Disproof of a conjecture on the minimum Wiener index of signed trees

Songlin Guo Wei Wang* Chuanming Wang

School of Mathematics, Physics and Finance, Anhui Polytechnic University, Wuhu 241000, P. R. China

Abstract

The Wiener index of a connected graph is the sum of distances between all unordered pairs of vertices. Sam Spiro [The Wiener index of signed graphs, Appl. Math. Comput., 416(2022)126755] recently introduced the Wiener index for a signed graph and conjectured that the path P_n with alternating signs has the minimum Wiener index among all signed trees with n vertices. By constructing an infinite family of counterexamples, we prove that the conjecture is false whenever n is at least 30.

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1 Introduction

A *signed graph* is a graph where each edge has a positive or negative sign. We usually write a signed graph as a pair (G, σ), where G is the underlying graph and $\sigma\colon\ E(G) \mapsto \{+1, -1\}$ describes the sign of each edge. For a path P in (G, σ), the *length* of P (under the signing σ) is $\ell_\sigma(P) = |\Sigma_{e\in E(P)}\sigma(e)|$. A path P in (G, σ) is called a *uv-path* if it has u and v as its endvertices. For two distinct vertices $u, v \in V(G)$, the *signed distance* [3] of u, v in (G, σ), is

$$d_\sigma(u, v) = \min\{\ell_\sigma(P)\colon\ P \text{ is a } uv\text{-path in } (G, \sigma)\}.$$

Definition 1 ([3])**.** Let (G, σ) be a signed graph. The Wiener index of (G, σ), denoted by $W_\sigma(G)$, is $\sum d_\sigma(u, v)$, where the summation is taken over all unordered pairs $\{u, v\}$ of distinct vertices in G.

Let $(G, +)$ denote a signed graph where each edge is positive. It is easy to see that the Wiener index $W_+(G)$ coincides with the classic Wiener index $W(G)$ of the ordinary graph G, introduced by Harry Wiener [5] in 1947. As the oldest topological index of a molecule, Wiener index has many applications in molecular chemistry, see the monograph [4].

*Corresponding author. Email: wangwei.math@gmail.com

A tree is a connected graph with no cycles. There are numerous studies of properties of the Wiener indices of trees, see the survey paper [1]. Entringer, Jackson and Snyder [2] proved that, among all trees of any fixed order n, the path P_n (resp. the star $K_{1,n}$) has the maximum (resp. minimum) Wiener index. Note that for any connected graph G together with any signing σ, we have $W_\sigma(G) \le W_+(G) = W(G)$. Consequently, the above result of Entringer et al. indicates that $W_\sigma(T) \le W(P_n)$ for any signed n-vertex tree (T, σ).

Let σ be a signing of the path P_n. We call σ (or (P_n, σ)) *alternating* if any two adjacent edges have opposite signs. We usually use α to denote an alternating signing of a path. The following interesting conjecture was proposed recently by Spiro [3].

Conjecture 1 ([3]). *Among all signed trees of order n, the alternating path (P_n, α) has the minimum Wiener index.*

In this short note, we disprove Conjecture 1 by constructing infinite counterexamples.

Theorem 1. *Conjecture 1 fails for every $n \ge 30$.*

The proof of Theorem 1 is given at the end of the next section.

2 An infinite family of counterexamples

Let $k \ge 0$ and $a_1, a_2, \ldots, a_k$ be k nonnegative integers. Let $T(a_1, a_2, \ldots, a_k)$ denote a rooted tree with $1 + k + \sum_{i=1}^k a_i$ vertices constructing by the following two rules:
(i) The root vertex has k neighbors $u_1, u_2, \ldots, u_k$; such k vertices will be called *branch* vertices.
(ii) For each $i \in \{1, 2, \ldots, k\}$, the branch vertex u_i has a_i neighbors other than the root vertex; such a_i neighbors will be called *leaf* vertices.

Definition 2. Let σ be a signing of a rooted tree $T(a_1, a_2, \ldots, a_k)$. We call σ *nice* if it satisfies the following two conditions:
(i) Among k edges incident to the root vertex, the numbers of positive edges and negative edges differ by at most one.
(ii) For each branch vertex u, all edges connecting u and leaf vertices have the same sign which is opposite to the sign of the edge connecting u and the root vertex.

