Fall 2019

Inverse Problems Related to the Wiener and Steiner-Wiener Indices

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INVERSE PROBLEMS RELATED TO THE WIENER AND STEINER-WIENER INDICES

by

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(Under the Direction of Hua Wang)

ABSTRACT

In a graph, the generalized distance between multiple vertices is the minimum number of edges in a connected subgraph that contains these vertices. When we consider such distances between all subsets of k vertices and take the sum, it is called the Steiner k-Wiener index and has important applications in Chemical Graph Theory. In this thesis we consider the inverse problems related to the Steiner Wiener index, i.e. for what positive integers is there a graph with Steiner Wiener index of that value?

INDEX WORDS: Inverse problems, Steiner Wiener indices, Molecular graphs

2009 Mathematics Subject Classification: 15A15, 41A10

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B.S., Dalton State College, 2015

A Thesis Submitted to the Graduate Faculty of Georgia Southern University in Partial Fulfillment of the Requirements for the Degree

MASTER OF SCIENCE

STATESBORO, GEORGIA

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Electronic Version Approved:
December 2019

DEDICATION

This thesis is dedicated to Dwight and Susan Gentry. For their unending and selfless support to help me accomplish this goal.

ACKNOWLEDGMENTS

I want to thank all the professors and fellow students of the Mathematics department at Georgia Southern University. I also want to thank my collaborators, Dr. Jie Zhang and Dr. Xiaodong Zhang. Last but certainly not the least, I am grateful for all the help from my thesis committee.

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LIST OF SYMBOLS

$\mathbb{R}$	Real Numbers
$\mathbb{C}$	Real Numbers
$\mathbb{Z}$	Integers
$\mathbb{N}$	Natural Numbers
$\mathbb{N}_0$	Natural Numbers including 0
G_n	Graphs on n vertices
K_n	Complete graphs on n vertices
S_n	Star graph on n vertices

CHAPTER 1

INTRODUCTION

1.1 BASIC GRAPH THEORY

Graph Theory is the study of graphs. In this context, graphs are mathematical structures that are used to model pairwise relations between objects.

Graph Theory has a long and interesting history and is one of the branches of mathematics that is understood to have a precise date of origination. In 1736, Leonhard Euler solved a celebrated problem known as the Seven Bridges of Königsberg problem. The question was posed as whether it was possible to walk over all of the seven bridges spanning the river Pregel in the town of Königsberg only once and without retracing one's steps. Euler was able to approach this problem from a graph theoretical perspective and found an ingenious solution. Euler's approach to this problem was not only instrumental to the introduction of the discipline of graph theory, but it also serves as the first application of the discipline to a specific problem. Since its inception, graph theory has been utilized for the studying numerous practical problems.

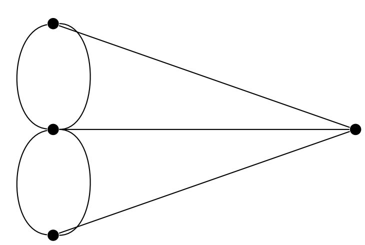


Figure 1.1: Euler's graph to illustrate the Seven Bridges of Königsberg

Formally speaking, a graph G is a collection that consists of an ordered pair $G = (V, E)$, where V represents the set of vertices and E represents the set of edges.

Definition 1.1. *A graph is a mathematical structure consisting of a set of vertices and a set of edges which form connections between pairs of vertices. Typically, we do not allow* *loops (edges connecting a vertex to itself), nor multiple edges joining the same two vertices. If the graph is directed, its edges are ordered pairs of vertices.*

Before introducing Chemical Graph Theory we first list some basic definitions that will be used.

Definition 1.2. *Two vertices v, v' of a graph are said to be adjacent if v, v' are connected by an edge of the graph.*

Definition 1.3. *For any graph G, the compliment of G is the graph with the same vertices as the vertices of G but with all of the edges not in G. For example, if G is a pentagon, then the compliment of G is a pentagram.*

Definition 1.4. *A graph in which every pair of vertices is adjacent is a complete graph. Such a graph is usually denoted by K_n, where n is the number of vertices. For example, a triangle is a complete graph, but no other polygon is.*

Definition 1.5. *A graph is connected if between every pair of vertices $x, y \in G$ there exists at least one path from x to y.*

Definition 1.6. *The degree of a vertex of a graph G is the number of other vertices that it is adjacent to. For example, the vertices in a polygon have degree 2. The vertices of the Peterson graph have degree 3. The vertices in the complete graph K_n have degree $n - 1$.*

Definition 1.7. *The diameter of a graph is the maximal distance between any two points on the graph. If the graph is not connected, then its diameter is infinity.*

Definition 1.8. *A graph is said to be regular if all of its vertices have the same degree.*

