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On the Inverse Steiner Wiener Problem*

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Abstract

The well-known Wiener index is defined as the sum of all distances between pairs of vertices. Motivated from applications in biochemistry the inverse Wiener problem asks, for any given positive integer, the structure that has its Wiener index of this value. This problem was completely solved through a series of studies. When distances are replaced with the Steiner distances, the k-Steiner Wiener index was introduced recently. Naturally, the inverse Steiner Wiener problem was also brought forward. In this paper we show that all but finitely many positive integers are Steiner 3-Wiener indices of some graphs, consequently solving the inverse Steiner

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Wiener problem for $k = 3$. We then generalize our approach to show, that pending some initial condition, it is likely that all but finitely many positive integers are Steiner k-Wiener indices of graphs. This is confirmed for small values of k with the help of computer. We also comment on potential future work.

1 Introduction

In Chemical Graph Theory one often uses graph invariants to represent the structural information of a molecular graph, in the hope of predicting the behavior of the corresponding chemical compound. One of the most well-known such graph invariants is the sum of distances between all pair of vertices in a graph, also known as the *Wiener index* [20, 21]. This is formally defined as

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

where $d(u, v)$ is the distance between vertices u and v in G. Motivated from practical needs, the so-called inverse Wiener problem was proposed:

Question 1.1 *For any positive integer x, does there exist a graph G (a tree T) such that*

$$W(G) = x, (W(T) = x)?$$

The problem was solved [3] for general graphs as all but finitely positive integers are Wiener indices of some graph. For trees the same conclusion was first conjectured [4, 7] and then shown in [15, 16, 19]. Other related work can also be found in [8, 17].

For a set $S \subset V(G)$ of vertices, the *Steiner distance* $d(S)$ is the minimum size of a connected subgraph of G whose vertex set contains S. When $|S| = 2$, $d(S)$ is exactly the distance between two vertices. Replacing distances with the Steiner distances, a natural generalization of the Wiener index was introduced in [9], called the *Steiner k-Wiener index* and defined as

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

It appears that $SW_k(G)$ was also introduced and studied under the term *average Steiner distance* much earlier in [1, 2]. More recently, as a chemical index the Steiner k-Wiener index received more attention as various related questions are examined [5, 6, 10–14, 18]. In particular, some preliminary studies of the inverse Steiner Wiener problem were conducted in [10]. In this note we first solve the inverse Steiner Wiener problem for $k = 3$ by proving the following.

Theorem 1.1 *All but finitely many positive integers are Steiner 3-Wiener indices of graphs.*

The proof of Theorem 1.1 will be presented in Section 2. We then further apply our approach to general values of k, proving that similar conclusion is likely to hold, provided that a initial condition can be established. This discussion is presented in Section 3. We then apply our result to small values of k and solve the inverse Steiner Wiener problem for $k = 4$ and 5. We present the corresponding statements with some concluding remarks in Section 4.

2 The inverse Steiner Wiener problem for $k = 3$

First we point out that

$$SW_3(K_n) = 2\binom{n}{3}$$

and

$$\begin{aligned} SW_3(S_n) = 2\binom{n-1}{2} + 3\binom{n-1}{3} &= (n-1) \cdot \binom{n-1}{2} \\ &= SW_3(K_n) + \binom{n-1}{3} \end{aligned}$$

for the complete graph K_n and the star S_n on n vertices. This is because:

- In K_n, $d(S) = 2$ for every one of the $\binom{n}{3}$ 3-vertex subsets of vertices;
- In S_n, depending on whether the center is in a 3-vertex subset S of vertices, we have $d(S) = 2$ or 3;
- From K_n to S_n, the $\binom{n-1}{3}$ subsets of 3 vertices that does not include the center has $d(S)$ increased from 2 to 3.

For instance, Table 1 shows the values of $SW_3(K_n)$ and $SW_3(S_n)$ for small n's.

We will show that, for large enough n, every positive integer between $SW_3(S_n)$ and $SW_3(K_n)$ can be represented as the Steiner 3-Wiener index of some graph. Note that by adding edges to a star we create a graph with diameter 2. More precisely, we have the following.

