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THE STEINER WIENER INDEX OF A GRAPH

Xueliang Li[1 2]

Center for Combinatorics and LPMC-TJKLC
Nankai University
Tianjin 300071, China

e-mail: lxl@nankai.edu.cn

Yaping Mao[3]

Department of Mathematics
Qinghai Normal University
Qinghai 810008, China

e-mail: maoyaping@ymail.com

and

Ivan Gutman

Faculty of Science P. O. Box 60
34000 Kragujevac, Serbia, and
State University of Novi Pazar, Novi Pazar, Serbia

e-mail: gutman@kg.ac.rs

Abstract

The Wiener index $W(G)$ of a connected graph G, introduced by Wiener in 1947, is defined as $W(G)=\sum_{u,v\in V(G)} d(u,v)$ where $d_G(u,v)$ is the distance between vertices u and v of G. The Steiner distance in a graph, introduced by Chartrand et al. in 1989, is a natural generalization of the concept of classical graph distance. For a connected graph G of order at least 2 and $S\subseteq V(G)$, the *Steiner distance* $d(S)$ of the vertices of S is the minimum size of a connected subgraph whose vertex set is S. We now introduce the concept of the Steiner Wiener index of a graph. The *Steiner k-Wiener index* $SW_k(G)$ of G is defined by $SW_k(G)=\sum_{\substack{S\subseteq V(G)\\ |S|=k}} d(S)$. Expressions for SW_k for some special graphs are obtained. We also give sharp upper and lower

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[2]Corresponding author
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bounds of SW_k of a connected graph, and establish some of its properties in the case of trees. An application in chemistry of the Steiner Wiener index is reported in our another paper.

Keywords: distance; Steiner distance; Wiener index; Steiner Wiener k-index..

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1. Introduction

All graphs in this paper are undirected, finite, and simple. We refer to [3] for graph theoretical notation and terminology not described here. Distance is one of the 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. If v is a vertex of a connected graph G, then the *eccentricity* $\varepsilon(v)$ of v is defined by $\varepsilon(v) = \max\{d(u, v) \,|\, u \in V(G)\}$. Furthermore, the *radius* $rad(G)$ and *diameter* $diam(G)$ of G are defined by $rad(G) = \min\{\varepsilon(v) \,|\, v \in V(G)\}$ and $diam(G) = \max\{\varepsilon(v) \,|\, v \in V(G)\}$. These latter two concepts are related by the inequalities $rad(G) \leq diam(G) \leq 2rad(G)$. Goddard and Oellermann gave a survey paper on this subject [13].

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

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

The first investigations of this distance–based graph invariant were done by Harold Wiener in 1947, who realized that there exist correlations between the boiling points of paraffins and their molecular structure, see [21, 22, 23]. Mathematicians study the Wiener index since the 1970s [11].

The Wiener index obtained wide attention and numerous results have been worked out, see the surveys [10, 15, 16, 24], the recent papers [2, 7, 17, 18, 19] and the references cited therein.

The Steiner distance of a graph, introduced by Chartrand et al. [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 $S \subseteq V(G)$ of at least two vertices, *an S-Steiner tree* or *a Steiner tree connecting S* (or simply, *an S-tree*) is a such 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 subgraphs 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 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 $d(S) \geq k - 1$. If G is the graph depicted in Figure 1 (a) and $S = \{x, u, v\}$, then $d(S) = 4$. There could be several trees of size 4 containing S. One such tree is shown in Figure 1 (b).

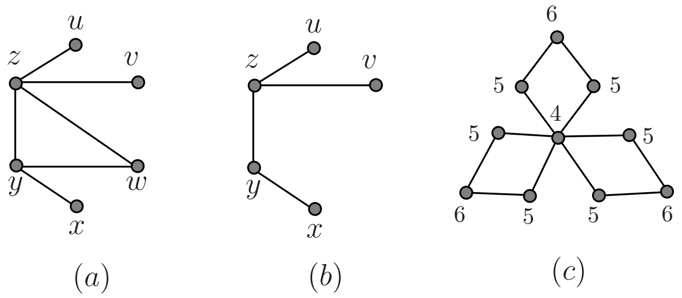

Figure 1: Graphs used to illustrate the basic definitions.

