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A Path Counterexample to Li's Steiner–Gutman Index Conjecture

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Abstract

We disprove a conjectured upper bound for the Steiner–Gutman index of trees, proposed by Li in *MATCH Commun. Math. Comput. Chem.* **95** (2026) 125–139. The path P_8 gives a counterexample for $k = 5$. More generally, every path P_n with $n \geq 8$ violates the conjectured bound for $k = 5$, and for every $k \geq 6$ the bound fails on all paths P_n with $n \geq k + 2$. The proof uses an exact path identity and an elementary monotonicity argument. We also establish a valid universal upper bound based on pairwise distances and vertex degrees. The conjecture's proved $k = 4$ case is unaffected.

1 Introduction

The Gutman index is a degree-weighted distance index used in mathematical chemistry to describe the structure of molecular graphs [2]. Its Steiner generalization replaces the distance between two vertices by the number of edges in a smallest connected subgraph spanning a selected vertex set [1,4]. Paths are especially natural test graphs: they describe linear chains, and their Steiner distances admit explicit formulas.

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In *The Steiner Gutman Index of Trees*, Li [3] proved an upper bound for the Steiner–Gutman 4-index (Theorem 2.3) and proposed an extension to every $k \geq 4$ (Conjecture 1). We show that this proposed extension is false for all $k \geq 5$. A counterexample occurs already on the eight-vertex path, and the failure persists in infinite path families.

The formula for the Steiner–Gutman index of a path is due to Mao and Das [4] and is also recorded by Li [3, Proposition 1.3]. We include a short derivation to make the comparison self-contained. The contributions of this note are the comparison with Li's coefficient, the infinite counterexample families, and a valid replacement upper bound for all trees.

2 Definitions and the conjecture

Let T be a tree with n vertices. Write $d_T(v)$ for the degree of v, $\mathrm{dist}_T(u,v)$ for the number of edges on the unique path between u and v, and $d_T(S)$ for the number of edges in the smallest subtree containing a set $S \subseteq V(T)$. The Gutman and Steiner–Gutman indices are

$$\mathrm{Gut}(T) = \sum_{\{u,v\}\subseteq V(T)} d_T(u) d_T(v) \,\mathrm{dist}_T(u,v), \tag{1}$$

$$\mathrm{SGut}_k(T) = \sum_{\substack{S\subseteq V(T)\\ |S|=k}} \left(\prod_{v\in S} d_T(v)\right) d_T(S), \qquad 2 \leq k \leq n. \tag{2}$$

In particular, $\mathrm{SGut}_2(T) = \mathrm{Gut}(T)$. Let $\Delta = \max_{v\in V(T)} d_T(v)$.

Conjecture 1 (Li [3], Conjecture 1)**.** *For every tree T of order $n \geq k \geq 4$,*

$$\mathrm{SGut}_k(T) \leq \frac{2\Delta^{k-2}}{k(k-1)}(n-k+1)(n-k+2)\ \mathrm{Gut}(T). \tag{3}$$

For $k = 4$ this is Li's proved theorem. Our counterexamples concern only the proposed generalization to $k \geq 5$.

3 The path identity

Write $P_n = v_1 v_2 \cdots v_n$. Its endpoints have degree 1; the other $n-2$ vertices have degree 2.

Lemma 1 (Mao–Das path formula [4]). *For $n \geq 4$ and $2 \leq k \leq n-2$,*

$$\mathrm{SGut}_k(P_n) = 2^k(k-1)\binom{n}{k+1} + 2^{k-2}(n-1)\binom{n-2}{k-2}, \tag{4}$$

$$\mathrm{Gut}(P_n) = 4\binom{n}{3} + n - 1 = \frac{(n-1)(2n^2-4n+3)}{3}. \tag{5}$$

Proof. For a selected set $S = \{v_{i_1}, \ldots, v_{i_k}\}$ with $i_1 < \cdots < i_k$, the Steiner subtree has $i_k - i_1$ edges. Counting the contribution of every path edge gives

$$\sum_{1 \leq i_1 < \cdots < i_k \leq n} (i_k - i_1) = (k-1)\binom{n+1}{k+1}. \tag{6}$$

For subsets that contain a specified endpoint, the unweighted sum of their spans is

$$\sum_{j=k}^{n} (j-1)\binom{j-2}{k-2} = (k-1)\sum_{j=k}^{n}\binom{j-1}{k-1} = (k-1)\binom{n}{k}.$$

