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A sharp lower bound on Steiner Wiener index for trees with given diameter

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ABSTRACT

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For a subset S of $V(G)$, the *Steiner distance* $d(S)$ of S is the minimum size of a connected subgraph whose vertex set contains S. For an integer k with $2 \leq k \leq n-1$, the *Steiner k-Wiener index* $\mathrm{SW}_k(G)$ is $\sum_{S\subseteq V(G),|S|=k} d(S)$. In this paper, we introduce some transformations for trees that do not increase their Steiner k-Wiener index for $2 \leq k \leq n-1$. Using these transformations, we get a sharp lower bound on Steiner k-Wiener index for trees with given diameter, and obtain the corresponding extremal graph as well.

1. Introduction

Throughout this paper all graphs are connected and simple, and all notations and terminologies not described here are standard in [1]. For a graph G and two vertices $u, v \in V(G)$, the *distance* between u and v, denoted by $d_G(u, v)$, is the length of a shortest path connecting u and v. The *diameter* $d(G)$ of G is the largest distance between any two vertices. The *Wiener index* $W(G)$ of a graph G is the sum of distances between each pair of vertices, that is,

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

The Wiener index is an important distance-based graph invariant. It was proposed by Harold Wiener [11] in 1947. He found that there exist correlations between the boiling points of paraffins and their molecular structure. The study of the Wiener index in mathematics dates back to the 1970s [4]. Since then, the Wiener index obtained wide attention and many splendid results have been obtained, see the surveys [3,6,7,12].

Let G be a graph with vertex set V and edge set E. For a subset S of V, the *Steiner distance* $d_G(S)$ of S is the minimum size of a connected subgraph whose vertex set contains S, that is,

$$d_G(S) = \min\{|E(H)| : H \text{ is a connected subgraph of } G \text{ with } S \subseteq V(H)\}.$$

This concept was proposed by Chartrand et al. [2] in 1989. Note that the size of the spanning tree of H is not greater than $|E(H)|$. Therefore, the Steiner distance can be written as

$$d_G(S) = \min\{|E(T)| : T \text{ is a subtree of } G \text{ with } S \subseteq V(T)\}.$$

Taking $S = \{u, v\}$, we see that $d_G(S) = d_G(u, v)$. Thus the concept of Steiner distance is a natural generalization of the concept of classical distance.

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With respect to the concept of Steiner distance, Li et al. [8] generalized the concept of Wiener index by Steiner Wiener index. For an integer k with $2 \le k \le n-1$, the *Steiner k-Wiener index* $\mathrm{SW}_k(G)$ of G is the sum of Steiner k-distances of all subsets S of V with $|S| = k$, that is,

$$\mathrm{SW}_k(G) = \sum_{S \subseteq V, |S|=k} d_G(S).$$

The classical Wiener index is just the special case of Steiner k-Wiener index for $k = 2$. The application of Steiner Wiener index was introduced in [5]. Recently, Mao et al. [10] established expressions for the Steiner k-Wiener index on the join, corona, cluster, lexicographical product, and Cartesian product of graphs.

In 1976, Entringer et al. [4] obtained the lower and upper bounds on Wiener index for trees, that is,

$$(n-1)^2 \le W(T) \le \binom{n+1}{3}$$

and the star S_n minimizes the Wiener index and the path P_n maximizes the Wiener index. Recently, Li et al. [8] generalized this result to the Steiner Wiener index, that is,

$$\binom{n-1}{k-1}(n-1) \le \mathrm{SW}_k(T) \le (k-1)\binom{n+1}{k+1}$$

for $2 \le k \le n-1$, and the star S_n and the path P_n attain the lower and upper bounds, respectively. In 2008, Liu et al. [9] characterized the tree with smallest Wiener index among all trees with given diameter. Naturally, we would like to generalize this result to the Steiner Wiener index. In Section 2, we introduce some transformations for a tree which do not increase its Steiner Wiener index. In Section 3, we give a sharp lower bound on the Steiner Wiener index for trees with given diameter, and obtain the corresponding extremal graph as well.

2. Transformations for trees

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, denote by $d(v)$ and $N(v)$ the degree and the neighbourhood of v, respectively. As usual, we write P_n, C_n and $K_{a,b}$ for the path, the cycle and the complete bipartite graphs, respectively. For two integers n and d with $2 \le d \le n-1$, let $\mathcal{T}(n)$ be the family of trees on n vertices and $\mathcal{T}(n,d) = \{T \in \mathcal{T}(n) : d(T) = d\}$. Clearly, $\mathcal{T}(2) = \{P_2\}$, $\mathcal{T}(3) = \{P_3\}$, $\mathcal{T}(n,2) = \{K_{1,n-1}\}$ and $\mathcal{T}(n,n-1) = \{P_n\}$. Each of them contains only one graph whose Steiner Wiener index is clear. Therefore, we only consider $\mathcal{T}(n,d)$ with $n \ge 4$ and $3 \le d \le n-2$. In this part, we will introduce some transformations for a tree, which do not increase its Steiner Wiener index.

We start with a useful combinatorial inequality.

Lemma 2.1. *Let a, b and k be three positive integers such that $a \le b$. If $2 \le k \le b+1$, then $\binom{a}{k} + \binom{b}{k} < \binom{a-1}{k} + \binom{b+1}{k}$; if $k \ge b+2$, then $\binom{a}{k} + \binom{b}{k} = \binom{a-1}{k} + \binom{b+1}{k}$.*

Proof. Note that $\binom{n-1}{m-1} + \binom{n-1}{m} = \binom{n}{m}$ for two positive integers m and n. It follows that

$$\left[\binom{a-1}{k} + \binom{b+1}{k}\right] - \left[\binom{a}{k} + \binom{b}{k}\right] = \left[\binom{b+1}{k} - \binom{b}{k}\right] - \left[\binom{a}{k} - \binom{a-1}{k}\right] = \binom{b}{k-1} - \binom{a-1}{k-1}.$$

If $2 \le k \le b+1$ then $\binom{b}{k-1} - \binom{a-1}{k-1} > 0$; if $k \ge b+2$ then $\binom{b}{k-1} - \binom{a-1}{k-1} = 0 - 0 = 0$. This completes the proof. $\square$