Figure 1 illustrates a nice signing for the rooted tree $T(3, 4, 4, 4, 4, 4)$, where we use dashed (resp. solid) lines to represent negative (resp. positive) edges.

Theorem 2. *If σ is a nice then*

$$W_\sigma(T(a_1, a_2, \ldots, a_k)) = 2\sum_{i=1}^k \binom{a_i}{2} + 2\binom{\lfloor \frac{k}{2} \rfloor}{2} + 2\binom{\lceil \frac{k}{2} \rceil}{2} + k\left(1 + \sum_{i=1}^k a_i\right).$$

Proof. Write $T = T(a_1, a_2, \ldots, a_k)$ and let P be any path in (T, σ). Clearly, P contains at most four edges. Since σ is nice, one easily sees from Definition 2(ii) that any path in (T, σ) with 4 edges have exactly 2 positive edges and hence satisfies $\ell_\sigma(P) = 0$. Similarly, if P has

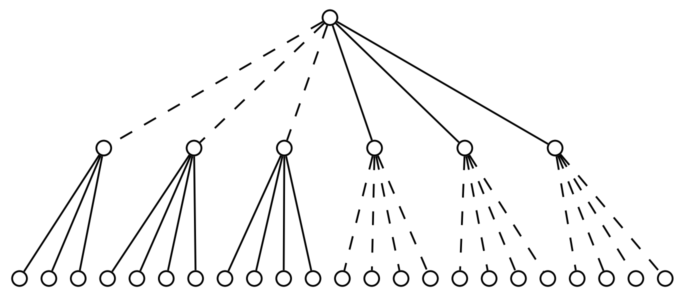

Figure 1: $T(3,4,4,4,4,4)$ with a nice signing.

exactly 2 edges and $\ell_\sigma(P) > 0$ then the two endvertices of P must be either two leaf vertices adjacent to a common branch vertex, or two branch vertices adjacent to the root vertex by two edges sharing the same sign. Note that the numbers of positive edges and negative edges are $\lfloor \frac{k}{2} \rfloor$ and $\lceil \frac{k}{2} \rceil$ (or in reverse order) by Definition 2(i). Thus, the contribution of such paths to $W_\sigma(T)$ is

$$2\sum_{i=1}^{k} \binom{a_i}{2} + 2\binom{\lfloor \frac{k}{2} \rfloor}{2} + 2\binom{\lceil \frac{k}{2} \rceil}{2}.$$

Furthermore, noting that each path P with exactly one or three edges satisfies $\ell_\sigma(P) = 1$ and there exists such a path between branch vertices and the remaining vertices, we see that the contribution of path with one or three edges is exactly

$$k\left(1 + \sum_{i=1}^{k} a_i\right).$$

Adding the above two expressions completes the proof. $\square$

Lemma 1. *Let α be an alternating signing of P_n. Then $W_\alpha(P_n) = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$.*

Proof. Let (U, V) be the bipartition of P_n as a bipartite graph, where we assume $|U| \leq |V|$. Then $|U| = \lfloor \frac{n}{2} \rfloor$ and $|V| = \lceil \frac{n}{2} \rceil$. Let u, v be any two vertices of P_n. It is easy to see that $d_\alpha(u, v) = 0$ if u and v are in the same part, and $d_\alpha(u, v) = 1$ otherwise. Thus, $W_\alpha(P_n) = |U||V| = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$, as desired. $\square$

Noting that $T(3,4,4,4,4,4)$ has exactly 30 vertices, the following proposition gives a counterexample to Conjecture 1.

Proposition 1. *Let α be an alternating signing of P_{30} and σ be a nice signing of $T = T(3,4,4,4,4,4)$. Then $W_\sigma(T) < W_\alpha(P_{30})$.*

Proof. Using Theorem 2 and Lemma 1, we find that $W_\sigma(T) = 222$ while $W_\alpha(P_{30}) = 225$. Thus $W_\sigma(T) < W_\alpha(P_{30})$, as desired. $\square$

We shall show that for any $n \geq 30$, there exists a counterexample to Conjecture 1.

