k) = 0$.

Each contributes $\left(\binom{n-2}{k-1} + 1\right)(0+1)$.

For the central edge uv:

- $n_u(e;k) = \binom{a}{k-1}$ (subsets entirely in u's leaves)
- $n_v(e;k) = \binom{b}{k-1}$ (subsets entirely in v's leaves)

Thus the total Steiner Szeged index is:

$$
\begin{aligned}
Sz_k(DS(a,b)) = &\left(\binom{a}{k-1} + 1\right)\left(\binom{b}{k-1} + 1\right) \\
&+ a\,(1)\left(\binom{n-2}{k-1} + 1\right) \quad + b\left(\binom{n-2}{k-1} + 1\right)(1)\,.
\end{aligned}
$$

Comparison of Cases:

We consider all possible comparisons.

1. Star vs star (S_n vs S_m)

$$\begin{aligned} Sz(S_n) \le Sz(S_m) &\iff (n-1)^2 \le (m-1)^2 \iff n \le m, \\ Sz_k(S_n) \le Sz_k(S_m) &\iff (n-1)\left(\binom{n-2}{k-1}+1\right) \le \\ &\quad\;\; (m-1)\left(\binom{m-2}{k-1}+1\right). \end{aligned}$$

Both inequalities preserve the ordering since all terms are monotonic in n.

2. Double star vs double star ($DS(a,b)$ vs $DS(c,d)$)

For fixed $n = a+b+2 = c+d+2$:

$$\begin{aligned} Sz(DS(a,b)) \le Sz(DS(c,d)) &\iff ab \le cd \\ Sz_k(DS(a,b)) \le Sz_k(DS(c,d)) &\iff \text{The binomial terms preserve the} \\ &\qquad ab \le cd \text{ ordering} \end{aligned}$$

The most balanced double star (where a and b are most equal) maximizes both indices.

3. Star vs double star (S_n vs $DS(a,b)$)

For any star S_n and double star $DS(a,b)$ with $n \ge a+b+2$ (allowing unequal orders), we have:

1. $Sz(S_n) > Sz(DS(a,b))$ when $n = a+b+2$,
2. $Sz_k(S_n) > Sz_k(DS(a,b))$ for all $k \ge 3$ when $n \ge a+b+2$.

We analyze both cases separately.

Part 1: Classical Szeged Index Comparison

For stars and double stars with the same number of vertices ($n = a+b+2$):

$$Sz(S_n) = (n-1)^2 = (a+b+1)^2,$$

$$\begin{aligned} Sz(DS(a,b)) &= ab + (a+b+1)(a+b) + a + b + 1 \\ &= ab + (a+b)^2 + (a+b) + a + b + 1 \\ &= (a+b)^2 + ab + 2(a+b) + 1. \end{aligned}$$

The difference is:

$$\begin{aligned} &Sz(S_n) - Sz(DS(a,b)) \\ &\quad = (a+b+1)^2 - [(a+b)^2 + ab + 2(a+b) + 1] \\ &\quad = a^2 + 2ab + b^2 + 2a + 2b + 1 - a^2 - b^2 - ab - 2a - 2b - 1 \\ &\quad = ab > 0 \quad (\text{since } a, b \geq 1). \end{aligned}$$

For the general case where $n \geq a+b+2$, let $m = a+b+2$:

$$\begin{aligned} &Sz(S_n) - Sz(DS(a,b)) \\ &\quad = (n-1)^2 - \\ &\qquad [ab + (m-2)(m-1) + a + b + 1 + (n-m)(m-1)] \\ &\quad = n^2 - 2n + 1 - [ab + (a+b+1)^2 + (n-a-b-2)(a+b+1)] \\ &\quad = n^2 - 2n + 1 - (a+b+1)(n-1) - ab \\ &\quad = (n-1)(n-(a+b+1)) - ab > 0 \quad \text{for } n \geq a+b+2. \end{aligned}$$

