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

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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.

Keywords: Wiener index; signed tree; signed graph

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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 $(G, \sigma)$, where $G$ is the underlying graph and $\sigma: E(G) \mapsto \{+1, -1\}$ describes the sign of each edge. For a path $P$ in $(G, \sigma)$, the length of $P$ (under the signing $\sigma$) is $\ell_\sigma(P) = |\Sigma_{e \in E(P)} \sigma(e)|$. A path $P$ in $(G, \sigma)$ 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 $(G, \sigma)$, is

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

Definition 1 ([3]). Let $(G, \sigma)$ be a signed graph. The Wiener index of $(G, \sigma)$, denoted by $W_\sigma(G)$, is $\Sigma d_\sigma(u,v)$, 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].

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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 \( \sigma \), we have \( W_\sigma(G) \leq W_+(G) = W(G) \). Consequently, the above result of Entringer et al. indicates that \( W_\sigma(T) \leq W(P_n) \) for any signed \( n \)-vertex tree \((T, \sigma)\).

Let \( \sigma \) be a signing of the path \( P_n \). We call \( \sigma \) (or \((P_n, \sigma)\)) alternating if any two adjacent edges have opposite signs. We usually use \( \alpha \) 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 \((P_n, \alpha)\) has the minimum Wiener index.

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

**Theorem 1.** Conjecture [1] fails for every \( n \geq 30 \).

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

### 2 An infinite family of counterexamples

Let \( k \geq 0 \) 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 \( \sigma \) be a signing of a rooted tree \( T(a_1, a_2, \ldots, a_k) \). We call \( \sigma \) 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 \( \sigma \) is a nice then

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

**Proof.** Write \( T = T(a_1, a_2, \ldots, a_k) \) and let \( P \) be any path in \((T, \sigma)\). Clearly, \( P \) contains at most four edges. Since \( \sigma \) is nice, one easily sees from Definition [2]ii) that any path in \((T, \sigma)\) 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

$$2 \sum_{i=1}^{k} \frac{a_i}{2} + 2 \left( \lfloor \frac{k}{2} \rfloor \right)^2 + 2 \left( \lceil \frac{k}{2} \rceil \right)^2.$$

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. \qed

**Lemma 1.** Let $\alpha$ 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. \qed

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 $\alpha$ be an alternating signing of $P_{30}$ and $\sigma$ 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. \qed

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

**Definition 3.**

$$T_k = \bigcup_{0 \leq s \leq k} \left\{ T(k-1, \ldots, k-1, k, \ldots, k), T(k, \ldots, k, k+1, \ldots, k+1) \right\}.$$
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 $\mathcal{T}_2$.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{trees.png}
\caption{The family $\mathcal{T}_2$.}
\end{figure}

**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 $\sigma$ is nice while $\alpha$ 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 $T_M = T(k+1, \ldots, k+1)$.

By Theorem 2 we have

$$W_\sigma(T_M) = 2k \left( \frac{k+1}{2} \right) + 2 \left( \frac{k}{2} \right) + 2 \left( \frac{k+1}{2} \right) + k(1 + k(k+1)) \quad (1)$$

$$< 2k \left( \frac{k+1}{2} \right) + 2 \left( \frac{k}{2} \right) + 2 \left( \frac{k+1}{2} \right) + k(1 + k(k+1))$$

$$= 2k^3 + \frac{5}{2}k^2 + \frac{1}{2}k - \frac{1}{4}.$$ 

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.

**Proof of Theorem 7.** Let $\mathcal{T} = \bigcup_{k=0}^\infty \mathcal{T}_k$. 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 $\sigma$ be a nice signing of $T_n$ and $\alpha$ 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
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 \(T_{31} \in T_5\) 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 \(W_\alpha(P_{31}) = \left\lfloor \frac{31}{2} \right\rfloor \left\lceil \frac{31}{2} \right\rceil = 240\). Thus \(W_\sigma(T_n) < W_\alpha(P_n)\) for \(n = 31\). The proof is complete.

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 \(\sigma\). 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 \(\sigma\) 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 \((T_n, \sigma)\) be the \(n\)-vertex tree in \(\cup_{k=0}^\infty T_k\) with a nice signing \(\sigma\). One referee kindly points out that \((T_n, \sigma)\) is optimal up to a constant factor. Precisely,

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

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 \(T_m = T(k, \ldots, k)\) and \(T_M = T(k+1, \ldots, k+1)\). Using Theorem 2 we have

\[
W_\sigma(T_m) = 2k \left( \frac{k}{2} \right) + 2 \left( \frac{\lfloor \frac{k}{2} \rfloor}{2} \right) + 2 \left( \frac{\lceil \frac{k}{2} \rceil}{2} \right) + k(1 + k^2) = (2 + o(1))k^3 \tag{2}
\]

and

\[
W_\sigma(T_M) = 2k \left( \frac{k+1}{2} \right) + 2 \left( \frac{\lfloor \frac{k}{2} \rfloor}{2} \right) + 2 \left( \frac{\lceil \frac{k}{2} \rceil}{2} \right) + k(1 + k(k+1)) = (2 + o(1))k^3. \tag{3}
\]

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.

The following lower bound is due to Sam Spiro.

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

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

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

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

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

$$W_\sigma(\hat{T}_n) \geq k(n - k) + 4k \left( \frac{n-1}{2k} \right).$$

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

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

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

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

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

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

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

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

**Theorem 3.**

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

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

**Problem 1.** Is it true that

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