Definition 3.

$$\mathcal{T}_k = \bigcup_{0 \leq s \leq k} \left\{ T(\underbrace{k-1, \ldots, k-1}_{k-s}, \underbrace{k, \ldots, k}_{s}), T(\underbrace{k, \ldots, k}_{k-s}, \underbrace{k+1, \ldots, k+1}_{s}) \right\}.$$

Note that $\mathcal{T}_k$ contains exactly $2k+1$ rooted trees of consecutive orders from k^2+1 to $(k+1)^2$, see Figure 2 for the five rooted trees in $\mathcal{T}_2$.

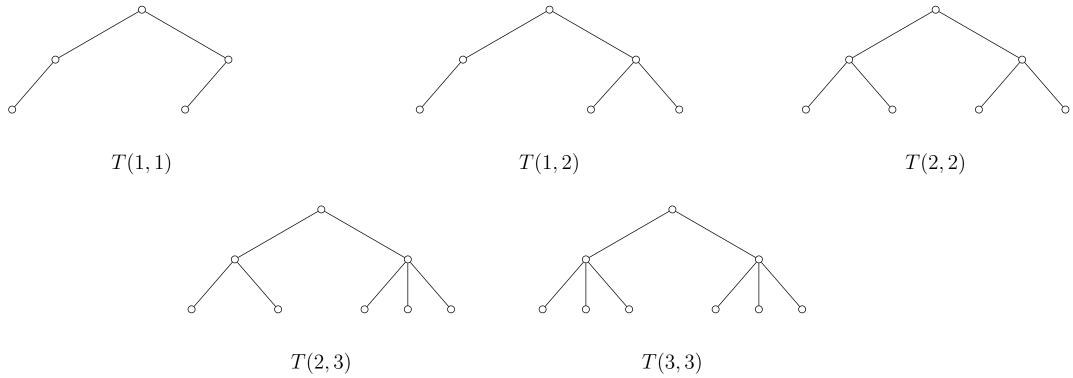

Figure 2: The family $\mathcal{T}_2$.

Lemma 2. *Let $k \geq 10$ and T be any rooted tree in $\mathcal{T}_k$. Let $n = |V(T)|$. Then $W_\sigma(T) < W_\alpha(P_n)$ where σ is nice while α is alternating.*

Proof. Write $m = k^2+1$ and $M = (k+1)^2$. By Theorem 2 and Lemma 1, it is not difficult to see that both $W_\sigma(T)$ and $W_\alpha(P_n)$ are increasing as a function of $n = |V(T)|$. Thus we are done if we can show that $W_\sigma(T_M) < W_\alpha(P_m)$ where $T_M = T(\underbrace{k+1,\ldots,k+1}_{k})$.

By Theorem 2 we have

$$\begin{aligned} W_\sigma(T_M) &= 2k\binom{k+1}{2} + 2\binom{\lfloor \frac{k}{2} \rfloor}{2} + 2\binom{\lceil \frac{k}{2} \rceil}{2} + k(1+k(k+1)) \qquad (1) \\ &< 2k\binom{k+1}{2} + 2\binom{\frac{k}{2}}{2} + 2\binom{\frac{k+1}{2}}{2} + k(1+k(k+1)) \\ &= 2k^3 + \frac{5}{2}k^2 + \frac{1}{2}k - \frac{1}{4}. \end{aligned}$$

On the other hand, by Lemma 1, we have

$$W_\alpha(P_m) = \left\lfloor \frac{m}{2} \right\rfloor \left\lceil \frac{m}{2} \right\rceil = \left\lfloor \frac{k^2+1}{2} \right\rfloor \left\lceil \frac{k^2+1}{2} \right\rceil > \frac{1}{4}k^4.$$

It follows that

$$\frac{W_\sigma(T_M)}{W_\alpha(P_m)} < \frac{8}{k} + \frac{10}{k^2} + \frac{2}{k^3} - \frac{1}{k^4} < \frac{8}{k} + \frac{10}{k^2} + \frac{2}{k^3} \leq \frac{8}{10} + \frac{10}{10^2} + \frac{2}{10^3} < 1.$$

