INVERSE PROBLEM ON THE STEINER WIENER INDEX

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Abstract

The Wiener index $W(G)$ of a connected graph $G$, introduced by Wiener in 1947, is defined as $W(G) = \sum_{u,v \in V(G)} d_G(u,v)$, where $d_G(u,v)$ is the distance (the length a shortest path) between the vertices $u$ and $v$ in $G$. For $S \subseteq V(G)$, the Steiner distance $d(S)$ of the vertices of $S$, introduced by Chartrand et al. in 1989, is the minimum size of a connected subgraph of $G$ whose vertex set contains $S$. The $k$-th Steiner Wiener index $SW_k(G)$ of $G$ is defined as $SW_k(G) = \sum_{|S|=k} d(S)$. We investigate the following problem: Fixed a positive integer $k$, for what kind of positive integer $w$ does there exist a connected graph $G$ (or a tree $T$) of order $n \geq k$ such that $SW_k(G) = w$ (or $SW_k(T) = w$)? In this paper, we give some solutions to this problem.

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1. Introduction

All graphs in this paper are assumed to be undirected, finite and simple. We refer to [3] for graph theoretical notation and terminology not specified here. A distance is one of basic concepts of graph theory [4]. If $G$ is a connected graph and $u, v \in V(G)$, then the distance $d(u, v) = d_G(u, v)$ between $u$ and $v$ is the length of a shortest path connecting $u$ and $v$. For more details on this subject, see [13].

The Wiener index $W(G)$ of a connected graph $G$ is defined by

$$ W(G) = \sum_{u,v \in V(G)} d_G(u,v). $$

Mathematicians have studied this graph invariant since the 1970s in [11]; for details see the surveys [10, 33], the recent papers [2, 7, 14, 17, 15, 20] and the references cited therein. Information on chemical applications of the Wiener index can be found in [27, 28].

The Steiner distance of a graph, introduced by Chartrand et al. in [6] in 1989, is a natural and nice generalization of the concept of the classical graph distance. For a graph $G = (V, E)$ and a set $S \subseteq V$ of at least two vertices, an $S$-Steiner tree or a Steiner tree connecting $S$ (or simply, an $S$-tree) is a subgraph $T = (V', E')$ of $G$ that is a tree with $S \subseteq V'$. Let $G$ be a connected graph of order at least 2 and let $S$ be a nonempty set of vertices of $G$. Then the Steiner distance $d(S)$ among the vertices of $S$ (or simply the distance of $S$) is the minimum size of a connected subgraph whose vertex set contains $S$. Note that if $H$ is a connected subgraph of $G$ such that $S \subseteq V(H)$ and $|E(H)| = d(S)$, then $H$ is a tree. Clearly, $d(S) = \min\{|E(T)| : S \subseteq V(T)\}$, where $T$ is a subtree of $G$. Furthermore, if $S = \{u, v\}$, then $d(S) = d(u, v)$ is nothing new, but the classical distance between $u$ and $v$. Clearly, if $|S| = k$, then $d(S) \geq k - 1$. For more details on Steiner distance, we refer to [1, 5, 6, 8, 13, 26].

In [23], we proposed a generalization of the Wiener index concept, using Steiner distance. Thus, the $k$-th Steiner Wiener index $SW_k(G)$ of a connected graph $G$ is defined by

$$ SW_k(G) = \sum_{S \subseteq V(G) \atop |S|=k} d(S). $$

For $k = 2$, the Steiner Wiener index coincides with the ordinary Wiener index. It is usual to consider $SW_k$ for $2 \leq k \leq n - 1$, but the above definition implies $SW_1(G) = 0$ and $SW_n(G) = n - 1$ for a connected graph $G$ of order $n$. For more details on Steiner Wiener index, we refer to [23, 24, 25].

A chemical application of $SW_k$ was recently reported in [16].
It should be noted that in the 1990s, Dankelmann et al. in [8, 9] studied the \textit{average Steiner distance}, which is related to our Steiner Wiener index via $SW_k(G)/\binom{n}{k}$.