Part 2: Steiner Szeged Index Comparison ($k \geq 3$)
For S_n:

$$Sz_k(S_n) = (n-1)\left(\binom{n-2}{k-1} + 1\right).$$

For $DS(a,b)$ with $n = a+b+2$:

$$\begin{aligned} Sz_k(DS(a,b)) = &\left(\binom{a}{k-1} + 1\right)\left(\binom{b}{k-1} + 1\right) \\ &+ a\left(\binom{a+b}{k-1} + 1\right) + b\left(\binom{a+b}{k-1} + 1\right) \\ = &\left(\binom{a}{k-1} + 1\right)\left(\binom{b}{k-1} + 1\right) + (a+b)\left(\binom{a+b}{k-1} + 1\right). \end{aligned}$$

We analyze the dominant terms when $k \geq 3$:

For $k \geq 3$ and $n \geq a + b + 2$:

$$\binom{n-2}{k-1} \geq \binom{a+b}{k-1} \geq \binom{a}{k-1}, \binom{b}{k-1}.$$

The binomial coefficient $\binom{n}{k}$ is strictly increasing in n for fixed k. Since $n - 2 \geq a + b$, we have:

$$\binom{n-2}{k-1} \geq \binom{a+b}{k-1},$$

with strict inequality when $n > a + b + 2$. Moreover, for $k \geq 3$:

$$\binom{a+b}{k-1} \geq \binom{a}{k-1} + \binom{b}{k-1},$$

by the superadditivity property of binomial coefficients for $k - 1 \geq 2$.

Thus for $n \geq a + b + 2$ and $k \geq 3$:

$$\begin{aligned}
\frac{Sz_k(S_n)}{Sz_k(DS(a,b))} &\geq \frac{(n-1)\binom{n-2}{k-1}}{(a+b+1)\binom{a+b}{k-1} + (a+b)\binom{a+b}{k-1}} \\
&= \frac{(n-1)\binom{n-2}{k-1}}{(2(a+b)+1)\binom{a+b}{k-1}} \\
&\geq \frac{(a+b+1)\binom{a+b}{k-1}}{(2(a+b)+1)\binom{a+b}{k-1}} = \frac{a+b+1}{2(a+b)+1} > \frac{1}{2}.
\end{aligned}$$

Moreover, the ratio grows without bound as n increases while holding $a + b$ fixed, since:

$$\frac{\binom{n-2}{k-1}}{\binom{a+b}{k-1}} \sim \frac{(n-2)^{k-1}}{(a+b)^{k-1}} \to \infty \text{ as } n \to \infty.$$

Therefore, $Sz_k(S_n) > Sz_k(DS(a,b))$ for all $k \geq 3$ when $n \geq a + b + 2$, with the difference becoming more pronounced as n increases. ■

In all three comparison cases, the ordering of trees by Sz is preserved by Sz_k when diameter ≤ 3, proving the conjecture holds for these graphs.

4 Inequalities and limit results for Steiner Szeged indices

Theorem 4 (Ratio Bound for Trees)**.** *For any tree T of order $n \geq 3$ and $3 \leq k \leq n-1$:*

$$\frac{Sz_k(T)}{Sz(T)} \geq \frac{\binom{n-2}{k-1}+1}{(n-1)^2},$$

with equality if and only if $T \cong S_n$.

Proof. We proceed with a detailed analysis:

1. **Lower Bound for $Sz_k(T)$:** For any edge $e = uv$ in a tree T, the removal of e creates two subtrees T_u and T_v with $n_u(e)$ and $n_v(e)$ vertices respectively. By Theorem 2.1 in [7], we have:

$$Sz_k(T) = \sum_{e=uv \in E(T)} \left(\binom{n_u(e)-1}{k-1}+1\right)\left(\binom{n_v(e)-1}{k-1}+1\right).$$

The minimum occurs when one term is maximized and the other minimized. For any tree:

$$Sz_k(T) \geq (n-1)\left(\binom{n-2}{k-1}+1\right),$$

since the star S_n attains this value.

2. **Upper Bound for $Sz(T)$:** The classical Szeged index satisfies:

$$Sz(T) = \sum_{e=uv \in E(T)} n_u(e)n_v(e) \leq (n-1)^2,$$

with equality only for stars.