Definition 1.9. *A graph is called simple if it has no loops or multiple edges.*

Definition 1.10. *A connected graph that has no cycles is defined as a tree.*

Definition 1.11. *Vertices of degree 1 are called terminal vertices or leaves and edges that are incident with terminal vertices are called terminal or pendant edges.*

Definition 1.12. *Two mathematical objects, A and B are isomorphic if they have the same structure, that is, if there exists a bijective map from A to B that preserves all of the structure relevant to these objects. Such maps are defined as isomorphisms.*

1.2 Chemical Graph Theory

Chemical graph theory is a branch of mathematical chemistry that uses nontrivial applications of graph theory to examine molecular structures. In Chemical graph theory, we approach the problem by using a graph to represent a molecule by representing the atoms as the vertices and the molecular bonds as the edges. The components of graphs that represent chemical compounds are observed differently than typical graphs. In a graph that represents a chemical compound, the vertices represent the atoms and the edges represent the chemical bonds that link the atoms (See, for instance, Figure 1.2). The primary focus of chemical graph theory is to use algebraic invariants to study the topological structure of a molecule as a whole or its orbitals, its molecular branching, structural fragments, and its electronic structures.

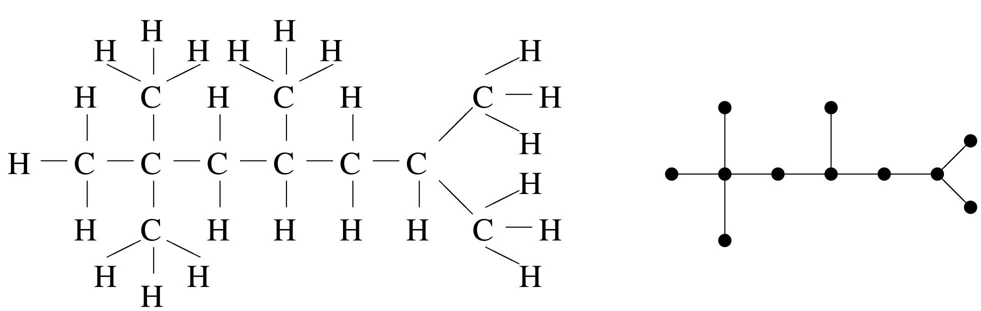


Figure 1.2: Structural formula for 2,2,4,6-tetramethylheptane (on the left) and its corresponding molecular graph (on the right) [17].

Examples of the studies of molecular structures include Cayley's attempts to enumerate chemical isomers and Kirchhoff's study of electrical circuits [5, 6]. Our work mainly concerns the so-called chemical indices defined as the following.

Definition 1.13. *A graph-based molecular descriptor, also known as a chemical index, is a graph-theoretic invariant that numerically characterizes the topological structure of a molecule.*

Among numerous different chemical indices, the Wiener index was introduced by Harry Wiener in 1947 [22, 23]. The Wiener index $W(G)$ of a connected graph G is defined as

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

where $d_G(u, v)$ is the distance between the vertices u and v in G (the number of edges on the shortest path connecting them).

Example 1.14. *For example, in Figure 3.2, the distance* $d(u, v)$ *is 2.*

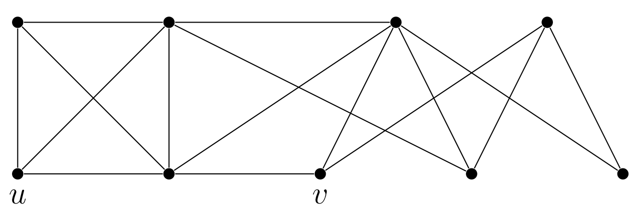


Figure 1.3: The vertices u and v in a graph.

The notion of distance between a pair of vertices can be generalized to the following.

Definition 1.15 ([2])**.** *The Steiner distance* $d(S)$ *for* $S \subset V(G)$ *is the minimum size (number of edges) of a connected subgraph of* G *whose vertex set contains* S*.*

Remark 1.16. *When* $|S| = 2$*, the Steiner distance is equal to the usual distance.*

Using the Steiner distance the following generalization of the Wiener index was introduced.

Definition 1.17. *The k-th Steiner Wiener index, or Steiner k-Wiener index, $SW_k(G)$ is defined as as*

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

Next figure shows an example the Steiner distances.

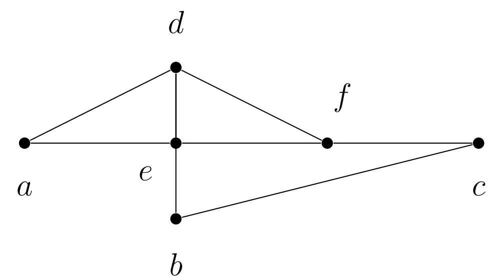


Figure 1.4: An example with labelled vertices.