Let $T \in \mathcal{T}(n)$ and $e \in E(T)$ such that $e = v_1v_2$. We say that v_1 and v_2 are the *left end* and the *right end* of e, respectively. Denote by

$$N_l^{(T)}(e) = \{v \in V(T) : d(v, v_1) < d(v, v_2)\},\ N_r^{(T)}(e) = \{v \in V(T) : d(v, v_1) > d(v, v_2)\}$$

and $n_l^{(T)}(e) = |N_l^{(T)}(e)|$, $n_r^{(T)}(e) = |N_r^{(T)}(e)|$. In other words, $N_l^{(T)}(e)$ and $N_r^{(T)}(e)$ are the vertex sets of the components of $G - e$ containing v_1 and v_2, respectively. By the definitions, $V(T) = N_l^{(T)}(e) \cup N_r^{(T)}(e)$ and $n = n_l^{(T)}(e) + n_r^{(T)}(e)$. Denote by $\gamma^{(T)}(e) = \min\{n_l^{(T)}(e), n_r^{(T)}(e)\}$ and $\eta^{(T)}(e) = \max\{n_l^{(T)}(e), n_r^{(T)}(e)\}$. Obviously, $n_l^{(T)}(v_1v_2)$ and $n_r^{(T)}(v_1v_2)$ depend on the order of v_1 and v_2, but $\gamma^{(T)}(v_1v_2)$ and $\eta^{(T)}(v_1v_2)$ do not. When the tree T is clear from the context, we delete T from the notations like $N_l^{(T)}(e)$, $n_l^{(T)}(e)$ and $\gamma^{(T)}(e)$. Li et al. give a useful formula to calculate the Steiner Wiener index of a tree.

Lemma 2.2 (*Theorem 4.3 of [8]*)**.** *Let k be an integer such that $2 \le k \le n$. If T is a tree, then for its Steiner k-Wiener index holds*

$$SW_k(T) = \sum_{e \in E(T)} \sum_{i=1}^{k-1} \binom{n_l(e)}{i}\binom{n_r(e)}{k-i}.$$

Note that $\mathrm{SW}_n(T) = n-1$ for all trees on n vertices. We only consider $\mathrm{SW}_k(T)$ for $2 \le k \le n-1$. Since $\{\gamma(e), \eta(e)\} = \{n_l(e), n_r(e)\}$, the formula given in Lemma 2.2 can be simplified as follows.

Lemma 2.3. *Let k be an integer such that $2 \le k \le n-1$. If T is a tree, then for its Steiner k-Wiener index holds*

$$SW_k(T) = (n-1)\binom{n}{k} - \sum_{e\in E(T)} \left[\binom{\gamma(e)}{k} + \binom{\eta(e)}{k}\right].$$

Proof. Note the combinatorial identity $\sum_{i=0}^{k}\binom{a}{i}\binom{b}{k-i} = \binom{a+b}{k}$. Since $\{\gamma(e), \eta(e)\} = \{n_l(e), n_r(e)\}$ and $\gamma(e)+\eta(e) = n_l(e)+n_r(e) = n$ for $e \in E(T)$, Lemma 2.2 implies that

$$\begin{aligned}
\mathrm{SW}_k(T) &= \sum_{e\in E(T)}\sum_{i=1}^{k-1}\binom{n_l(e)}{i}\binom{n_r(e)}{k-i} = \sum_{e\in E(T)}\sum_{i=1}^{k-1}\binom{\gamma(e)}{i}\binom{\eta(e)}{k-i}\\
&= \sum_{e\in E(T)}\left[\sum_{i=0}^{k}\binom{\gamma(e)}{i}\binom{\eta(e)}{k-i} - \binom{\gamma(e)}{0}\binom{\eta(e)}{k} - \binom{\gamma(e)}{k}\binom{\eta(e)}{0}\right]\\
&= \sum_{e\in E(T)}\left[\binom{n}{k} - \left[\binom{\gamma(e)}{k} + \binom{\eta(e)}{k}\right]\right]\\
&= (n-1)\binom{n}{k} - \sum_{e\in E(T)}\left[\binom{\gamma(e)}{k} + \binom{\eta(e)}{k}\right].
\end{aligned}$$

It follows our result. □

Let T and T' be two trees in $\mathcal{T}(n)$. For $\epsilon \in E(T)$ and a positive integer s, a *feasible map* from T to T' with respect to ϵ and s is a bijection ϕ: $E(T) \to E(T')$ such that:
(i) $\gamma^{(T)}(\epsilon) - s = \gamma^{(T')}(\phi(\epsilon))$,
(ii) $\gamma^{(T)}(e) = \gamma^{(T')}(\phi(e))$ for $e \in E(T) \setminus \{\epsilon\}$.

Denote by $\mathcal{F}_{\epsilon,s}(T, T')$ the set of all feasible maps from T to T' with respect to ϵ and s. Now we give a criterion to compare the Steiner Wiener indices of two trees.

Theorem 2.1. *Let T and T' be two trees in $\mathcal{T}(n)$. If there exist $\epsilon \in E(T)$ and a positive integer s such that $\mathcal{F}_{\epsilon,s}(T, T') \neq \emptyset$, then $SW_k(T) > SW_k(T')$ for $2 \le k \le \eta^{(T)}(\epsilon) + s$ and $SW_k(T) = SW_k(T')$ for $\eta^{(T)}(\epsilon) + s < k \le n-1$.*

Proof. Assume $\phi \in \mathcal{F}_{\epsilon,s}(T, T')$. We consider $\mathrm{SW}_k(T) - \mathrm{SW}_k(T')$ for $2 \le k \le n-1$. By Lemma 2.3, we have

$$\begin{aligned}
\mathrm{SW}_k(T) - \mathrm{SW}_k(T') &= \left[(n-1)\binom{n}{k} - \sum_{e\in E(T)}\left[\binom{\gamma^{(T)}(e)}{k} + \binom{\eta^{(T)}(e)}{k}\right]\right]\\
&\quad - \left[(n-1)\binom{n}{k} - \sum_{e\in E(T')}\left[\binom{\gamma^{(T')}(e)}{k} + \binom{\eta^{(T')}(e)}{k}\right]\right]\\
&= \sum_{e\in E(T')}\left[\binom{\gamma^{(T')}(e)}{k} + \binom{\eta^{(T')}(e)}{k}\right] - \sum_{e\in E(T)}\left[\binom{\gamma^{(T)}(e)}{k} + \binom{\eta^{(T)}(e)}{k}\right]\\
&= \sum_{e\in E(T)}\left[\binom{\gamma^{(T')}(\phi(e))}{k} + \binom{\eta^{(T')}(\phi(e))}{k}\right] - \sum_{e\in E(T)}\left[\binom{\gamma^{(T)}(e)}{k} + \binom{\eta^{(T)}(e)}{k}\right]\\
&= \left[\binom{\gamma^{(T')}(\phi(\epsilon))}{k} + \binom{\eta^{(T')}(\phi(\epsilon))}{k}\right] - \left[\binom{\gamma^{(T)}(\epsilon)}{k} + \binom{\eta^{(T)}(\epsilon)}{k}\right].
\end{aligned}$$