The seemingly elementary question: “Which natural numbers are Wiener indices of graphs?” was much investigated in the past; see [12, 19, 21, 29, 31, 32]. We now consider the analogous question for Steiner Wiener indices.

\textbf{Problem.} Fixed a positive integer $k$, for what kind of positive integer $w$ does there exist a connected graph $G$ (or a tree $T$) of order $n \geq k$ such that $SW_k(G) = w$ (or $SW_k(T) = w$)?

For $k = 2$, the authors have nice results in [30, 32], completely solved a conjecture by Lepović and Gutman [22] for trees, which states that for all but 49 positive integers $w$ one can find a tree with Wiener index $w$. This is different from our problem for trees, since here we consider graphs or trees with order $n$.

2. \textsc{The Cases} $k = n$ and $k = n - 1$

At first, let us consider the case $k = n$.

If $G$ is a connected graph or a tree of order $n$, then for $k = n$, $SW_k(G) = n - 1$. Thus the following result is immediate.

\textbf{Proposition 2.1.} For a positive integer $w$, there exists a connected graph $G$ or a tree $T$ of order $n$ such that $SW_n(G) = w$ or $SW_n(T) = w$ if and only if $w = n - 1$.

For the case $k = n - 1$, we need the following results in [23].

\textbf{Lemma 2.2} [23]. Let $T$ be a tree of order $n$, possessing $p$ pendant vertices. Then

$$SW_{n-1}(T) = n(n-1) - p$$

irrespective of any other structural detail of $T$.

\textbf{Lemma 2.3} [23]. Let $K_n$ be the complete graph of order $n$, and let $k$ be an integer such that $2 \leq k \leq n$. Then

$$SW_k(K_n) = \binom{n}{k}(k-1).$$

\textbf{Lemma 2.4} [23]. Let $G$ be a connected graph of order $n$, and let $k$ be an integer such that $2 \leq k \leq n$. Then

$$\binom{n}{k}(k-1) \leq SW_k(G) \leq (k-1)\binom{n+1}{k+1}.$$  

Moreover, the lower bound is sharp.
From the previous results, we can derive the following proposition.

**Proposition 2.5.** For a positive integer \( w \), there exists a connected graph \( G \) of order \( n \) such that \( SW_{n-1}(G) = w \) if and only if \( n^2 - 2n \leq w \leq n^2 - n - 2 \).

**Proof.** By Lemma 2.4, if \( G \) is a connected graph of order \( n \), then

\[
n(n-2) \leq SW_{n-1}(G) \leq (n+1)(n-2).
\]

Therefore, \( n^2 - 2n \leq w \leq n^2 - n - 2 \).

By Lemma 2.3, \( SW_{n-1}(K_n) = n^2 - 2n \).

Let \( T \) be a tree of order \( n \) with \( p \) pendant vertices with \( 2 \leq p \leq n - 1 \). By Lemma 2.2, \( SW_{n-1}(T) = n^2 - n - p \), and thus for any integer \( w \) with \( n^2 - n - (n - 1) \leq w \leq n^2 - n - 2 \), there exists a tree \( T \) of order \( n \) such that \( SW_{n-1}(T) = w \).

From the proof of Proposition 2.5 the next result immediately follows.

**Proposition 2.6.** For a positive integer \( w \), there exists a tree \( T \) of order \( n \) such that \( SW_{n-1}(T) = w \) if and only if \( n^2 - 2n + 1 \leq w \leq n^2 - n - 2 \).

3. **The Case \( k = n - 2 \)**

Similarly to Lemma 2.2, we can derive the following result.

**Lemma 3.1.** Let \( T \) be a tree of order \( n \), possessing \( p \) pendant vertices. Let \( q \) be the number of vertices of degree 2 in \( T \) that are adjacent to a pendant vertex. Then

\[
SW_{n-2}(T) = \frac{1}{2} \left( n^3 - 2n^2 + n - 2np + 2p - 2q \right).
\]

**Proof.** For any \( S \subseteq V(T) \) and \( |S| = n - 2 \), let \( \bar{S} = \{u, v\} \). If \( d_T(u) = d_T(v) = 1 \), then \( d_T(S) = n - 3 \), and this case contributes to \( SW_{n-2} \) by

\[
\sum_{d_T(u)=d_T(v)=1, u,v \in S} d_T(S) = \frac{p}{2}(n-3).
\]

