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

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

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 *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.

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. 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.

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].

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.

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*

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

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*

$$SW_{n-2}(T) = \frac{1}{2}\big(n^3 - 2n^2 + n - 2np + 2p - 2q\big). \tag{1}$$

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

$$\sum_{\substack{u,v\in\bar{S}\\ d_T(u)=d_T(v)=1}} d_T(S) = \binom{p}{2}(n-3).$$

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

$$\sum_{\substack{u,v\in\bar{S}\\ d_T(u)\geq 2,\ d_T(v)\geq 2}} d_T(S) = \binom{n-p}{2}(n-1)\,.$$

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

$d_T(S) = n-2$. 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

$$\begin{aligned}\sum_{\substack{u,v\in\bar{S}\\ d_T(u)=1,\ d_T(v)\geq 2}} d_T(S) &= \sum_{\substack{u,v\in\bar{S},uv\in E(T)\\ d_T(u)=1,\ d_T(v)=2}} d_T(S) + \sum_{\substack{u,v\in\bar{S},uv\in E(T)\\ d_T(u)=1,\ d_T(v)\geq 3}} d_T(S) + \sum_{\substack{u,v\in\bar{S},uv\notin E(T)\\ d_T(u)=1,\ d_T(v)\geq 2}} d_T(S)\\ &= q(n-3)+(p-q)(n-2)+p(n-p-1)(n-2)\,.\end{aligned}$$

From the above argument, we have

$$\begin{aligned}SW_{n-2}(T) &= \binom{p}{2}(n-3)+\binom{n-p}{2}(n-1)+q(n-3)\\ &\quad+(p-q)(n-2)+p(n-p-1)(n-2)\\ &= \frac{1}{2}\left(n^3-2n^2+n-2np+2p-2q\right).\end{aligned}$$

■

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 $w = \frac{1}{2}\left(n^3-2n^2+n-2np+2p-2q\right)$, 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 $w = \frac{1}{2}\left(n^3-2n^2+n-2np+2p-2q\right)$, 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 $SW_{n-2}(T) = \frac{1}{2}\big(n^3 - 2n^2 + n - 2np + 2p - 2q\big) = w$, as desired.

Conversely, for any tree T of order n $(n \geq 5)$ with p pendant vertices, from Lemma 3.1, $SW_{n-2}(T) = \frac{1}{2}\big(n^3 - 2n^2 + n - 2np + 2p - 2q\big)$. 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*

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

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 $k\binom{n-t}{k}$. If $S \subseteq V(P_t)$, then it contributes to SW_k by $(k-1)\binom{t+1}{k+1}$ 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 $|S \cap V(S_{n-t+1} - v)| = i$, $|S \cap V(P_t)| = k - i$ and $P_t = u_1 u_2 \cdots u_t$, where $v = u_1$. 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 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

$$\begin{aligned}\binom{j-1}{k-i-1}(j+i-1) &= \binom{j-1}{k-i-1} j + \binom{j-1}{k-i-1}(i-1) \\ &= (k-i)\binom{j}{k-i} + (i-1)\binom{j-1}{k-i-1},\end{aligned}$$

it follows that

$$\begin{aligned}\sum_{j=k-i}^{t} \binom{j-1}{k-i-1}(j+i-1) &= (k-i)\sum_{j=k-i}^{t}\binom{j}{k-i} + (i-1)\sum_{j=k-i}^{t}\binom{j-1}{k-i-1} \\ &= (k-i)\binom{t+1}{k-i+1} + (i-1)\binom{t}{k-i},\end{aligned}$$

and hence

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

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

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

Let

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

Then

$$\begin{aligned}
Y &= \sum_{i=1}^{k-1}(k-i+1)\binom{t}{k-i+1}\binom{n-t}{i} - \sum_{i=1}^{k-1}\binom{t}{k-i+1}\binom{n-t}{i} \\
&= t\sum_{i=1}^{k-1}\binom{t-1}{k-i}\binom{n-t}{i} - \sum_{i=1}^{k-1}\binom{t}{k+1-i}\binom{n-t}{i} \\
&= t\left[\binom{n-1}{k} - \binom{t-1}{k} - \binom{n-t}{k}\right] \\
&\quad - \left[\binom{n}{k+1} - \binom{t}{k+1} - t\binom{n-t}{k} - \binom{n-t}{k+1}\right],
\end{aligned}$$