Theorem 2.1 *For any given $n \geq 6$ and any $x \in \left[2\binom{n}{3}, (n-1)\binom{n-1}{2}\right]$, there exists a connected graph G with diameter 2 such that $SW_3(G) = x$.*

Table 1. The values of $SW_3(S_n)$ and $SW_3(K_n)$.

n	$SW_3(K_n)$	$SW_3(S_n)$
3	2	2
4	8	9
5	20	24
6	40	50
7	70	90
8	112	147
9	168	224
10	240	324
11	330	450
12	440	605

Proof. We will show, by induction on n, that every $x \in [2\binom{n}{3}, (n-1)\binom{n-1}{2}]$ is the Steiner 3-Wiener index of some graph created from adding some edges to a star. It is obvious that such graphs have diameter 2. For example, the graphs in Figure 1 has Steiner 3-Wiener index value from

$$SW_3(K_6) = SW_3(G_1) = 40$$

to

$$SW_3(S_6) = SW_3(G_{11}) = 50.$$

Thus, by Figure 1, the conclusion holds for $n = 6$. Suppose now that the conclusion holds for $n = m \geq 6$. That is, for any

$$x \in \left[2\binom{m}{3}, (m-1)\binom{m-1}{2}\right]$$

we have $SW_3(G) = x$ for some graph of order m with diameter 2. Now, in the case of $n = m+1$, we are interested in the interval

$$\left[2\binom{m+1}{3}, m\binom{m}{2}\right]. \tag{1}$$

Through simple algebra we have

$$m\binom{m}{2} - \binom{m-1}{3} \leq 2\binom{m+1}{3} + \binom{m-1}{3}$$

and hence

$$\left[2\binom{m+1}{3}, m\binom{m}{2}\right] \subset \left[2\binom{m+1}{3}, 2\binom{m+1}{3} + \binom{m-1}{3}\right] \cup \left[m\binom{m}{2} - \binom{m-1}{3}, m\binom{m}{2}\right].$$

Consequently, to consider every x in (1) it suffices to consider two cases.

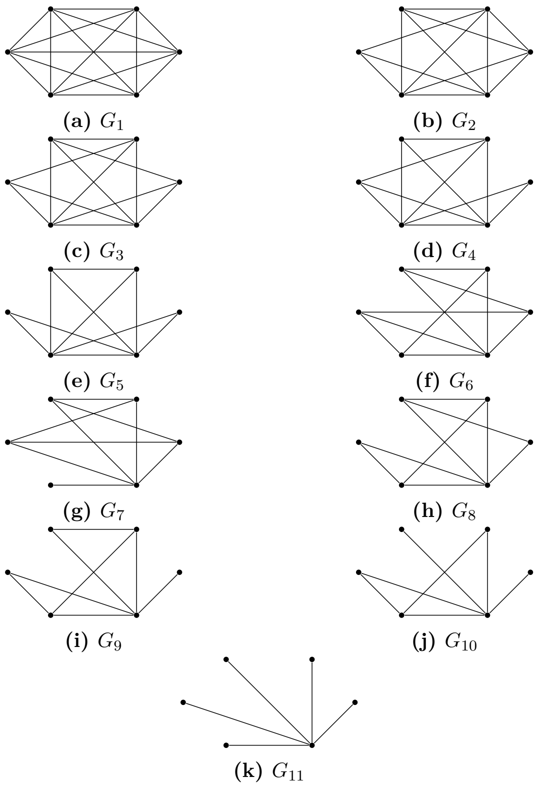

Figure 1. The Steiner 3-Wiener index of graphs of order $n = 6$.

Case I . If $x \in \left[2\binom{m+1}{3}, 2\binom{m+1}{3} + \binom{m-1}{3}\right]$, let

$$x = 2\binom{m+1}{3} + x_1$$

for some $0 \leq x_1 \leq \binom{m-1}{3}$. Then we have

$$x' = 2\binom{m}{3} + x_1 \in \left[2\binom{m}{3}, (m-1)\binom{m-1}{2}\right].$$

By our induction hypothesis, there is a graph G' on m vertices with diameter 2 such that $SW_3(G') = x'$. We now consider the graph G of order $m+1$, obtained from G' by joining an additional vertex w with all vertices of G'. It is easy to see that G is also of diameter 2 (Figure 2).

To evaluate $SW_3(G)$, we consider $d(S)$ for each 3-vertex subset S in G:

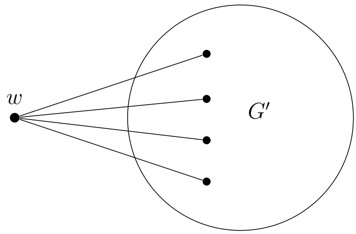

Figure 2. The graph G obtained from G' (Case I).

- If S does not contain w, then $d(S)$ is the same in G as in G'. And the sum of all such Steiner distances is exactly $SW_3(G')$;
- If S does contain w, then $d(S) = 2$ and there are $\binom{m}{2}$ ways to choose the other two vertices.