Let n and k be integers such that $2 \leq k \leq n$. The *Steiner k-eccentricity* $\varepsilon_k(v)$ of a vertex v of G is defined by $\varepsilon_k(v) = \max\{d(S) \,|\, S \subseteq V(G),\ |S| = k, \text{and } v \in S\}$. The *Steiner k-radius* of G is $srad_k(G) = \min\{\varepsilon_k(v) \,|\, v \in V(G)\}$, while the *Steiner k-diameter* of G is $sdiam_k(G) = \max\{\varepsilon_k(v) \,|\, v \in V(G)\}$. Note that for every connected graph G, $\varepsilon_2(v) = \varepsilon(v)$ for all vertices v of G, $srad_2(G) = rad(G)$ and $sdiam_2(G) = diam(G)$. Each vertex of the graph G of Figure 1 (c) is labeled with its Steiner 3-eccentricity, so that $srad_3(G) = 4$ and $sdiam_3(G) = 6$. For more details on Steiner distance, we refer to [1, 5, 6, 8, 13, 20].

The following observation is easily seen.

Observation 1.1. *Let k be an integer such that $2 \leq k \leq n$. If H is a spanning subgraph of G, then $sdiam_k(G) \leq sdiam_k(H)$.*

We now generalize the concept of Wiener index by Steiner distance. The *Steiner k-Wiener index* $SW_k(G)$ of G is defined by

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

For $k = 2$, the above defined 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 $SW_n(G) = n - 1$.

In Section 2, we obtain the exact values of the Steiner Wiener k-index of the path, star, complete graph, and complete bipartite graph. In Section 3, we obtain sharp lower and upper bounds for SW_k for connected graphs and for trees. In Section 4 we establish some relations for SW_k of trees. An application in chemistry of the Steiner Wiener index is reported in our another paper [14].

2. RESULTS FOR SOME SPECIAL GRAPHS

Beginning this section, we note that the special case for $k = 2$ of all formulas derived here for the Steiner Wiener index, thus pertaining to the ordinary Wiener index, are well known and mentioned many times in the earlier literature.

Recently, we found the following concept about the Wiener distance. The *average Steiner distance* $\mu_k(G)$ of a graph G is defined as the average of the Steiner distances of all k-subsets of $V(G)$, i.e.,

$$\mu_k(G) = \binom{n}{k}^{-1} \sum_{S \subseteq V(G), |S|=k} d_G(S),$$

which was introduced by Dankelmann, Oellermann and Swart in [8]. This concept is similar to our Steiner Wiener index. However, their motivation is to analyse transportation or communication networks, but ours is from chemical applications of the famous Wiener index. Therefore, fortunately most of their results are different from ours. For more details on the average Steiner distance, we refer to [8, 9].

For a connected graph G, one can easily see that

$$SW_k(G) = \mu_k(G)\binom{n}{k}, \tag{1}$$

Corollary 2.1 of [8] implies that $\mu_k(K_n) = (k-1)\mu_2(K_n)$. Then from Eq. (1) one can immediately get the following result.

Proposition 2.1. Let K_n be the complete graph of order n, and let k be an integer such that $2 \leq k \leq n$. Then $SW_k(K_n) = \binom{n}{k}(k-1)$.

For complete bipartite graphs, we have the following result.

Proposition 2.2. Let $K_{a,b}$ be the complete bipartite graph of order $a + b$ ($1 \leq a \leq b$), and let k be an integer such that $2 \leq k \leq a + b$. Then

$$SW_k(K_{a,b}) = \begin{cases} (k-1)\binom{a+b}{k} + \binom{a}{k} + \binom{b}{k}, & if\ 1 \leq k \leq a; \\ (k-1)\binom{a+b}{k} + \binom{b}{k}, & if\ a < k \leq b; \\ (k-1)\binom{a+b}{k}, & if\ b < k \leq a+b. \end{cases}$$

Proof. Let $G = K_{a,b}$, and let $U = \{u_1, u_2, \ldots, u_a\}$ and $W = \{w_1, w_2, \ldots, w_b\}$ be the two parts of $G = K_{a,b}$.