Subsets containing both endpoints number $\binom{n-2}{k-2}$, and each has span $n-1$. If all degrees were 2, the weighted sum would be 2^k times (6). Correcting the factor at each endpoint by inclusion–exclusion yields

$$\begin{aligned}\mathrm{SGut}_k(P_n) &= 2^k(k-1)\left[\binom{n+1}{k+1} - \binom{n}{k}\right] + 2^{k-2}(n-1)\binom{n-2}{k-2} \\ &= 2^k(k-1)\binom{n}{k+1} + 2^{k-2}(n-1)\binom{n-2}{k-2}.\end{aligned}$$

Taking $k = 2$ gives (5). ∎

An equivalent form of (4), useful below, is

$$\mathrm{SGut}_k(P_n) = B_{n,k}\left(1 + \frac{4n(n-k)}{k(k+1)}\right), \qquad B_{n,k} = 2^{k-2}(n-1)\binom{n-2}{k-2}. \tag{7}$$

Indeed, $\binom{n}{k+1}/\binom{n-2}{k-2} = n(n-1)(n-k)/[(k+1)k(k-1)]$.

4 Infinite families of counterexamples

Since $\Delta(P_n) = 2$, the right-hand side of (3) on P_n is

$$L_{n,k} = \frac{2^{k-1}}{k(k-1)}(n-k+1)(n-k+2)G_n, \qquad G_n = \mathrm{Gut}(P_n). \tag{8}$$

Theorem 1. *Li's conjectured inequality* (3) *is false for* $k \geq 5$. *In fact:*

1. $\mathrm{SGut}_5(P_n) > L_{n,5}$ *for every* $n \geq 8$;
2. $\mathrm{SGut}_k(P_n) > L_{n,k}$ *for every* $k \geq 6$ *and* $n \geq k+2$.

In particular,

$$\mathrm{Gut}(P_8) = 231, \quad \mathrm{SGut}_5(P_8) = 4704, \quad L_{8,5} = 3696, \tag{9}$$

so the conjectured bound is exceeded by 1008.

Proof. For $k = 5$, equations (4), (5) and (8) give

$$\begin{aligned}\mathrm{SGut}_5(P_n) - L_{n,5} = {} & \frac{4}{45}(n-1)(n-3)(n-4) \\ & \times (2n^3 - 20n^2 + 47n - 39).\end{aligned} \tag{10}$$

If $n = 8 + t$ with $t \geq 0$, the last factor is $2t^3 + 28t^2 + 111t + 81 > 0$. This proves the first assertion; (9) follows by direct evaluation.

Fix $k \geq 6$. We show that $\mathrm{SGut}_k(P_n)/L_{n,k}$ is strictly increasing in n for $n \geq k+2$. The second factor in (7) is positive and strictly increasing. Also

$$\frac{B_{n+1,k}}{B_{n,k}} = \frac{n}{n-k+1}, \qquad \frac{L_{n+1,k}}{L_{n,k}} = \frac{n-k+3}{n-k+1}\frac{G_{n+1}}{G_n}.$$

Thus $B_{n,k}/L_{n,k}$ increases if $nG_n - (n-k+3)G_{n+1} > 0$. By (5),

$$nG_n - (n-k+3)G_{n+1} = \frac{n}{3}\big[(2k-12)n^2 + 6n + k - 6\big] > 0 \tag{11}$$

for $k \geq 6$. The full ratio therefore increases.

At the first value $n = k + 2$, direct substitution gives

$$\frac{\mathrm{SGut}_k(P_{k+2})}{L_{k+2,k}} = \frac{k(k-1)^2(k^2+9k+16)}{16(k+1)(2k^2+4k+3)}. \tag{12}$$

The numerator minus the denominator is

$$H(k) = k^5 + 7k^4 - 33k^3 - 119k^2 - 96k - 48.$$

Putting $k = 6 + s$, where $s \geq 0$, gives

$$\begin{aligned} H(6+s) = {} & s^5 + 37s^4 + 495s^3 \\ & + 2959s^2 + 7440s + 4812 > 0. \end{aligned}$$

Hence (12) exceeds 1, and monotonicity completes the proof. ■

Remark. The path P_7 does not violate the bound for $k = 5$: $\mathrm{SGut}_5(P_7) = 1376 < 7008/5 = L_{7,5}$. Thus the threshold $n = 8$ is exact within this path family. This does not affect Li's proved $k = 4$ inequality.