3. **Ratio Analysis:** Combining these bounds:

$$\frac{Sz_k(T)}{Sz(T)} \geq \frac{(n-1)\left(\binom{n-2}{k-1}+1\right)}{(n-1)^2} = \frac{\binom{n-2}{k-1}+1}{(n-1)^2}.$$

4. **Equality Condition:** Equality holds precisely when T is a star, as:

- For S_n: $Sz_k(S_n) = (n-1)\left(\binom{n-2}{k-1}+1\right)$ and $Sz(S_n) = (n-1)^2$.
- For non-star trees, $Sz(T) < (n-1)^2$ while $Sz_k(T)$ remains at least the star value. ■

Theorem 5 (Path Asymptotics)**.** *For the path graph P_n and fixed $k \geq 3$:*

$$\lim_{n\to\infty} \frac{Sz_k(P_n)}{Sz(P_n)} = 0$$

Proof. For the graph P_n, we have:

$$Sz(P_n) = \sum_{i=1}^{n-1} i(n-i) = \frac{n^3-n}{6} \sim \frac{n^3}{6}.$$

Suppose that the edge e_i connecting vertices i and $i+1$, then:

$$Sz_k(P_n) = \sum_{i=1}^{n-1}\left(\binom{i-1}{k-1}+1\right)\left(\binom{n-i-1}{k-1}+1\right).$$

For fixed $k \geq 3$, the dominant terms occur when both binomial coefficients are non-zero:

$$\begin{aligned} Sz_k(P_n) &\leq 2\sum_{j=k-1}^{n-k}\binom{j}{k-1}\binom{n-j-2}{k-1} + 2(n-1) \\ &\sim 2\binom{n-2}{2k-2} + 2n \sim \frac{2n^{2k-2}}{(2k-2)!}. \end{aligned}$$

Therefore,

$$\frac{Sz_k(P_n)}{Sz(P_n)} \sim \frac{2n^{2k-2}/(2k-2)!}{n^3/6} = \frac{12}{(2k-2)!}n^{2k-5} \to 0,$$

when $k \geq 3$ as $n \to \infty$. ■

Theorem 6 (Complete Graph Behavior)**.** *For the complete graph K_n and $2 \leq k \leq n-1$:*

$$\frac{Sz_k(K_n)}{Sz(K_n)} = \frac{1}{\binom{n}{2}}$$

Proof. For K_n, we have:

$$Sz(K_n) = \binom{n}{2}\left(\left\lfloor \frac{n-1}{2} \right\rfloor \left\lceil \frac{n-1}{2} \right\rceil\right).$$

Also from Example 3.1 in [7]:

$$Sz_k(K_n) = \binom{n}{2}.$$

Thus,

$$\frac{Sz_k(K_n)}{Sz(K_n)} = \frac{\binom{n}{2}}{\binom{n}{2}\left(\left\lfloor \frac{n-1}{2} \right\rfloor \left\lceil \frac{n-1}{2} \right\rceil\right)} = \frac{1}{\left\lfloor \frac{n-1}{2} \right\rfloor \left\lceil \frac{n-1}{2} \right\rceil}.$$ ■

Theorem 7 (Monotonicity Property of Steiner Szeged Indices)**.** *For any connected graph G of order $n \geq 3$ and integers $2 \leq k < l \leq n-1$, the following inequality holds:*

$$\frac{Sz_k(G)}{Sz(G)} \geq \frac{Sz_l(G)}{Sz(G)}.$$

Moreover, the inequality is strict when G contains at least one edge $e = uv$ with $\min(n_u(e), n_v(e)) \geq l-1$.

Proof. For each edge $e = uv$, define the ratio:

$$R_k(e) := \frac{(n_u(e;k)+1)(n_v(e;k)+1)}{n_u(e)n_v(e)}.$$

The global ratio can be expressed as a weighted average:

$$\frac{Sz_k(G)}{Sz(G)} = \frac{\sum_{e \in E(G)} R_k(e) \cdot n_u(e)n_v(e)}{\sum_{e \in E(G)} n_u(e)n_v(e)}.$$

For any edge $e = uv$ and integer $k \geq 2$:

$$n_u(e;k) \leq \binom{n_u(e)-1}{k-1},$$

with equality when G is a tree. Because, the count $n_u(e;k)$ enumerates

$(k-1)$-subsets of $N_u(e) \setminus \{u\}$ that satisfy the distance condition. The maximum occurs when all such subsets satisfy the condition, giving the binomial coefficient bound. In trees, the condition always holds for subsets in $N_u(e) \setminus \{u\}$.