By Lemma 2.1, we have

$$\begin{aligned}
&\left[\binom{\gamma^{(T)}(\epsilon)}{k} + \binom{\eta^{(T)}(\epsilon)}{k}\right]\\
&\le \left[\binom{\gamma^{(T)}(\epsilon)-1}{k} + \binom{\eta^{(T)}(\epsilon)+1}{k}\right]\\
&\le \cdots\\
&\le \left[\binom{\gamma^{(T)}(\epsilon)-(s-1)}{k} + \binom{\eta^{(T)}(\epsilon)+(s-1)}{k}\right]
\end{aligned}$$

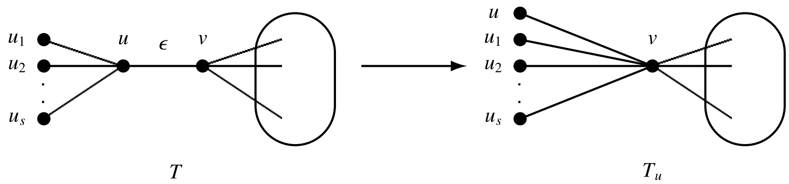

Fig. 1. The star-root transformation of T on u.

$$\leq \left[\binom{\gamma^{(T)}(\epsilon)-s}{k}+\binom{\eta^{(T)}(\epsilon)+s}{k}\right]$$
$$=\left[\binom{\gamma^{(T')}(\phi(\epsilon))}{k}+\binom{\eta^{(T')}(\phi(\epsilon))}{k}\right].$$

Rather, if $k \leq \eta^{(T)}(\epsilon)+s$ then the last inequality above must be strict; if $k > \eta^{(T)}(\epsilon)+s$ then all above inequalities become equalities. Thus we have

$$\begin{cases} \mathrm{SW}_k(T)-\mathrm{SW}_k(T')>0 & \text{if } k \leq \eta^{(T)}(\epsilon)+s\,, \\ \mathrm{SW}_k(T)-\mathrm{SW}_k(T')=0 & \text{if } k > \eta^{(T)}(\epsilon)+s. \end{cases}$$

It follows our result. □

By Theorem 2.1 we will give some transformations for a tree, which do not increase its Steiner Wiener index. In fact, they are all special cases of Theorem 2.1 for some specific ϵ and s.

For a tree $T \in \mathcal{T}(n)$, a vertex $u \in V(T)$ is a *star-root* if $N(u)=\{v,u_1,\ldots,u_s\}$ such that $d(v)>1$ and $d(u_i)=1$ for $1 \leq i \leq s$ and $s \geq 1$. Clearly, each tree $T \in \mathcal{T}(n)$ has at least two star-roots unless $T=K_{1,n-1}$. Let T be a tree in $\mathcal{T}(n)$ and u a star root in $V(T)$ with $N(u)=\{v,u_1,\ldots,u_s\}$ such that $d(v)>1$. We construct the new tree T_u from T by deleting the edges uu_i and adding the edges vu_i (see Fig. 1). The *star-root switching* of T on u is the transformation from T to T_u, and T_u is the corresponding *star-root switching graph*. By simple observations, T_u contains one more pendant vertex than T.

Corollary 2.1. *Let T be a tree in $\mathcal{T}(n)$. If u is a star-root of T, then $SW_k(T) > SW_k(T_u)$ for $2 \leq k \leq n-1$.*

Proof. Assume that $N(u)=\{v,u_1,\ldots,u_s\}$, where $d(v)>1$. We define the bijection $f\colon E(T)\to E(T_u)$ by $f(uu_i)=vu_i$ for $1 \leq i \leq s$ and $f(xy)=xy$ for $xy \in E(T)\setminus\{uu_1,\ldots,uu_s\}$. Denote by $\epsilon=uv$. It is easy to see that

$$\begin{cases} n_l^{(T)}(\epsilon)=s+1,\ n_r^{(T)}(\epsilon)=n-(s+1) \\ \gamma^{(T)}(e)=\gamma^{(T_u)}(f(e)),\ \text{ for } e \in E(T)\setminus\{\epsilon\} \\ \gamma^{(T_u)}(f(\epsilon))=1,\ \eta^{(T_u)}(f(\epsilon))=n-1. \end{cases}$$

If $s+1 \leq \frac{n}{2}$, then $\gamma^{(T)}(\epsilon)=n_l^{(T)}(\epsilon)=s+1$ and $\eta^{(T)}(\epsilon)=n_r^{(T)}(\epsilon)=n-(s+1)$. It means that $\gamma^{(T_u)}(f(\epsilon))=1=\gamma^{(T)}(\epsilon)-s$. Thus $f \in \mathcal{F}_{\epsilon,s}(T,T_u)$. By Theorem 2.1, we have $\mathrm{SW}_k(T)>\mathrm{SW}_k(T_u)$ for $2 \leq k \leq \eta^{(T)}(\epsilon)+s$. Note that $\eta^{(T)}(\epsilon)+s=n-1$. The result follows.

If $s+1 > \frac{n}{2}$, then $\gamma^{(T)}(\epsilon)=n-(s+1)$ and $\eta^{(T)}(\epsilon)=n-(n-(s+1))=s+1$. It means that $\gamma^{(T_u)}(f(\epsilon))=1=\gamma^{(T)}(\epsilon)-(n-s-2)$. Note that $s \leq n-3$. We have $n-s-2 \geq 1$, and thus $f \in \mathcal{F}_{\epsilon,n-s-2}$. By Theorem 2.1, we have $\mathrm{SW}_k(T)>\mathrm{SW}_k(T_u)$ for $2 \leq k \leq \eta^{(T)}(\epsilon)+(n-s-2)$. Note that $\eta^{(T)}(\epsilon)+(n-s-2)=n-1$. The result follows. □

Let $T \in \mathcal{T}(n)$ and $u \in V(T)$. Denote by $P(u)=\{v \in N(u): d(v)=1\}$ and $P(u)^*=\{v \in N(u): d(u)>1\}$. We say that u is a *pseudo star-root* if $|P(u)| \geq 1$ and $|P(u)^*| \geq 1$. Particularly, a star-root x is a pseudo star-root with $|P(x)^*|=1$. Suppose that v_1 is a pseudo star-root of T. For $v_2 \in P(v_1)^*$ and $U=\{u_1,\ldots,u_s\}\subseteq P(v_1)$, we construct the new tree $T^{(U)}_{v_1\to v_2}$ from T by deleting the edges v_1u_i and adding the edges v_2u_i for $1 \leq i \leq s$ (see Fig. 2). The *pseudo star-root switching* of T from v_1 to v_2 with respect to U is the transformation from T to $T^{(U)}_{v_1\to v_2}$, and $T^{(U)}_{v_1\to v_2}$ is the corresponding *pseudo star-root switching graph*. The pseudo star-root switching is *complete* if $U=P(v_1)$. For convenience, denote by $T_{v_1\to v_2}=T^{(P(v_1))}_{v_1\to v_2}$.