Corollary. *For each fixed $k \geq 5$, as $n \to \infty$,*

$$\frac{\mathrm{SGut}_k(P_n)}{L_{n,k}} \sim \frac{3k(k-1)^2}{(k+1)!}\, n^{k-4}. \tag{13}$$

In particular, the failure becomes unbounded along the path family.

Proof. The respective leading terms of (4) and (8) are $2^k(k-1)n^{k+1}/(k+1)!$ and $2^k n^5/[3k(k-1)]$. Their quotient proves the claim. ■

5 A valid bound for all trees

For a finite list $x = (x_1, \ldots, x_m)$, let $e_j(x)$ be its jth elementary symmetric polynomial, with $e_0(x) = 1$.

Theorem 2. *Let T be a tree on $n \geq 3$ vertices, $2 \leq k \leq n$, $d_v = d_T(v)$*

and $\Delta = \max_v d_v$. *Then*

$$\mathrm{SGut}_k(T) \le \frac{1}{k-1} \sum_{\{u,v\}\subseteq V(T)} d_u d_v \,\mathrm{dist}_T(u,v) e_{k-2}\big((d_w)_{w\notin\{u,v\}}\big) \tag{14}$$

$$\le \frac{\binom{n-2}{k-2}}{k-1} \sum_{\{u,v\}\subseteq V(T)} d_u d_v \,\mathrm{dist}_T(u,v) \left(\frac{2(n-1)-d_u-d_v}{n-2}\right)^{k-2} \tag{15}$$

$$\le \frac{2^{k-2}}{k-1}\binom{n-2}{k-2}\,\mathrm{Gut}(T) \tag{16}$$

$$\le \frac{\Delta^{k-2}}{k-1}\binom{n-2}{k-2}\,\mathrm{Gut}(T). \tag{17}$$

For $k = 2$ *all displayed inequalities are equalities.*

Proof. Fix a k-element vertex set S. Each edge e of its Steiner subtree partitions S into two nonempty parts of sizes a_e and $k - a_e$. Exactly $a_e(k - a_e)$ unordered vertex pairs of S use e, and $a_e(k - a_e) \ge k - 1$. Summing over the subtree edges gives

$$(k-1)d_T(S) \le \sum_{\{u,v\}\subseteq S} \mathrm{dist}_T(u,v). \tag{18}$$

Multiplying by $\prod_{x\in S} d_x$ and summing over all k-subsets yields (14), because a fixed pair $\{u, v\}$ leaves an elementary symmetric sum in the remaining $k - 2$ vertex degrees.

For each pair, the other $n - 2$ degrees have sum $2(n - 1) - d_u - d_v$. Maclaurin's inequality gives

$$e_{k-2}\big((d_w)_{w\notin\{u,v\}}\big) \le \binom{n-2}{k-2}\left(\frac{2(n-1)-d_u-d_v}{n-2}\right)^{k-2},$$

including $k = 2$ with the usual zero-th power convention. This proves (15). Since $d_u, d_v \ge 1$, the mean in parentheses is at most 2, giving (16). Finally $\Delta \ge 2$ for every tree of order at least 3, so (17) follows. For $k = 2$, (18) and all remaining steps are equalities. ∎

Remark. The replacement bounds need not be sharp and do not improve

Li's proved $k = 4$ inequality.

A An edge-cut identity

For each edge e of a tree T, let A_e, B_e be the vertex sets of the components of $T - e$.

Proposition 3. *For $2 \le k \le |V(T)|$, writing $d_v = d_T(v)$, we have*

$$\mathrm{Gut}(T) = \sum_{e \in E(T)} \left(\sum_{v \in A_e} d_v \right) \left(\sum_{v \in B_e} d_v \right), \tag{19}$$

$$\mathrm{SGut}_k(T) = \sum_{e \in E(T)} \left[e_k\big((d_v)_{v \in V(T)}\big) - e_k\big((d_v)_{v \in A_e}\big) - e_k\big((d_v)_{v \in B_e}\big) \right], \tag{20}$$

where $e_k = 0$ for a list containing fewer than k variables.

Proof. An edge lies on the path between two vertices exactly when those vertices are on opposite sides of its cut. This proves (19) by counting contributions edge by edge. An edge belongs to the Steiner subtree of S exactly when S meets both sides of the cut. Subtracting the degree-product sums over sets entirely in A_e or B_e from the sum over all k-sets proves (20). ∎

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