First, we consider the case $1 \leq k \leq a$. For any $S \subseteq V(G)$ and $|S| = k$, we have $S \cap U = \varnothing$, or $S \cap W = \varnothing$, or $S \cap U \neq \varnothing$ and $S \cap W \neq \varnothing$. If $S \cap U = \varnothing$, then $S \subseteq W$. Without loss of generality, let $S = \{w_1, w_2, \ldots, w_k\}$. Then the tree T induced by the edges in $\{u_1w_1, u_1w_2, \ldots, u_1w_k\}$ is a Steiner tree connecting S. This implies $d(S) \leq k$. Since $G = K_{a,b}$ is a complete bipartite graph, it follows that any tree connecting S must use at least k edges, and hence $d(S) \geq k$. Therefore, $d(S) = k$. Similarly, if $S \cap W = \varnothing$, then $d(S) = k$. Suppose $S \cap U \neq \varnothing$ and $S \cap W \neq \varnothing$. Without loss of generality, let $S = \{u_1, u_2, \ldots, u_x, w_1, w_2, \ldots, w_{k-x}\}$. Then the tree T induced by the edges in $\{u_1w_1, w_1u_2, w_1u_3, \ldots, w_1u_x, u_1w_2, u_1w_3, \ldots, u_1w_{k-x}\}$ is a Steiner tree connecting S, which implies $d(S) \leq k-1$. Since $|S| = k$, it follows that any tree connecting S must use at least $k-1$ edges, and hence $d(S) = k-1$. Thus,

$$
\begin{aligned}
SW_k(G) &= \sum_{\substack{S \subseteq V(G) \\ S \cap U = \varnothing}} d(S) + \sum_{\substack{S \subseteq V(G) \\ S \cap U = \varnothing}} d(S) + \sum_{\substack{S \subseteq V(G) \\ S \cap U \neq \varnothing, S \cap U \neq \varnothing}} d(S) \\
&= k\binom{a}{k} + k\binom{b}{k} + (k-1)\left[\sum_{x=1}^{a} \binom{a}{x}\binom{b}{k-x}\right] \\
&= k\binom{a}{k} + k\binom{b}{k} + (k-1)\left[\binom{a+b}{k} - \binom{b}{k} - \binom{a}{k}\right] \\
&= (k-1)\binom{a+b}{k} + \binom{a}{k} + \binom{b}{k}.
\end{aligned}
$$

Next, we consider the case $a < k \leq b$. For any $S \subseteq V(G)$ and $|S| = k$, we have $S \cap U = \varnothing$ or $S \cap U \neq \varnothing$. If $S \cap U = \varnothing$, then $S \subseteq W$. Without loss of generality, let $S = \{w_1, w_2, \ldots, w_k\}$. Then the tree T induced by the edges in $\{u_1w_1, u_1w_2, \ldots, u_1w_k\}$ is a Steiner tree connecting S, which implies $d(S) \leq k$. Since $G = K_{a,b}$ is a complete bipartite graph, it follows that any tree connecting S must use at least k edges, and hence $d(S) \geq k$. Therefore, $d(S) = k$. Suppose $S \cap U \neq \varnothing$. Without loss of generality, let $S = \{u_1, u_2, \ldots, u_x, w_1, w_2, \ldots, w_{k-x}\}$ $(1 \leq x \leq a)$. Then the tree T induced by the edges in $\{u_1w_1, w_1u_2, w_1u_3, \ldots, w_1u_x, u_1w_2, u_1w_3, \ldots, u_1w_{k-x}\}$ is a Steiner tree connecting S, which implies $d(S) \leq k-1$. Since $|S| = k$, it follows that any tree connecting S must use at least $k-1$ edges, and hence $d(S) = k-1$. Thus,

$$\begin{aligned} SW_k(G) &= \sum_{\substack{S\subseteq V(G)\\ S\cap U=\varnothing}} d(S) + \sum_{\substack{S\subseteq V(G)\\ S\cap U\neq\varnothing}} d(S) \\ &= k\binom{b}{k} + (k-1)\left[\sum_{x=1}^{a}\binom{a}{x}\binom{b}{k-x}\right] \\ &= k\binom{b}{k} + (k-1)\left[\sum_{x=1}^{\infty}\binom{a}{x}\binom{b}{k-x}\right] \\ &= k\binom{b}{k} + (k-1)\left[\binom{a+b}{k} - \binom{b}{k}\right] \\ &= (k-1)\binom{a+b}{k} + \binom{b}{k}. \end{aligned}$$