Corollary 2.2. *Let T be a tree in $\mathcal{T}(n)$ and v_1 a pseudo star-root of T. Let U be a nonempty subset of $P(v_1)$ and $v_2 \in P(v_1)^*$. If $n_l^{(T)}(v_1v_2) \leq n_r^{(T)}(v_1v_2)$, then $SW_k(T) > SW_k(T^{(U)}_{v_1\to v_2})$ for $2 \leq k \leq \eta^{(T)}(v_1v_2)+|U|$ and $SW_k(T)=SW_k(T^{(U)}_{v_1\to v_2})$ for $\eta^{(T)}(v_1v_2)+|U| < k \leq n-1$.*

Proof. Define the bijection $f\colon E(T)\to E(T^{(U)}_{v_1\to v_2})$ by $f(v_1u)=v_2u$ for $u \in U$ and $f(xy)=xy$ for $xy \in E(T)\setminus\{v_1u : u \in U\}$. Denote by $\epsilon=v_1v_2$. Obviously, $\gamma^{(T)}(e)=\gamma^{(T^{(U)}_{v_1\to v_2})}(f(e))$ for $e \in E(T)\setminus\{\epsilon\}$. Since $n_l^{(T)}(v_1v_2) \leq n_r^{(T)}(v_1v_2)$, we have

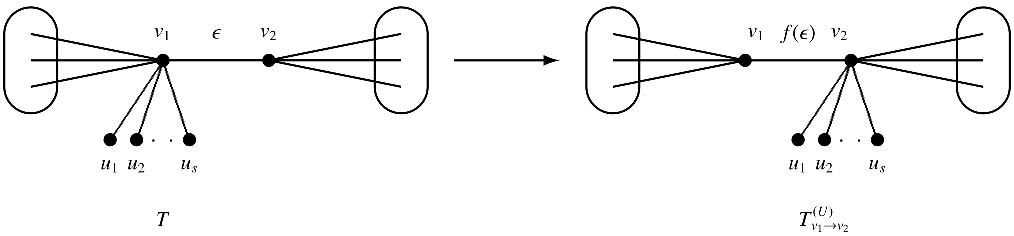

Fig. 2. The pseudo star-root switching from v_1 to v_2 with respect to U.

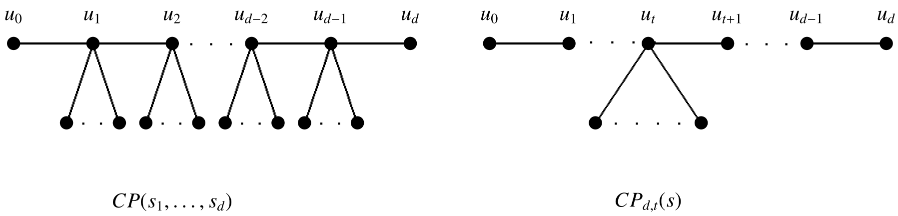

Fig. 3. The caterpillar graphs.

$\gamma^{(T)}(\epsilon) = n_l^{(T)}(\epsilon)$ and $\gamma^{(T^{(U)}_{v_1\to v_2})}(f(\epsilon)) = n_l^{(T)}(\epsilon) - |U| = \gamma^{(T)}(\epsilon) - |U|$. Thus $f \in \mathcal{F}_{\epsilon,|U|}$, and so the result follows from Theorem 2.1. $\square$

The *caterpillar tree* with respect to $P_d = u_0u_1\cdots u_d$, denoted by $CP(s_1,\ldots,s_{d-1})$, is the tree obtained from P_d by attaching s_i new vertices to u_i for $1 \le i \le d-1$ (see Fig. 3). Especially, the path P_d itself can be regarded as the caterpillar tree $CP(\underbrace{0,0,\ldots,0}_{d-1})$ and the star $K_{1,n-1}$ can be regarded as the caterpillar tree $CP(n-3)$. Obviously, $CP(s_1,s_2,\ldots,s_{d-1}) \in \mathcal{T}(n,d)$, where $n = \sum_{i=1}^{d-1} s_i + d + 1$. Particularly, if $s_i = 0$ for $i \ne t$ and $s_t = s \ne 0$, then such a caterpillar tree is denoted by $CP_{d,t}(s)$ (see Fig. 3), that is,

$$CP_{d,t}(s) = CP(\underbrace{0,\ldots,0}_{t-1}, s, \underbrace{0,\ldots,0}_{d-1-t}).$$

Note that $CP_{d,t}(s) \cong CP_{d,d-t}(s)$. We always assume that $t \le \frac{d}{2}$ in the notation $CP_{d,t}(s)$.

Corollary 2.3. *Let $CP_{d,t}(s)$ be a caterpillar tree with respect to $P_d = u_0u_1\cdots u_d$ such that $s \ge 1$. If $t \le \frac{d}{2} - 1$, then $SW_k(CP_{d,t}(s)) > SW_k(CP_{d,t+1}(s))$ for $2 \le k \le d-t+s$ and $SW_k(CP_{d,t}(s)) = SW_k(CP_{d,t+1}(s))$ for $d-t+s < k \le n-1$.*

Proof. Denote by $T = CP_{d,t}(s)$ and $T' = CP_{d,t+1}(s)$ (see Fig. 4). Define the bijection $f\colon E(T) \to E(T')$ by $f(u_tu) = u_{t+1}u$ for $u \in P(u_t)$ and $f(xy) = xy$ for $xy \in E(T)\setminus\{u_tu : u \in P(u_t)\}$. Denote by $\epsilon = u_tu_{t+1}$. Obviously, $n_l^{(T)}(\epsilon) = s+t+1$, $n_r^{(T)}(\epsilon) = d-t$ and $\gamma^{(T)}(e) = \gamma^{(T')}(f(e))$ for $e \ne \epsilon$.