Thus $W_\sigma(T_M) < W_\alpha(P_m)$, as desired. The proof is complete. $\square$

Proof of Theorem 1. Let $\mathcal{T} = \cup_{k=0}^{\infty} \mathcal{T}_k$. It is clear that $\mathcal{T}$ contains exactly one n-vertex (rooted) tree for every positive integer n. We use T_n to denote the unique n-vertex tree in the family $\mathcal{T}$. Let σ be a nice signing of T_n and α be an alternating signing of P_n. By Lemma 2, we see that $W_\sigma(T_n) < W_\alpha(P_n)$ whenever $n \geq 10^2+1$. On the other hand, we know from Proposition 1 that there does exist a 30-vertex tree T (with a nice signing σ) such that $W_\sigma(T) < W_\alpha(P_{30})$. It remains to consider the case that $n \in \{31, 32, \ldots, 100\}$.

We claim that $W_\sigma(T_n) < W_\alpha(P_n)$ for each $n \in \{31, 32, \ldots, 100\}$. This can be checked directly using Theorem 2 and Lemma 1. Take $n = 31$ as an example. As $31 \in [5^2+1, (5+1)^2]$, we find that $T_{31} \in \mathcal{T}_5$ and moreover $T_{31} = T(5, 5, 5, 5, 5)$. Using Theorem 2 for T_{31}, we obtain that $W_\sigma(T_{31}) = 238$. By Lemma 1, we have $W_\alpha(P_{31}) = \lfloor \frac{31}{2} \rfloor \lceil \frac{31}{2} \rceil = 240$. Thus $W_\sigma(T_n) < W_\alpha(P_n)$ for $n = 31$. The proof is complete. $\square$

We remark that the counterexamples constructed in this note also disprove another conjecture of Spiro. For a graph G, the *minimal signed Wiener index* of G, denoted by $W_*(G)$, is the minimum of $W_\sigma(G)$ for all possible signings σ. Spiro [3] conjectured that $W_*(T) \geq W_*(P_n)$ for any n-vertex tree T. Let $n \geq 30$ and T_n be the tree used in the proof of Theorem 1. Clearly, $W_*(T_n) \leq W_\sigma(T_n)$, where σ is a nice signing of T_n. On the other hand, it is easy to see that $W_*(P_n) = W_\alpha(P_n)$. Since $W_\sigma(T_n) < W_\alpha(P_n)$, we obtain $W_*(T_n) < W_*(P_n)$, disproving this conjecture.

3 Asymptotic property

It is still unknown which signed trees have the minimum Wiener index among all signed trees of a fixed order n. We use $(\hat{T}_n, \hat{\sigma})$ to denote an n-vertex signed tree whose Wiener index is minimum among all signed trees of order n. And let (T_n, σ) be the n-vertex tree in $\cup_{k=0}^{\infty} \mathcal{T}_k$ with a nice signing σ. One referee kindly points out that (T_n, σ) is optimal up to a constant factor. Precisely,

$$\limsup_{n \to \infty} \frac{W_\sigma(T_n)}{W_{\hat{\sigma}}(\hat{T}_n)} \leq C,$$

for some constant C.

Lemma 3. $W_\sigma(T_n) = (2 + o(1))n^{\frac{3}{2}}$.

Proof. Let $k = \lfloor \sqrt{n-1} \rfloor$, $m = k^2 + 1$ and $M = (k+1)^2$. Then we have $m \leq n \leq M$. Note that $T_m = T(\underbrace{k, \ldots, k}_{k})$ and $T_M = T(\underbrace{k+1, \ldots, k+1}_{k})$. Using Theorem 2, we have

$$W_\sigma(T_m) = 2k\binom{k}{2} + 2\binom{\lfloor \frac{k}{2} \rfloor}{2} + 2\binom{\lceil \frac{k}{2} \rceil}{2} + k(1 + k^2) = (2 + o(1))k^3 \tag{2}$$

and

$$W_\sigma(T_M) = 2k\binom{k+1}{2} + 2\binom{\lfloor \frac{k}{2} \rfloor}{2} + 2\binom{\lceil \frac{k}{2} \rceil}{2} + k(1 + k(k+1)) = (2 + o(1))k^3. \tag{3}$$

Noting that $k^3 \sim n^{\frac{3}{2}}$ and $W_\sigma(T_m) \leq W_\sigma(T_n) \leq W_\sigma(T_M)$, we have $W_\sigma(T_n) = (2 + o(1))n^{\frac{3}{2}}$ by Squeeze Theorem. $\square$

The following lower bound is due to Sam Spiro.