If \( d_T(u) \geq 2 \) and \( d_T(v) \geq 2 \), then \( d_T(S) = n - 1 \), and this case contributes to \( SW_{n-2} \) by

\[
\sum_{d_T(u) \geq 2, d_T(v) \geq 2, u,v \in S} d_T(S) = \frac{n-p}{2}(n-1).
\]

Suppose that \( d_T(u) = 1 \) and \( d_T(v) \geq 2 \). If \( d_T(u) = 1 \), \( d_T(v) = 2 \) and \( uv \in E(G) \), then \( d_T(S) = n - 3 \). If \( d_T(u) = 1 \), \( d_T(v) \geq 3 \) and \( uv \in E(T) \), then
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If \( d_T(u) = 1 \), \( d_T(v) \geq 2 \) and \( uv \notin E(T) \), then \( d_T(S) = n - 2 \). Therefore, this case contributes to \( SW_{n-2} \) by

\[
\sum_{\substack{u,v \in S \\colon d_T(u) = 1, \ d_T(v) \geq 2 \\quad \text{or} \quad \text{if } d_T(u) = 1, \ d_T(v) = 2}} d_T(S) = q(n - 3) + (p - q)(n - 2) + p(n - p - 1)(n - 2).
\]

From the above argument, we have

\[
SW_{n-2}(T) = \frac{p}{2}(n - 3) + \frac{(n - p)}{2}(n - 1) + q(n - 3) + (p - q)(n - 2) + p(n - p - 1)(n - 2)
\]

\[
= \frac{1}{2} (n^3 - 2n^2 + n - 2np + 2p - 2q).
\]

Li et al. obtained the following sharp lower and upper bounds of \( SW_k(T) \) for a tree \( T \).

**Lemma 3.2 [23].** Let \( T \) be a tree of order \( n \), and let \( k \) be an integer such that \( 2 \leq k \leq n \). Then

\[
\binom{n-1}{k-1}(n - 1) \leq SW_k(T) \leq (k - 1)\binom{n+1}{k+1}.
\]

Moreover, among all trees of order \( n \), the star \( S_n \) minimizes the Steiner Wiener \( k \)-index, whereas the path \( P_n \) maximizes the Steiner Wiener \( k \)-index.

For trees, we have the following result.

**Theorem 3.3.** For a positive integer \( w \), there exists a tree \( T \) of order \( n \) (\( n \geq 5 \)), possessing \( p \) pendant vertices, such that \( SW_{n-2}(T) = w \) if and only if \( w = \frac{1}{2}(n^3 - 2n^2 + n - 2np + 2p - 2q) \), where \( q \) is the number of vertices of degree 2 in \( T \) that are adjacent to a pendant vertex, and one of the following holds:

1. \( 2 \leq q \leq \left\lfloor \frac{n-1}{2} \right\rfloor \) and \( q \leq p \leq n - q - 1 \);
2. \( q = 1 \) and \( 3 \leq p \leq n - 2 \);
3. \( q = 0 \) and \( 4 \leq p \leq n - 1 \).

**Proof.** Suppose that \( w = \frac{1}{2}(n^3 - 2n^2 + n - 2np + 2p - 2q) \), where \( 0 \leq q \leq \left\lfloor \frac{n-1}{2} \right\rfloor \), \( q \leq p \leq n - q - 1 \). Let \( K_{1,p-1} \) be a star of order \( p \), and let \( v \) be the center of \( K_{1,p-1} \). Then \( K_{1,p-1}^* \) is a graph obtained from \( K_{1,p-1} \) by picking up \( q - 1 \) edges and then replacing each of them by a path of length 2. Note that \( K_{1,p-1}^* \) is a
subdivision of $K_{1,p−1}$. Let $G$ be a graph obtained by $K_{1,p−1}^*$ and a path $P_{n−p−q+2}$ by identifying $v$ and one endvertex of the path. Clearly, $G$ is a tree of order $n$ with $p$ pendant vertices, and there are exactly $q$ vertices of degree 2 in $T$ such that each of them is adjacent to a pendant vertex. From Lemma 3.1, we have $SW_{n−2}(T) = \frac{1}{2}(n^3 - 2n^2 + n - 2np + 2p - 2q) = w$, as desired.