If $s+t+1 \le d-t$, then $\gamma^{(T)}(\epsilon) = n_l^{(T)}(\epsilon) = s+t+1$ and $\eta^{(T)}(\epsilon) = n_r^{(T)}(\epsilon) = d-t$. Therefore, $\gamma^{(T')}(f(\epsilon)) = t+1 = \gamma^{(T)}(\epsilon) - s$. Thus $f \in \mathcal{F}_{\epsilon,s}(T,T')$, and so the result follows from Theorem 2.1.

If $s+t+1 > d-t$, then $\gamma^{(T)}(\epsilon) = n_r^{(T)}(\epsilon) = d-t$ and $\eta^{(T)}(\epsilon) = n_l^{(T)}(\epsilon) = s+t+1$. Since $t \le \frac{d}{2} - 1$, we have $n_r^{(T')}(f(\epsilon)) - n_l^{(T')}(f(\epsilon)) = (d-t+s) - (t+1) = d-2t+s-1 \ge s+1 > 0$. It means that $\gamma^{(T')}(f(\epsilon)) = n_l^{(T')}(f(\epsilon)) = t+1$. Therefore, $\gamma^{(T')}(f(\epsilon)) = t+1 = \gamma^{(T)}(\epsilon) - (d-2t-1)$. Note that $d-2t-1 \ge 1$. We have $f \in \mathcal{F}_{\epsilon,d-2t-1}(T,T')$, and so the result follows from Theorem 2.1. $\square$

3. The sharp lower bound for trees in $\mathcal{T}(n,d)$

In this section, we first prove that the caterpillar tree $CP_{d,\lfloor\frac{d}{2}\rfloor}(n-d-1)$ minimizes the Steiner k-Wiener index in $\mathcal{T}(n,d)$ for $2 \le k \le n-1$ by using the transformations given in Section 2. Next, we get the lower bound by computing the Steiner k-Wiener index of $CP_{d,\lfloor\frac{d}{2}\rfloor}(n-d-1)$. Keep in mind that we always assume $n \ge 4$ and $3 \le d \le n-2$ for $\mathcal{T}(n,d)$.

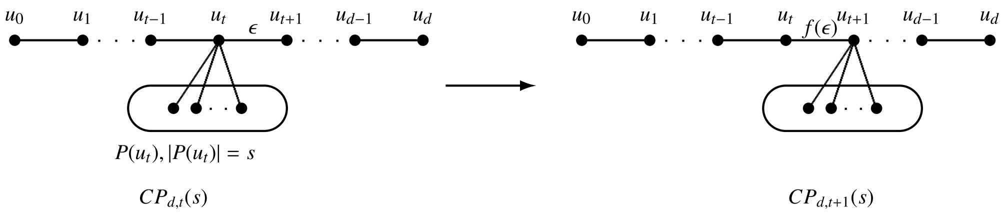

Fig. 4. The caterpillar trees $CP_{d,t}(s)$ and $CP_{d,t+1}(s)$.

Lemma 3.1. *Let T be a tree in $\mathcal{T}(n, d)$ and $P = u_0u_1 \ldots u_d$ an induced path of T. Then there exists a caterpillar tree $CP(s_1, s_2, \ldots, s_{d-1}) \in \mathcal{T}(n, d)$ with respect to P such that*

$$SW_k(T) \geq SW_k(CP(s_1, s_2, \ldots, s_{d-1}))$$

for $2 \leq k \leq n-1$ with equality if and only if $T \cong CP(s_1, s_2, \ldots, s_{d-1})$.

Proof. Recall the definition of star-roots. It is easy to see that a tree is a caterpillar tree if and only if it contains exactly two star-roots. Note that u_1 and u_{d-1} are two star-roots of T. If u_1 and u_{d-1} are the only star-roots of T, then T is a caterpillar tree with respect to P, and there is nothing to prove. Otherwise T contains a star-root u different from u_1 and u_{d-1}. By star-root switching on u, we transform T to T_u. By Corollary 2.1, we have $\mathrm{SW}_k(T) > \mathrm{SW}_k(T_u)$ for $2 \leq k \leq n-1$. Note that u_1 and u_{d-1} are still star-roots of T_u. We regard T_u as T and repeat this process. We will end up in finite times because T_u contains one more pendant vertex than T. At last we always get the caterpillar tree $CP(s_1, s_2, \ldots, s_{d-1})$ with respect to P. □

Lemma 3.2. *If $CP(s_1, \ldots, s_{d-1})$ is a caterpillar tree in $\mathcal{T}(n, d)$ with respect to $P = u_0u_1 \ldots u_d$, then there exists an integer $a \in \left[1, \lfloor \frac{d}{2} \rfloor\right]$ such that*

$$SW_k(CP(s_1, \ldots, s_{d-1})) \geq SW_k(CP_{d,a}(n-d-1))$$

for $2 \leq k \leq n-1$. Furthermore, the equality holds for all k if and only if $CP(s_1, \ldots, s_{d-1}) \cong CP_{d,a}(n-d-1)$.

Proof. Denote by $T = CP(s_1, \ldots, s_{d-1})$ and $i_0 = \max\{1 \leq i \leq n-1 : n_l^{(T)}(u_iu_{i+1}) = i + 1 + \sum_{j=1}^{i} s_j \leq \frac{n}{2}\}$. Therefore, $n_l^{(T)}(u_iu_{i+1}) \leq n_r^{(T)}(u_iu_{i+1})$ if and only if $i \leq i_0$, that is,

$$n_l^{(T)}(u_iu_{i+1}) \leq n_r^{(T)}(u_iu_{i+1}), \text{ for } 1 \leq i \leq i_0 \tag{1}$$

and

$$n_l^{(T)}(u_{i+1}u_i) \leq n_r^{(T)}(u_{i+1}u_i), \text{ for } i_0 + 1 \leq i \leq d-2. \tag{2}$$

In what follows we prove that $\mathrm{SW}_k(CP(s_1, \ldots, s_{d-1})) \geq \mathrm{SW}_k(CP_{d,i_0+1}(n-d-1))$.