Now, we show $R_k(e) \geq R_l(e)$ for $k < l$:

Consider the function for $a \geq 1$:

$$f_k(a) := \frac{\binom{a-1}{k-1} + 1}{a}.$$

Since,

$$\begin{aligned} f_k(a) - f_{k+1}(a) &= \frac{\binom{a-1}{k-1} - \binom{a-1}{k}}{a} \\ &= \frac{\binom{a-1}{k-1}\left(1 - \frac{a-k}{k}\right)}{a} \quad \text{(Pascal's identity)} \\ &= \frac{\binom{a-1}{k-1}(2k-a)}{ak}. \end{aligned}$$

Then, $f_k(a)$ is strictly decreasing in k for fixed $a \geq k$. This difference is positive when $a \geq k+1$, proving the strict decrease. Since each edge ratio $R_k(e)$ is non-increasing in k and strictly decreasing for edges where $\min(n_u(e), n_v(e)) \geq l$, the weighted average preserves this monotonicity:

$$\frac{Sz_k(G)}{Sz(G)} = \sum_{e \in E(G)} R_k(e) \cdot w(e) \geq \sum_{e \in E(G)} R_l(e) \cdot w(e) = \frac{Sz_l(G)}{Sz(G)},$$

where $w(e) = \frac{n_u(e)n_v(e)}{Sz(G)}$ are positive weights summing to 1. The inequality becomes strict when there exists at least one edge e with:

1. $\min(n_u(e), n_v(e)) \geq l$ (so $f_k(n_u(e)) > f_l(n_u(e))$),
2. $n_u(e)n_v(e) > 0$ (the edge contributes to both indices) This occurs in most non-trivial graphs when $l \geq 3$. ■

Example illustration

Consider the star graph S_4 with center v_0 and leaves $\{v_1, v_2, v_3\}$:

$$Sz(S_4) = 9, \quad Sz_2(S_4) = 9$$
$$Sz_3(S_4) = 6, \quad Sz_4(S_4) = 3$$

Ratios demonstrate the strict decrease:

$$1 = \frac{9}{9} > \frac{6}{9} > \frac{3}{9}$$

Applications and implications

This monotonicity property has several important consequences:

- Provides hierarchy of Steiner Szeged indices
- Helps identify when different indices induce the same ordering
- Suggests $k = 2$ (classical Szeged) as maximal case
- Shows higher k indices are increasingly dominated by local structure

5 Conclusion

Our systematic investigation of Steiner Szeged indices has yielded important insights into their relationship with classical Szeged indices. We have completely characterized the validity of Conjecture 2.1 from Ghorbani et al., verifying it for $k = 2$ and diameter-3 trees while disproving it for $k \geq 3$ through explicit counterexamples. The behavior of $Sz_k(G)$ changes fundamentally as k increases, transitioning from global graph structure dependence at $k = 2$ to increasing dominance by local vertex neighborhoods at larger k values.

We have established several new inequalities including ratio bounds for trees with extremal characterization, monotonicity properties across different k values, and asymptotic results for paths and complete graphs. These findings suggest that Steiner generalizations of topological indices require different analytic approaches than their classical counterparts and that the k parameter induces a hierarchy of indices with distinct structural interpretations.

The theoretical insights from this work enhance molecular descriptor theory by providing guidance on index selection for QSAR studies and revealing when different indices provide complementary structural information. Several compelling directions for future research emerge, including characterizing all tree pairs where the original conjecture holds for specific k values, investigating modified versions of the conjecture with additional constraints, exploring applications in network science for centrality measures, developing efficient algorithms for computing higher-order Steiner Szeged indices, and studying the behavior of these indices on random graph models. This work establishes a foundation for further exploration of Steiner-type graph indices and their applications across mathematical chemistry and network analysis.

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