Conversely, for any tree $T$ of order $n$ ($n \geq 5$) with $p$ pendant vertices, from Lemma 3.1, $SW_{n−2}(T) = \frac{1}{2}(n^3 - 2n^2 + n - 2np + 2p - 2q)$. We now show that $p, q$ satisfy one of (1), (2), (3). Clearly, $p \geq 2, 0 \leq q \leq \left\lfloor \frac{n−1}{2} \right\rfloor$ and $q \leq p$.

**Claim 1.** $p + q \leq n − 1$.

**Proof.** Assume, to the contrary, that $p + q = n$. Then $T$ is a path of order $n$. Since $n \geq 5$, it follows that there exists a vertex of degree 2 having no adjacent pendant vertex, which contradicts to $p + q = n$.

If $q \geq 2$, then it follows from Claim 1 and $q \leq p$ that $q \leq p \leq n − q − 1$. If $q = 1$, then it follows from Claim 1 that $2 \leq p \leq n − 2$. Furthermore, if $p = 2$, then $T$ is a path of order $n$. Since $n \geq 5$, it follows that $q = 2$, a contradiction. If $q = 0$, then it follows from Claim 1 that $2 \leq p \leq n − 1$. Furthermore, if $p = 2$, then $T$ is a path of order $n$. Since $n \geq 5$, it follows that $q = 2$, a contradiction. If $p = 3$, then $T$ is a tree of order $n$. Since $n \geq 5$, it follows that $q \geq 1$, a contradiction.

4. The Case for General $k$

For trees, we have the following result.

**Theorem 4.1.** Let $T$ be a graph obtained from a path $P_t$ and a star $S_{n−t+1}$ by identifying a pendant vertex of $P_t$ and the center $v$ of $S_{n−t+1}$, where $1 \leq t \leq n−1$ and $k \leq n$. Then

$$SW_k(T) = t \left( \binom{n−1}{k} \right) + \left( \binom{t}{k+1} \right) + \left( \binom{n−t+1}{k+1} \right) + (k−1) \left( \binom{n}{k} \right).$$

**Proof.** For any $S \subseteq V(T)$ and $|S| = k$, if $S \subseteq V(S_{n−t+1}−v)$, then $d_G(S) = k$. There are $\binom{n−t}{k}$ such subsets, contributing to $SW_k$ by $k \left( \binom{n−t}{k} \right)$. If $S \subseteq V(P_t)$, then it contributes to $SW_k$ by $\binom{t}{k+1}$ from Lemma 3.2. Suppose that $S \cap V(P_t) \neq \emptyset$ and $S \cap (V(S_{n−t+1}−v)) \neq \emptyset$. Let $|S \cap V(S_{n−t+1}−v)| = i$, $|S \cap V(P_t)| = j$. Without loss of generality, let $S \cap V(P_t) = \{u_{j_1}, u_{j_2}, \ldots, u_{j_{k−i}}\}$, where $1 \leq j_1 < j_2 < \cdots < j_{k−i} \leq t$. Then $k−i \leq j_{k−i} \leq t$. Let $j_{k−i} = j$. Then $d_G(S) = i + j − 1$, and $k−i \leq j \leq t$. Once the vertex $u_j$ is chosen, we have $\binom{j−2}{k−i−1}$ ways to choose $u_{j_1}, u_{j_2}, \ldots, u_{j_{k−i−1}}$. In
In this case, we contribute to $SW_k$ by

$$X = \sum_{i=1}^{k-1} \binom{n-t}{i} \left[ \sum_{j=k-i}^{t} \binom{j-1}{k-i-1} (j+i-1) \right].$$