For $1 \leq i \leq i_0 + 1$, we define $T(i) = CP(\underbrace{0, \ldots, 0}_{i-1}, \sum_{j=1}^{i} s_j, s_{i+1}, \ldots, s_{d-1})$. Without loss of generality, assume $s_1 > 0$. Thus u_i is a pseudo star-root of $T(i)$ for $1 \leq i \leq i_0$. Moreover, we have

$$\begin{cases} T(1) = T \\ T(2) = T(1)^{(U)}_{u_1 \to u_2}, \text{ where } U = P(u_1) \setminus \{u_0\} \\ T(i+1) = T(i)_{u_i \to u_{i+1}}, \text{ for } 2 \leq i \leq i_0. \end{cases}$$

By the definition of $T(i)$, we see that

$$n_l^{(T(i))}(u_iu_{i+1}) = i + 1 + \sum_{j=1}^{i} s_j = n_l^{(T)}(u_iu_{i+1}), \quad \text{for } 1 \leq i \leq i_0.$$

Therefore, from (1), we have $n_l^{(T(i))}(u_iu_{i+1}) \leq n_r^{(T(i))}(u_iu_{i+1})$ for $1 \leq i \leq i_0$. Thus Corollary 2.2 implies that

$$\mathrm{SW}_k(T(1)) \geq \mathrm{SW}_k(T(2)) \geq \cdots \geq \mathrm{SW}_k(T(i_0+1)) = \mathrm{SW}_k(CP(\underbrace{0, \ldots, 0}_{i_0}, \sum_{j=1}^{i_0+1} s_j, s_{i_0+2}, \ldots, s_{d-1})).$$

For $1 \leq i \leq d - i_0 - 1$, denote by

$$T'(i) = CP(\underbrace{0, \ldots, 0}_{i_0}, s'_{i_0+1}, s'_{i_0+2}, \ldots, s'_{d-(i+1)}, \sum_{j=d-i}^{d-1} s'_j, \underbrace{0, \ldots, 0}_{i-1}),$$

where $s'_{i_0+1} = \sum_{j=1}^{i_0+1} s_j$ and $s'_j = s_j$ for $i_0 + 2 \le j \le d - 1$. Without loss of generality, assume that $s_{d-1} > 0$. Thus u_{d-i} is a pseudo star-root of $T'(i)$ for $1 \le i \le d - i_0 - 2$. Moreover, we have

$$\begin{cases} T'(1) = T(i_0 + 1) \\ T'(2) = T'(1)^{(U')}_{u_{d-1}\to u_{d-2}}, \text{ where } U' = P(u_{d-1}) \setminus \{u_d\} \\ T'(i + 1) = T'(i)_{u_{d-i}\to u_{d-(i+1)}}, \text{ for } 2 \le i \le d - i_0 - 2. \end{cases}$$

Similarly, from (2), we have $n_l^{(T'(i))}(u_{d-i}u_{d-i-1}) \le n_r^{(T'(i))}(u_{d-i}u_{d-i-1})$ for $1 \le i \le d - i_0 - 2$. Thus Corollary 2.2 implies that

$$\mathrm{SW}_k(T'(1)) \ge \mathrm{SW}_k(T'(2)) \ge \cdots \ge \mathrm{SW}_k(T'(d - i_0 - 1)) = \mathrm{SW}_k(CP(\underbrace{0, \ldots, 0}_{i_0}, \sum_{j=1}^{d-1} s_j, \underbrace{0, \ldots, 0}_{d-i_0-2})).$$

By the arguments above, we have $\mathrm{SW}_k(T(1)) \ge \mathrm{SW}_k(T'(d - i_0 - 1))$, that is,

$$\mathrm{SW}_k(CP(s_1, \ldots, s_{d-1})) \ge \mathrm{SW}_k(CP_{d,i_0+1}(n - d - 1)).$$

If $i_0 + 1 \le \lfloor \frac{d}{2} \rfloor$, then take $a = i_0 + 1$ and the result follows. If $i_0 + 1 > \lfloor \frac{d}{2} \rfloor$, since $CP_{d,i_0+1}(n - 1 - d) \cong CP_{d,d-(i_0+1)}(n - 1 - d)$, then take $a = d - (i_0 + 1)$ and the result follows. □

Lemma 3.3. *If $CP_{d,t}(n - d - 1)$ is a caterpillar tree in $\mathcal{T}(n, d)$ with respect to $P = u_0u_1 \ldots u_d$, then we have*

$$SW_k(CP_{d,t}(n - d - 1)) \ge SW_k(CP_{d,\lfloor \frac{d}{2} \rfloor}(n - d - 1))$$

for $2 \le k \le n - 1$. Furthermore, the equality holds for all k if and only if $CP_{d,t}(n - d - 1) \cong CP_{d,\lfloor \frac{d}{2} \rfloor}(n - d - 1)$.

Proof. Since $CP_{d,t}(n - d - 1) \cong CP_{d,d-t}(n - d - 1)$, without loss of generality, we assume that $t \le \lfloor \frac{d}{2} \rfloor$. If $t = \lfloor \frac{d}{2} \rfloor$, there is nothing to prove. Otherwise $t \le \lfloor \frac{d}{2} \rfloor - 1$. By Corollary 2.3, we have $\mathrm{SW}_k(CP_{d,t+i}(n - d - 1)) \ge \mathrm{SW}_k(CP_{d,t+i+1}(n - d - 1))$ for $0 \le i \le \lfloor \frac{d}{2} \rfloor - t - 1$. It follows our result. □

Combining Lemmas 3.1–3.3, we get our main result immediately.

Theorem 3.1. *For $T \in \mathcal{T}(n, d)$ with $3 \le d \le n-2$, we have $SW_k(T) \ge SW_k(CP_{d,\lfloor \frac{d}{2} \rfloor}(n-d-1))$ for $2 \le k \le n-1$. Furthermore, the equality holds for all k if and only if $T \cong CP_{d,\lfloor \frac{d}{2} \rfloor}(n - d - 1)$.*

We recall that Theorem 3.1 provides a generalization of the result known for the Wiener index [9], i.e., it yields this result by setting $k = 2$. To make our results more clear, we present a specific example.