and hence

$$\begin{aligned}
SW_k(T) &= (k-1)\binom{t+1}{k+1} + k\binom{n-t}{k} + X \\
&= (k-1)\binom{t+1}{k+1} + k\binom{n-t}{k} + Y + (k-1)\left[\binom{n}{k} - \binom{t}{k} - \binom{n-t}{k}\right] \\
&= (k-1)\binom{t+1}{k+1} + k\binom{n-t}{k} + t\left[\binom{n-1}{k} - \binom{t-1}{k} - \binom{n-t}{k}\right] \\
&\quad - \left[\binom{n}{k+1} - \binom{t}{k+1} - t\binom{n-t}{k} - \binom{n-t}{k+1}\right] \\
&\quad + (k-1)\left[\binom{n}{k} - \binom{t}{k} - \binom{n-t}{k}\right]
\end{aligned}$$

$$
\begin{aligned}
&= (k-1)\binom{t}{k+1} + (k-1)\binom{t}{k} + k\binom{n-t}{k} + t\binom{n-1}{k} - t\binom{t-1}{k} \\
&\quad - t\binom{n-t}{k} - \binom{n}{k+1} + \binom{t}{k+1} + t\binom{n-t}{k} + \binom{n-t}{k+1} \\
&\quad + (k-1)\binom{n}{k} - (k-1)\binom{t}{k} - (k-1)\binom{n-t}{k} \\
&= (k-1)\binom{t}{k+1} + k\binom{n-t}{k} + t\binom{n-1}{k} - t\binom{t-1}{k} \\
&\quad - \binom{n}{k+1} + \binom{t}{k+1} + \binom{n-t}{k+1} + (k-1)\binom{n}{k} - (k-1)\binom{n-t}{k} \\
&= k\binom{t}{k+1} + \binom{n-t}{k} + t\binom{n-1}{k} - t\binom{t-1}{k} - \binom{n}{k+1} + \binom{n-t}{k+1} \\
&\quad + (k-1)\binom{n}{k} \\
&= k\binom{t}{k+1} + t\binom{n-1}{k} - t\binom{t-1}{k} - \binom{n}{k+1} + \binom{n-t+1}{k+1} + (k-1)\binom{n}{k} \\
&= t\binom{n-1}{k} - \binom{t}{k+1} - \binom{n}{k+1} + \binom{n-t+1}{k+1} + (k-1)\binom{n}{k}.
\end{aligned}
$$

■

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*

$$w = t\binom{n-1}{k} - \binom{t}{k+1} - \binom{n}{k+1} + \binom{n-t+1}{k+1} + (k-1)\binom{n}{k},$$

where $1 \leq t \leq n-1$ and $k \leq n$.

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 $k \leq r \leq n-1-k$,*

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

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 $\binom{r}{k}$ such subsets, contributing to SW_k by $k\binom{r}{k}$. 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 $\binom{n-r-1}{k-x-1}\binom{r}{x}$ 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 $\binom{n-r-1}{k-x}\binom{r}{x}$ such subsets, contributing to SW_k by $k\sum_{x=1}^{k-1}\binom{n-r-1}{k-x}\binom{r}{x}$. Then

$$
\begin{aligned}
& SW_k(G) \\
&= (k-1)\binom{n-r}{k} + k\binom{r}{k} + (k-1)\sum_{x=1}^{k-1}\binom{n-r-1}{k-x-1}\binom{r}{x} \\
&\quad + k\sum_{x=1}^{k-1}\binom{n-r-1}{k-x}\binom{r}{x} \\
&= (k-1)\binom{n-r}{k} + k\binom{r}{k} + (k-1)\left[\binom{n-1}{k-1} - \binom{n-1-r}{k-1}\right] \\
&\quad + k\left[\binom{n-1}{k} - \binom{n-1-r}{k} - \binom{r}{k}\right] \\
&= (k-1)\binom{n-r}{k} + (k-1)\left[\binom{n-1}{k-1} - \binom{n-1-r}{k-1}\right] \\
&\quad + k\left[\binom{n-1}{k} - \binom{n-1-r}{k}\right] \\
&= (k-1)\binom{n-r}{k} + (n-1)\binom{n-1}{k-1} - (k-1)\binom{n-1-r}{k-1} - k\binom{n-1-r}{k} \\
&= (n-1)\binom{n-1}{k-1} + (k-1)\binom{n-r-1}{k} - k\binom{n-1-r}{k} \\
&= (n-1)\binom{n-1}{k-1} - \binom{n-1-r}{k},
\end{aligned}
$$

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.*

(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* $1 \le t \le n-1$ *and* $k \le n$.
(2) $w = (n-1)\binom{n-1}{k-1} - \binom{n-r-1}{k}$, *where* $k \le r \le n-1-k$ *and* $k \le n$.

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