Since

$$\binom{j-1}{k-i-1}(j+i-1) = \binom{j-1}{k-i-1}j + \binom{j-1}{k-i-1}(i-1) = (k-i)\binom{j}{k-i} + (i-1)\binom{j-1}{k-i-1},$$

it follows that

$$\sum_{j=k-i}^{t} \binom{j-1}{k-i-1}(j+i-1) = (k-i) \sum_{j=k-i}^{t} \binom{j}{k-i} + (i-1) \sum_{j=k-i}^{t} \binom{j-1}{k-i-1}$$

$$= (k-i)\left(\binom{t+1}{k-i+1}\right) + (i-1)\left(\binom{t}{k-i}\right),$$

and hence

$$X = \sum_{i=1}^{k-1} \binom{n-t}{i} \left[ \sum_{j=k-i}^{t} \binom{j-1}{k-i-1} (j+i-1) \right]$$

$$= \sum_{i=1}^{k-1} \binom{n-t}{i} \left[ (k-i)\binom{t+1}{k-i+1} + (i-1)\binom{t}{k-i} \right]$$

$$= \sum_{i=1}^{k-1} \binom{n-t}{i}(k-i)\binom{t+1}{k-i+1} + \sum_{i=1}^{k-1} \binom{n-t}{i}(i-1)\binom{t}{k-i}$$

$$= \sum_{i=1}^{k-1} (k-i)\binom{t}{k-i+1}\binom{n-t}{i} + \sum_{i=1}^{k-1} (k-i)\binom{t}{k-i}\binom{n-t}{i}$$

$$+ \sum_{i=1}^{k-1} (i-1)\binom{t}{k-i}\binom{n-t}{i}.$$
\[
\sum_{i=1}^{k-1} (k-i) \left( \binom{t}{k-i+1} \binom{n-t}{i} \right) + (k-1) \sum_{i=1}^{k-1} \left( \binom{t}{k-i} \binom{n-t}{i} \right)
\]

\[
= \sum_{i=1}^{k-1} (k-i) \left( \binom{t}{k-i+1} \binom{n-t}{i} \right) + (k-1) \left[ \binom{n}{k} - \binom{t}{k} - \binom{n-t}{k} \right].
\]

Let

\[
Y = \sum_{i=1}^{k-1} (k-i) \left( \binom{t}{k-i+1} \binom{n-t}{i} \right).
\]

Then

\[
Y = \sum_{i=1}^{k-1} (k-i+1) \left( \binom{t}{k-i+1} \binom{n-t}{i} \right) - \sum_{i=1}^{k-1} \left( \binom{t}{k-i+1} \binom{n-t}{i} \right)
\]

\[
= t \sum_{i=1}^{k-1} \left( \binom{t}{k-i+1} \binom{n-t}{i} \right) - \sum_{i=1}^{k-1} \left( \binom{t}{k-i+1} \binom{n-t}{i} \right)
\]

\[
= t \left[ \binom{n-1}{k} - \binom{t-1}{k} - \binom{n-t}{k} \right]
\]

\[
- \left[ \binom{n}{k+1} - \binom{t}{k+1} - t \binom{n-t}{k+1} - \binom{n-t}{k+1} \right],
\]

and hence

\[
SW_k(T) = (k-1) \left( \binom{t+1}{k+1} + k \binom{n-t}{k} \right) + X
\]

\[
= (k-1) \left( \binom{t+1}{k+1} + k \binom{n-t}{k} \right) + Y + (k-1) \left[ \binom{n}{k} - \binom{t}{k} - \binom{n-t}{k} \right]
\]

\[
= (k-1) \left( \binom{t+1}{k+1} + k \binom{n-t}{k} + t \left[ \binom{n-1}{k} - \binom{t-1}{k} - \binom{n-t}{k} \right]
\]

\[
- \left[ \binom{n}{k+1} - \binom{t}{k+1} - t \binom{n-t}{k+1} - \binom{n-t}{k+1} \right]
\]

\[
+ (k-1) \left[ \binom{n}{k} - \binom{t}{k} - \binom{n-t}{k} \right]
\]
The following corollary is immediate from Theorem 4.1.