Example 1. The tree T given in Fig. 5 is in $\mathcal{T}(16, 6)$. Firstly, by star-root switching, we transform T into a caterpillar tree as the proof of Lemma 3.1. Since v_5 is a star-root of T, we transform T to $T' = T_{v_5}$. Since v_7 is a star-root of T', we transform T' to $T'' = T'_{v_7} = CP(1, 4, 2, 1, 1)$. Next, by pseudo star-root switching, we transform T'_{v_7} into $CP_{6,a}(9)$ for some $a \in [1, 3]$ as the proof of Lemma 3.2. By simple calculation, the i_0 defined in the proof of Lemma 3.2 is equal to 2. Denote by $T(1) = CP(1, 4, 2, 1, 1)$. Note that $i_0 + 1 = 3$. Since u_1 is a pseudo star-root of $T(1)$ and $n_l^{T(1)}(u_1u_2) \le n_l^{T(1)}(u_1u_2)$, we transform $T(1)$ to $T(2)$, where $T(2) = T(1)^{(\{v_1\})}_{u_1\to u_2} = CP(0, 5, 2, 1, 1)$. Similarly, we transform $T(2)$ to $T(3)$ where $T(3) = T(2)_{u_2\to u_3} = CP(0, 0, 7, 1, 1)$. Denote by $T'(1) = T(3)$. Note that $d - i_0 - 1 = 3$. Since u_5 is a pseudo star-root of $T'(1)$ and $n_l^{T'(1)}(u_5u_4) \le n_l^{T'(1)}(u_5u_4)$, we transform $T'(1)$ to $T'(2)$, where $T'(2)^{(\{v_9\})} = T'(1)_{u_5\to u_4} = CP(0, 0, 7, 2, 0)$. Similarly, we transform $T'(2)$ to $T'(3)$, where $T'(3) = T'(2)_{u_4\to u_3} = CP(0, 0, 9, 0, 0) = CP_{6,3}(9)$. Since $3 = \frac{6}{2}$, we get the extremal graph. Thus $\mathrm{SW}_k(T) > \mathrm{SW}_k(CP_{6,3}(9))$ for $2 \le k \le 15$.

In order to get the lower bound of Steiner Wiener index for the graphs in $\mathcal{T}(n, d)$, we only need to calculate the Steiner Wiener index of $CP_{d,\lfloor \frac{d}{2} \rfloor}(n - d - 1)$.

Theorem 3.2. *For $2 \le k \le n - d$, the Steiner k-Wiener index of $CP_{d,\lfloor \frac{d}{2} \rfloor}(n - d - 1)$ is given by*

$$SW_k(CP_{d,\lfloor \frac{d}{2} \rfloor}(n - d - 1)) = \Gamma(n, d, k),$$

where $\Gamma(n, d, k) = \frac{n(d+k)-k(d+1)}{n}\binom{n}{k} - 2\left[\binom{\frac{d}{2}+1}{k+1} + \binom{n}{k+1} - \binom{n-\frac{d}{2}}{k+1}\right]$ *for d even and* $\Gamma(n, d, k) = \frac{n(d+k)-k(d+1)}{n}\binom{n}{k} - \left[\binom{\frac{d+3}{2}}{k+1} + \binom{\frac{d+1}{2}}{k+1} + 2\binom{n}{k+1} + \binom{n-\frac{d+1}{2}}{k} - 2\binom{n-\frac{d-1}{2}}{k+1}\right]$ *for d odd.*

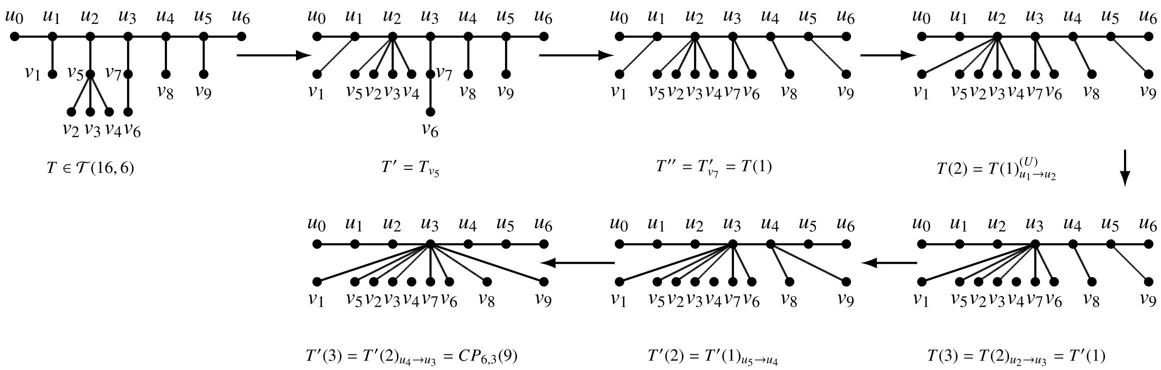

Fig. 5. The graphs in Example 1.

Proof. From Lemma 2.3, we have

$$\begin{aligned}
SW_k(CP_{d,\lfloor \frac{d}{2}\rfloor}(n-d-1)) &= (n-1)\binom{n}{k} - \sum_{e\in E(T)}\left[\binom{\gamma(e)}{k}+\binom{\eta(e)}{k}\right]\\
&= (n-1)\binom{n}{k} - \left[\sum_{i=1}^{\lfloor \frac{d}{2}\rfloor}\left[\binom{i}{k}+\binom{n-i}{k}\right] + \sum_{i=1}^{d-\lfloor \frac{d}{2}\rfloor}\left[\binom{i}{k}+\binom{n-i}{k}\right] + (n-d-1)\binom{n-1}{k}\right]\\
&= (n-1)\binom{n}{k} - (n-d-1)\binom{n-1}{k} - \left[\sum_{i=1}^{\lfloor \frac{d}{2}\rfloor}\left[\binom{i}{k}+\binom{n-i}{k}\right] + \sum_{i=1}^{d-\lfloor \frac{d}{2}\rfloor}\left[\binom{i}{k}+\binom{n-i}{k}\right]\right]\\
&= \frac{n(d+k)-k(d+1)}{n}\binom{n}{k} - \left[\sum_{i=1}^{\lfloor \frac{d}{2}\rfloor}\left[\binom{i}{k}+\binom{n-i}{k}\right] + \sum_{i=1}^{d-\lfloor \frac{d}{2}\rfloor}\left[\binom{i}{k}+\binom{n-i}{k}\right]\right].
\end{aligned}$$