In this end, we consider the remaining case $b < k \leq a+b$. For any $S \subseteq V(G)$ and $|S| = k$, we have $S \cap U \neq \varnothing$ and $S \cap U \neq \varnothing$. Without loss of generality, let $S = \{u_1, u_2, \ldots, u_x, w_1, w_2, \ldots, w_{k-x}\}$. Then the tree T induced by the edges in $\{u_1w_1, w_1u_2, w_1u_3, \ldots, w_1u_x, u_1w_2, u_1w_3, \ldots, u_1w_{k-x}\}$ is a Steiner tree connecting S, which implies $d(S) \leq k-1$. Since $|S| = k$, it follows that any tree connecting S must use at least $k-1$ edges, and hence $d(S) = k-1$. Thus,

$$SW_k(G) = \sum_{\substack{S\subseteq V(G)\\ S\cap U=\varnothing}} d(S) = (k-1)\binom{a+b}{k}.$$

The proof is now complete. ■

From the above proposition, we can derive the following corollary.

Corollary 2.3. *Let S_n be the star of order n ($n \geq 3$), and let k be an integer such that $2 \leq k \leq n$. Then*

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

Proof. From Proposition 2.2, we have that $SW_k(S_n) = SW_k(K_{1,n-1}) = \binom{n}{n}(n-1) = n-1$ for $k = n$ and $SW_k(S_n) = SW_k(K_{1,n-1}) = (k-1)\binom{n}{k} + \binom{n-1}{k}$ for $2 \leq k \leq n-1$. We conclude that

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

■

Lemma 2.1 of [8] says that $\mu_k(P_n) = \frac{k-1}{k+1}(n+1)$. Then from Eq. (1) one can easily get the following result.

Proposition 2.4. Let P_n be the path of order n ($n \geq 3$), and let k be an integer such that $2 \leq k \leq n$. Then

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

3. Lower and upper bounds for general graphs

The following observation is immediate.

Observation 3.1. *Let G be a connected graph of order n, $e \in E(G)$, and let k be an integer such that $2 \leq k \leq n$. Furthermore, let H be the graph with vertex set $V(H) = V(G)$ and edge set $E(G) \setminus e$. Then*

$$SW_k(G) \leq SW_k(H).$$

This straightforwardly leads to the following result.

Proposition 3.2. Let G be a connected graph of order n, and T a spanning tree of G. Let k be an integer such that $2 \leq k \leq n$. Then

$$SW_k(G) \leq SW_k(T)$$

with equality if and only if G is a tree.

For a tree T, Proposition 3.1 of [8] says that $k(1 - \frac{1}{n}) \leq \mu_k(T) \leq \frac{k-1}{k+1}(n+1)$. Then from Eq. (1) one can derive lower and upper bounds for the Steiner Wiener index of a tree.

Theorem 3.3. *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.

We recall that Theorem 3.3 provides a generalization of the much older results known for the Wiener index [11], i.e., it yields this previous result by setting $k = 2$.

For a connected graph G, Theorem 2.1 of [8] says that $k - 1 \leq SW_k(G) \leq \frac{k-1}{k+1}(n+1)$. Then from Eq. (1) one can get the following upper and lower bounds of $SW_k(G)$ for a general connected graph G.

Theorem 3.4. *Let G be a connected graph of order n, and let k be an integer such that $2 \le k \le n$. Then*

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

Moreover, the lower bound is sharp.

4. The Steiner Wiener index for trees

Theorem 4.1. *Let T be a tree of order n, possessing p pendent vertices. Then*

$$SW_{n-1}(T) = n(n-1) - p, \tag{2}$$

irrespective of any other structural detail of T.

Proof. Since $k = n-1$, the respective subsets S contain all except one vertices of T. If the vertex missing from S is pendent, then the vertices contained in S form a tree of order $n-1$. Therefore $d(S) = n-2$. There are p such subsets, contributing to SW_{n-1} by $p \times (n-2)$.

If the vertex of T, not present in S, is non-pendent, then the vertices contained in S cannot form a tree, and the respective Steiner tree must contain all the n vertices of T. Therefore, $d(S) = n-1$. There are $n-p$ such subsets, contributing to SW_{n-1} by $(n-p) \times (n-1)$.