**Corollary 4.2.** For a positive integer \( w \), there exists a tree \( T \) of order \( n \) such that \( SW_k(T) = w \) if

\[
\begin{align*}
    w &= t \binom{n-1}{k} - \binom{t}{k+1} - \binom{n}{k+1} + \binom{n-t+1}{k+1} + (k-1)\binom{n}{k},
\end{align*}
\]

where \( 1 \leq t \leq n-1 \) and \( k \leq n \).

For general graphs, we have the following.

**Theorem 4.3.** Let \( G \) be a graph obtained from a clique \( K_{n-r} \) and a star \( S_{r+1} \) by identifying a vertex of \( K_{n-r} \) and the center \( v \) of \( S_{r+1} \). For \( k \leq r \leq n-1-k \),

\[
    SW_k(G) = (n-1)\binom{n-1}{k-1} - \binom{n-r-1}{k-1}.
\]
Proof. For any \( S \subseteq V(G) \) and \(|S| = k\), if \( S \subseteq V(K_{n-r}) \), then \( d_G(S) = k - 1\). There are \( \binom{n-r}{k} \) such subsets, contributing to \( SW_k \) by \((k-1)\binom{n-r}{k}\). If \( S \subseteq V(S_{r+1}) - v \), then \( d_G(S) = k \). There are \( \binom{k}{r} \) such subsets, contributing to \( SW_k \) by \( k\binom{k}{r} \). Suppose that \( S \cap V(K_{n-r}) \neq \emptyset \) and \( S \cap (V(S_{r+1}) - v) \neq \emptyset \). If \( v \in S \), then \( d_G(S) = k - 1 \). There are \( \binom{n-r-1}{k-x-1} \) such subsets, contributing to \( SW_k \) by \((k-1)\sum_{x=1}^{k-1} \binom{n-r-1}{k-x-1} \binom{r}{x}\). If \( v \notin S \), then \( d_G(S) = k \). There are \( \binom{n-r-1}{k-x} \) such subsets, contributing to \( SW_k \) by \( k\sum_{x=1}^{k-1} \binom{n-r-1}{k-x} \binom{r}{x}\). Then

\[
SW_k(G) = (k-1)\binom{n-r}{k} + k\binom{r}{k} + (k-1)\sum_{x=1}^{k-1} \binom{n-r-1}{k-x-1} \binom{r}{x}
\]

\[
+ k\sum_{x=1}^{k-1} \binom{n-r-1}{k-x} \binom{r}{x}
\]

\[
= (k-1)\binom{n-r}{k} + k\binom{r}{k} + (k-1) \left[ \binom{n-1}{k-1} - \binom{n-1-r}{k-1} \right]
\]

\[
+ k \left[ \binom{n-1}{k} - \binom{n-1-r}{k} - \binom{r}{k} \right]
\]

\[
= (k-1)\binom{n-r}{k} + (k-1) \left[ \binom{n-1}{k-1} - \binom{n-1-r}{k-1} \right]
\]

\[
+ k \left[ \binom{n-1}{k} - \binom{n-1-r}{k} \right]
\]

\[
= (k-1)\binom{n-r}{k} + (n-1)\binom{n-1}{k-1} - (k-1)\binom{n-1-r}{k-1} - k\binom{n-1-r}{k}
\]

\[
= (n-1)\binom{n-1}{k-1} + (k-1)\binom{n-r-1}{k} - k\binom{n-1-r}{k}
\]

\[
= (n-1)\binom{n-1}{k-1} - \binom{n-1-r}{k},
\]

as desired.

The following corollary is immediate from Theorems 4.1 and 4.3.

Corollary 4.4. For a positive integer \( w \), there exists a connected graph \( G \) of order \( n \) such that \( SW_k(G) = w \) if \( w \) satisfies one of the following conditions.
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\( (1) \ w = t \binom{n-1}{k} - \binom{t}{k+1} - \binom{n}{k+1} + \binom{n-t+1}{k+1} + (k-1)\binom{n}{k}, \) where \( 1 \leq t \leq n-1 \) and \( k \leq n. \)

\( (2) \ w = (n-1)\binom{n-1}{k-1} - \binom{n-r-1}{k}, \) where \( k \leq r \leq n - 1 - k \) and \( k \leq n. \)

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