We only consider the case that d is even and the other case is similar. Now $\lfloor \frac{d}{2}\rfloor = d - \lfloor \frac{d}{2}\rfloor = \frac{d}{2}$. Note that $\binom{a}{k+1}+\binom{a}{k} = \binom{a+1}{k+1}$ for any positive integers a and k. We have,

$$\begin{aligned}
&\sum_{i=1}^{\frac{d}{2}}\left[\binom{i}{k}+\binom{n-i}{k}\right] + \sum_{i=1}^{d-\frac{d}{2}}\left[\binom{i}{k}+\binom{n-i}{k}\right]\\
=&2\sum_{i=1}^{\frac{d}{2}}\left[\binom{i}{k}+\binom{n-i}{k}\right]\\
=&2\sum_{i=1}^{\frac{d}{2}}\binom{i}{k} + 2\sum_{i=1}^{\frac{d}{2}}\binom{n-i}{k}\\
=&2\left[\binom{1}{k+1} + \sum_{i=1}^{\lfloor \frac{d}{2}\rfloor}\binom{i}{k}\right] + 2\left[\binom{n-\frac{d}{2}}{k+1} + \sum_{i=1}^{\frac{d}{2}}\binom{n-i}{k} - \binom{n-\frac{d}{2}}{k+1}\right]\\
=&2\binom{\frac{d}{2}+1}{k+1} + 2\binom{n}{k+1} - 2\binom{n-\frac{d}{2}}{k+1}.
\end{aligned}$$

It follows that

$$SW_k(CP_{d,\lfloor \frac{d}{2}\rfloor}(n-d-1)) = \frac{n(d+k)-k(d+1)}{n}\binom{n}{k} - 2\left[\binom{\frac{d}{2}+1}{k+1} + \binom{n}{k+1} - \binom{n-\frac{d}{2}}{k+1}\right]. \quad \square$$

Now we give the lower bound of Steiner Wiener index for trees in $\mathcal{T}(n,d)$.

Corollary 3.1. *For $T \in \mathcal{T}(n,d)$ with $3 \le d \le n-1$, we have*

$$SW_k(T) \ge \Gamma(n,d,k)$$

for $2 \le k \le n-1$. Furthermore, if the equality holds for all k then $T \cong CP_{d,\lfloor \frac{d}{2}\rfloor}(n-d-1)$.

Table 1
$\Gamma(n, d, k)$ for $5 \leq n \leq 19$ and $3 \leq d \leq 17$.

(n, d, k)	$\Gamma(n, d, k)$	(n, d, k)	$\Gamma(n, d, k)$	(n, d, k)	$\Gamma(n, d, k)$	(n, d, k)	$\Gamma(n, d, k)$
(5, 3, 2)	18	(5, 3, 3)	27	(6, 3, 2)	28	(6, 3, 3)	56
(6, 4, 2)	31	(6, 4, 3)	62	(7, 3, 2)	40	(7, 3, 3)	100
(7, 4, 2)	44	(7, 4, 3)	110	(7, 5, 2)	50	(7, 5, 3)	125
(8, 3, 2)	54	(8, 3, 3)	162	(8, 4, 2)	59	(8, 4, 3)	177
(8, 5, 2)	67	(8, 5, 3)	201	(8, 6, 2)	75	(8, 6, 3)	225
(9, 3, 2)	70	(9, 3, 3)	245	(9, 4, 2)	76	(9, 4, 3)	266
(9, 5, 2)	86	(9, 5, 3)	301	(9, 6, 2)	96	(9, 6, 3)	336
(9, 7, 2)	108	(9, 7, 3)	378	(10, 3, 2)	88	(10, 3, 3)	352
(10, 4, 2)	95	(10, 4, 3)	380	(10, 5, 2)	107	(10, 5, 3)	428
(10, 6, 2)	119	(10, 6, 3)	475	(10, 7, 2)	134	(10, 7, 3)	536
(10, 8, 2)	149	(10, 8, 3)	596	(11, 3, 2)	108	(11, 3, 3)	486
(11, 4, 2)	116	(11, 4, 3)	522	(11, 5, 2)	130	(11, 5, 3)	585
(11, 6, 2)	144	(11, 6, 3)	648	(11, 7, 2)	162	(11, 7, 3)	729
(11, 8, 2)	180	(11, 8, 3)	810	(11, 9, 2)	200	(11, 9, 3)	900
(12, 3, 2)	130	(12, 3, 3)	650	(12, 4, 2)	139	(12, 4, 3)	695
(12, 5, 2)	155	(12, 5, 3)	775	(12, 6, 2)	171	(12, 6, 3)	855
(12, 7, 2)	192	(12, 7, 3)	960	(12, 8, 2)	213	(12, 8, 3)	1065
(12, 9, 2)	237	(12, 9, 3)	1185	(12, 10, 2)	261	(12, 10, 3)	1305
(13, 3, 2)	154	(13, 3, 3)	847	(13, 4, 2)	164	(13, 4, 3)	902
(13, 5, 2)	182	(13, 5, 3)	1001	(13, 6, 2)	200	(13, 6, 3)	1100
(13, 7, 2)	224	(13, 7, 3)	1232	(13, 8, 2)	248	(13, 8, 3)	1364
(13, 9, 2)	276	(13, 9, 3)	1518	(13, 10, 2)	304	(13, 10, 3)	1672
(13, 11, 2)	334	(13, 11, 3)	1837				

For $k = 2, 3$, we list the lower bound $\Gamma(n, d, k)$ for $5 \leq n \leq 19$ and $3 \leq d \leq 17$ in Table 1.

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References

[1] J.A. Bondy, U.S.R. Murty, Graph Theory, Springer, 2008.
[2] G. Chartrand, O.R. Oellermann, S. Tian, H.B. Zou, Steiner distance in graphs, Časopis Pest. Mat. 114 (1989) 399–410.
[3] A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and application, Acta Appl. Math. 66 (2001) 211–249.
[4] R.C. Entringer, D.E. Jackson, D.A. Snyder, Distance in graphs, Czechoslovak Math. J. 26 (1976) 283–296.
[5] I. Gutman, B. Furtula, X. Li, Multicenter wiener indices and their applications, J. Serb. Chem. Soc. 80 (2015) 1009–1017.
[6] I. Gutman, S. Klavžar, B. Mohar, Fifty years of the wiener index, MATCH Commun. Math. Comput. Chem. 35 (1997) 1–159.
[7] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.
[8] X. Li, Y. Mao, I. Gutman, The steiner wiener index of a graph, Discuss. Math. Graph Theory 36 (2016) 455–465.
[9] H. Liu, X. Pan, On the wiener index of trees with fixed diameter, MATCH Commun. Math. Comput. Chem. 60 (2008) 85–94.
[10] Y. Mao, Z. Wang, I. Gutman, Steiner wiener index of graph products, Trans. Combin. 5 (2016) 39–50.
[11] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947) 17–20.
[12] K. Xu, M. Liu, K.C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance-based topological indices, MACTH Commun. Math. Comput. Chem. 71 (2014) 461–508.