Lemma 4. $W_{\hat{\sigma}}(\hat{T}_n) \geq (\sqrt{2} + o(1))n^{\frac{3}{2}}$.

Proof. Let U, V be the bipartition of $\hat{T}_n$ with $|U| \leq |V|$. Label vertices in U as $u_1, u_2, \ldots, u_k$, where $k = |U|$. Let d_i^+ (resp. d_i^-) denote the number of positive (resp. negative) edges incident with u_i for each i. It is not too difficult to show that

$$W_{\hat{\sigma}}(\hat{T}_n) \geq |U||V| + 2\sum_{i=1}^{k}\left(\binom{d_i^+}{2} + \binom{d_i^-}{2}\right). \tag{4}$$

Indeed, the first term comes from all paths of odd length and the term $\binom{d_i^+}{2} + \binom{d_i^-}{2}$ comes from the paths of length 2 between two neighbors of u_i with the same sign. As the function $\binom{x}{2} = \frac{1}{2}x(x-1)$ is convex, we have

$$\sum_{i=1}^{k}\left(\binom{d_i^+}{2} + \binom{d_i^-}{2}\right) \geq 2k\binom{\frac{1}{2k}\sum_{i=1}^{k}(d_i^+ + d_i^-)}{2}, \tag{5}$$

by Jensen's Inequality. As $|U| = k$, $|V| = n-k$ and $\sum_{i=1}^{k}(d_i^+ + d_i^-)$ equals $n-1$, which is the number of edges in $\hat{T}_n$, we obtain from Eqs. (4) and (5) that

$$\begin{aligned}
W_{\hat{\sigma}}(\hat{T}_n) &\geq k(n-k) + 4k\binom{\frac{n-1}{2k}}{2} \\
&= kn + \frac{n^2}{2k} - k^2 + \frac{1}{2k}((2k+1) - (2k+2)n) \\
&\geq kn + \frac{n^2}{2k} - k^2 - 2n. \qquad (6)
\end{aligned}$$

Using the basic inequality $a + b \geq 2\sqrt{ab}$ for $a, b > 0$, we have

$$kn + \frac{n^2}{2k} \geq 2\sqrt{\frac{n^3}{2}} = \sqrt{2}n^{\frac{3}{2}}. \tag{7}$$

Recall that $k \leq n/2$. Thus $n - k \geq n/2$. If $k \geq 2\sqrt{2n}$ then from the trivial inequality $W_{\hat{\sigma}}(\hat{T}_n) \geq k(n-k)$ we obtain

$$W_{\hat{\sigma}}(\hat{T}_n) \geq (2\sqrt{2n}) \cdot \frac{n}{2} = \sqrt{2}n^{\frac{3}{2}}.$$

Now assume $k < 2\sqrt{2n}$. Then by (6) and (7), we find

$$W_{\hat{\sigma}}(\hat{T}_n) \geq \sqrt{2}n^{\frac{3}{2}} - k^2 - 2n \geq \sqrt{2}n^{\frac{3}{2}} - 10n = (\sqrt{2} + o(1))n^{\frac{3}{2}}.$$

Thus we always have $W_{\hat{\sigma}}(\hat{T}_n) \geq (\sqrt{2} + o(1))n^{\frac{3}{2}}$, as desired. $\square$

The following theorem is a direct consequence of Lemmas 3 and 4.

Theorem 3.

$$\limsup_{n\to\infty} \frac{W_\sigma(T_n)}{W_{\hat{\sigma}}(\hat{T}_n)} \leq \sqrt{2}.$$

We end this note by leaving the following problem suggested by one referee.

Problem 1. *Is it true that*

$$\lim_{n\to\infty} \frac{W_\sigma(T_n)}{W_{\hat{\sigma}}(\hat{T}_n)} = 1?$$

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