Thus, $SW_{n-1}(T) = p(n-2) + (n-p)(n-1)$, which straightforwardly leads to Eq. (2). ■

Let G be any graph (not necessarily connected) with vertex set $V(G)$. Let e be an edge of G, connecting the vertices x and y. Define the sets

$$\begin{aligned} \mathcal{N}_1(e) &= \{u \,|\, u \in V(G), d(u,x) < d(u,y)\} \\ \mathcal{N}_2(e) &= \{u \,|\, u \in V(G), d(u,x) > d(u,y)\} \end{aligned}$$

and let their cardinalities be $n_1(e) = |\mathcal{N}_1(e)|$ and $n_2(e) = |\mathcal{N}_2(e)|$, respectively. In other words, $n_1(e)$ counts the vertices of G, lying closer to one end of the edge e than to its other end, and the meaning of $n_2(e)$ is analogous.

In his seminal paper [23], Wiener discovered the following result:

Proposition 4.2. If T is a tree, then for its Wiener index holds:

$$W(T) = \sum_{e \in E(T)} n_1(e)\, n_2(e).$$

We now state the generalization of Proposition 4.2 to Steiner Wiener indices:

Theorem 4.3. *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:*

$$SW_k(T) = \sum_{e \in E(T)} \sum_{i=1}^{k-1} \binom{n_1(e)}{i} \binom{n_2(e)}{k-i}. \tag{3}$$

Proof. The Steiner k-Wiener index is equal to the sum of distances of all k-element subsets S of the vertex set of T. Each such subset determines a unique subtree of T and its contribution to SW_k is just the number edges of this subtree. Now, instead of counting these edges and adding them over all subsets S, we can count how many times a given edge, say e, is contained in the subtrees formed by all subsets S, and add this over all edges.

Let e be an edge of the tree T. On its two sides there are $n_1(e)$ and $n_2(e)$ vertices, respectively. Choose i vertices on one side and $k - i$ vertices on the other side. Such a choice determines a k-element subset S, whose associated subtree contains the edge e. Evidently, the above described choice can be done in $\binom{n_1(e)}{i}\binom{n_2(e)}{k-i}$ different ways. If we sum these terms over all possible values of i, we obtain the total number of times the edge e is in a k-vertex Steiner tree of T. Eq. (3) thus follows. ■

Corollary 4.4. *Proposition 4.2 is obtained from Eq. (3) by setting $k = 2$.*

Corollary 4.5. *If $k = 3$, then the Steiner k-Wiener index of a tree of order n is directly related to the ordinary Wiener index as*

$$SW_3(T) = \frac{n-2}{2} W(T). \tag{4}$$

Proof. The special case of Eq. (3) for $k = 3$ reads:

$$\begin{aligned} SW_3(T) &= \sum_{e \in E(T)} \left[\binom{n_1(e)}{1}\binom{n_2(e)}{2} + \binom{n_1(e)}{2}\binom{n_2(e)}{1} \right] \\ &= \frac{1}{2} \sum_{e \in E(T)} n_1(e)\, n_2(e) \big[n_1(e) + n_2(e) \big] - \sum_{e \in E(T)} n_1(e) n_2(e)\,. \end{aligned}$$

Eq. (4) follows now from Proposition 4.2 and the fact that for any edge of an n-vertex tree, $n_1(e) + n_2(e) = n$. ■

Remark. The Wiener index or the Steiner 2-Wiener index for any graph can be computed in polynomial time since one needs only to compute the distances of $\binom{n}{2}$ pairs of vertices in a graph of order n. However, since the problem of “Steiner

Tree in Graphs" is NP-complete (see [12]), it is NP-hard to compute the Steiner k-Wiener index $SW_k(G)$ for a general graph G and a general positive integer k. Recall that the problem of "Steiner Tree in Graphs" is stated as follows: Given a graph $G = (V, E)$, a weight $w(e)$ (a positive integer) for each $e \in E$, a subset $R \subseteq V$ and a positive integer B, is there a subtree of G that includes all the vertices of R and such that the sum of the weights of the edges in the subtree is no more than B ? This problem remains NP-complete if all edge weights are equal.

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