Consequently we have, through simple algebra, that

$$\begin{aligned} SW_3(G) &= SW_3(G') + 2\binom{m}{2} \\ &= \left(2\binom{m}{3} + x_1\right) + 2\binom{m}{2} \\ &= 2\binom{m+1}{3} + x_1 \\ &= x. \end{aligned}$$

Case II . If $x \in \left[m\binom{m}{2} - \binom{m-1}{3}, m\binom{m}{2}\right]$, let

$$x = m\binom{m}{2} - x_2$$

for some $0 \leq x_2 \leq \binom{m-1}{3}$.

Then we have

$$x' = (m-1)\binom{m-1}{2} - x_2 \in \left[2\binom{m}{3}, (m-1)\binom{m-1}{2}\right].$$

By our inductive hypothesis, there is a graph G' on m vertices with diameter 2 such that $SW_3(G') = x'$.

Recall that G' can be viewed as a star with additional edges between the leaves, let the center of the star (i.e. the vertex adjacent to all other vertices in G') be v. We now consider the graph G of order $m+1$, obtained from G' by joining an additional vertex w with v. It is easy to see that G is also of diameter 2 (Figure 3).

To evaluate $SW_3(G)$, we consider $d(S)$ for each 3-vertex subset S in G:

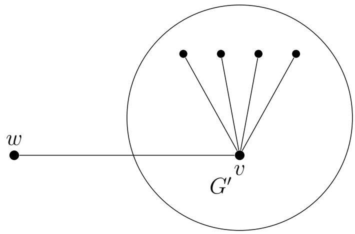

Figure 3. The graph G obtained from G' (Case II).

– If S does not contain w, then $d(S)$ is the same in G as in G'. And the sum of all such Steiner distances is exactly $SW_3(G')$;

– If S contains w but not v, then $d(S) = 3$ and there are $\binom{m-1}{2}$ ways to choose the other two vertices;

– If S contains both w and v, then $d(S) = 2$ and there are $\binom{m-1}{1}$ ways to choose the third vertex;

Consequently we have, through simple algebra, that

$$\begin{aligned} SW_3(G) &= SW_3(G') + 3\binom{m-1}{2} + 2\binom{m-1}{1} \\ &= \left((m-1)\binom{m-1}{2} - x_2\right) + 3\binom{m-1}{2} + 2\binom{m-1}{1} \\ &= m\binom{m}{2} - x_2 \\ &= x. \end{aligned}$$

The conclusion then follows from the fact that all x in (1) is considered in at least one of the above cases. ■

Theorem 2.1 claims that the interval

$$I_n := \left[2\binom{n}{3}, (n-1)\binom{n-1}{2}\right]$$

is “representable” by the Steiner 3-Wiener index for $n \geq 6$. Note that

$$(n-1)\binom{n-1}{2} \geq \binom{n+1}{3}$$

when n is sufficiently large. Hence all but finitely many positive integers are in I_n for some n, implying Theorem 1.1. With the help of computer one can easily check the values not included in $\cup I_n$ and find that the following positive integers are not the Steiner 3-Wiener index of any graph:

$$1,3,4,5,6,7,11,12,13,14,15,16,17,18,19,29,31,32,$$
$$33,34,35,36,37,38,39,57,59,60,63,65,66,67,68,69.$$

As a consequence we have the following stronger version of Theorem 1.1.

Theorem 2.2 *Except for the 34 numbers listed above, every positive integer is the Steiner 3-Wiener index of some simple connected graph.*

3 The inverse Steiner Wiener problem for general k

In this section we show how the argument from the previous section can be used to study the inverse Steiner Wiener problem for general k. Given $k \geq 4$, similar to before, it is easy to obtain

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

and

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

Again we wish to show that every integer in the interval $\left[(k-1)\binom{n}{k},(n-1)\binom{n-1}{k-1}\right]$ is the Steiner k-Wiener index of some connected simple graph. For the purpose of all related discussion we define the statement $\mathbb{P}_{n,k}$ as

For every integer x in $\left[(k-1)\binom{n}{k},(n-1)\binom{n-1}{k-1}\right]$ there is a connected simple graph G of order n with diameter 2 such that $SW_k(G) = x$.

The theorem below states that if $\mathbb{P}_{n,k}$ is true for some $n \geq 2k$ then the inverse Steiner Wiener problem is solved for that particular k.

Theorem 3.1 *For any given $k \geq 4$, if $\mathbb{P}_{n,k}$ holds for some $n \geq 2k$, then all but finitely many positive integers are Steiner k-Wiener indices of simple connected graphs.*

Proof. First suppose that $\mathbb{P}_{m,k}$ holds for some $m \geq 2k$. We will prove, by induction on n, that $\mathbb{P}_{n,k}$ holds for any $n \geq m$.

Assume $\mathbb{P}_{n,k}$, to consider $\mathbb{P}_{n+1,k}$ we first point out the fact that

$$\left[(k-1)\binom{n+1}{k}, n\binom{n}{k-1}\right] \subset I_1 \cup I_2,$$

where

$$I_1 = \left[(k-1)\binom{n+1}{k}, (k-1)\binom{n+1}{k} + \binom{n-1}{k}\right]$$

and

$$I_2 = \left[n\binom{n}{k-1} - \binom{n-1}{k}, n\binom{n}{k-1}\right].$$

For that we needed

$$(k-1)\binom{n+1}{k} + \binom{n-1}{k} \geq n\binom{n}{k-1} - \binom{n-1}{k},$$

which simplifies to $2\binom{n-1}{k} \geq \binom{n}{k}$ and is true when $n \geq m \geq 2k$. As in the proof of Theorem 2.1, we proceed by considering two cases:

1. For any $x \in I_1$, let $x = (k-1)\binom{n+1}{k} + x_1$ for some $0 \leq x_1 \leq \binom{n-1}{k}$. Then

$$x' = (k-1)\binom{n}{k} + x_1 \in \left[(k-1)\binom{n}{k}, (n-1)\binom{n-1}{k-1}\right]$$

and hence we have $SW_k(G') = x'$ for some G' of order n with diameter 2. Let G be obtained from G' by joining an additional vertex with every vertex in G'. Then we have

$$\begin{aligned} SW_k(G) &= SW_k(G') + (k-1)\binom{n}{k-1} \\ &= (k-1)\binom{n}{k} + (k-1)\binom{n}{k-1} + x_1 \\ &= (k-1)\binom{n+1}{k} + x_1 = x. \end{aligned}$$

2. For any $x \in \left[n\binom{n}{k-1} - \binom{n-1}{k}, n\binom{n}{k-1}\right]$, let $x = n\binom{n}{k-1} - x_2$ for some $0 \leq x_2 \leq \binom{n-1}{k}$. Then

$$x' = (n-1)\binom{n-1}{k-1} - x_2 \in \left[(k-1)\binom{n}{k}, (n-1)\binom{n-1}{k-1}\right]$$

and hence we have $SW_k(G') = x'$ for some G' of order n with diameter 2. Let G be obtained from G' by joining an additional vertex with the one vertex of G' adjacent with every other vertex in G'. Then we have

$$\begin{aligned} SW_k(G) &= SW_k(G') + k\binom{n-1}{k-1} + (k-1)\binom{n-1}{k-2} \\ &= (n-1)\binom{n-1}{k-1} - x_2 + k\binom{n-1}{k-1} + (k-1)\binom{n-1}{k-2} \\ &= n\binom{n}{k-1} - x_2 = x. \end{aligned}$$

Consequently we have shown $\mathbb{P}_{n+1,k}$ and by induction, $\mathbb{P}_{n,k}$ for all $n \geq m$.

We now claim that

$$\left[(k-1)\binom{n}{k}, (n-1)\binom{n-1}{k-1}\right] \cap \left[(k-1)\binom{n+1}{k}, n\binom{n}{k-1}\right] \neq \emptyset$$

when n is large. Indeed,

$$\frac{(n-1)\binom{n-1}{k-1}}{(k-1)\binom{n+1}{k}} \to \frac{k}{k-1}$$

as $n \to \infty$, for any fixed k.

Hence every large enough positive integer falls into $\left[(k-1)\binom{n}{k}, (n-1)\binom{n-1}{k-1}\right]$ for some n. The conclusion follows. ■

4 Concluding remarks

In this note we considered the inverse problem for the Steiner k-Wiener index. In the case of $k = 3$ we provided a definite answer for general graphs. Our proof can also be used to reconstruct the specific structure that has the corresponding Steiner 3-Wiener index. It would also be interesting to consider this problem, for $k = 3$ for trees, as many chemical compound has acyclic molecular structures.

For general k, we showed that our approach can show that every large enough positive integer is the Steiner k-Wiener index of some graph, provided that some general initial statement $\mathbb{P}_{2k,k}$ can be established. Through computer search we can easily verify this for small values such as $k = 4$ and 5. Consequently we have

All large enough positive integer is the Steiner k-Wiener index of some graph, for k=3, 4, and 5.

Naturally, it would be interesting to try to extend these to larger k's, and to find fast algorithms to check the statement $\mathbb{P}_{2k,k}$.

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