Recall that the Steiner distance is the minimum size of a set of vertices $S \subset G$ that contains every vertex in S. If we let S be the subset of vertices $\{a, b, c\}$ in G in Figure 1.4, we can observe that the Steiner distance is 3. Something important to note is that when we are computing the Steiner distance in a graph, the resulting subgraph will be a tree because the minimum number of edges to connect the subset of vertices S will eliminate any cycles and unnecessary edges to connect the vertices in S.

1.3 The regular and Steiner Wiener indices

We now provide examples of how to compute the Wiener index and the Steiner Wiener index of a given graph. This process will shed some light on the main idea of our proofs later.

Recall that the Wiener index is defined as $W(G) = \sum_{u,v \in V(G)} d_G(u, v)$, the sum of all distances of a graph G. For example, if we look at the graph of n-Butane (Figure 1.5) we notice that the molecule is composed of three pairs of vertices at a distance of one from

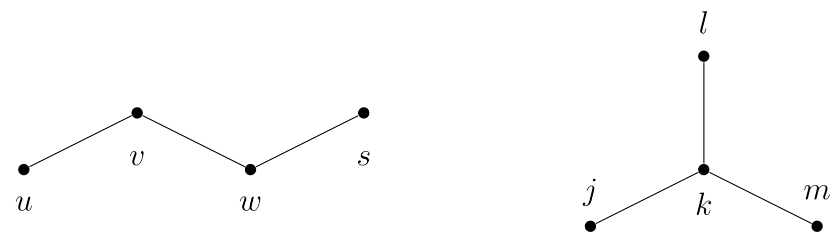


Figure 1.5: The molecular structure of n-Butane on the left and the molecular structure of Isobutane on the right.

each other, two pairs of vertices at distance two, and one pair of vertices at a distance of three. More specifically, we have:

- $d(u, s) = 3$.
- $d(u, w) = d(s, v) = 2$.
- $d(u, v) = d(v, w) = d(s, w) = 1$.

Thus the Wiener index of n-Butane is

$$3 \cdot 1 + 2 \cdot 2 + 1 \cdot 3 = 10.$$

As another example, consider the molecule of Isobutane (Figure 1.5). This molecule is composed of three pairs of vertices at a distance of one and three pairs of vertices at a distance of two. The pairs of vertices $(l, k), (j, k), (m, k)$ yield distance one and $(l, j), (l, m), (j, m)$ yield distance two. Hence The Wiener index of Isobutane is

$$3 \cdot 1 + 3 \cdot 2 = 9.$$

Note that the pairs of vertices that are composed of a leaf vertex and the center vertex will have a distance of one because it only takes one edge to connect the two chosen vertices and the pairs consisting of the leaves have a distance of two because it takes two edges to connect the two chosen vertices.

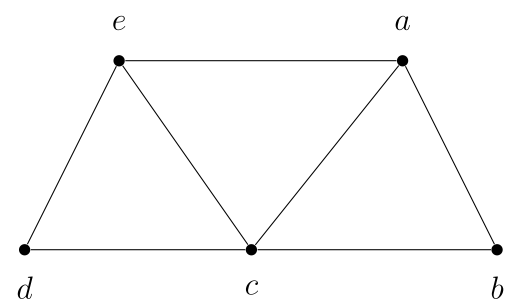


Figure 1.6: An example with labelled vertices.

Let us now use Figure 1.6 to illurstrate the Steiner 3-Wiener index. Recall that the Steiner k-Wiener index of a graph G is defined as

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

incorporating both concepts of the Steiner distance and the Wiener index. The Steiner k-Wiener index calculates the sum of the distances from all sets of vertices $S \in G$ with $|S| = k$. In figure 1.6, the Steiner Wiener index of G when $k = 3$ is

$$\begin{aligned} SW_3(G) = &\sum_{S \subseteq V(G),\ |S|=3} d(S) \\ &= d(a,b,c) + d(a,b,d) + d(a,b,e) + d(a,c,d) + d(a,c,e) \\ &\quad + d(b,c,d) + d(b,c,e) + d(b,d,e) + d(c,d,e) + d(a,d,e) \end{aligned}$$

Computing the distances of the subsets gives

$$2 + 3 + 2 + 2 + 2 + 2 + 2 + 3 + 2 + 2 = 22$$

Notice that we can observe that the number of k-sets will be $\binom{n}{k}$ with $n = |V(G)|$

1.4 The Inverse Steiner k-Wiener Problem

The Inverse Wiener problem asks that if we are given $n \in \mathbb{N}$, is there a graph G or a tree T that exists where $W(G) = n$. The Inverse Wiener problem for general graphs G is much easier than it is for trees. For trees the following conjecture has been proposed.

Conjecture 1.18. *For all but a finite set of positive integers n, we can find a tree with a Wiener index of n.*

For “small” positive integers, with the help of computers it has been found that for all but 49 positive numbers, there exists some tree with a Wiener index of that value. The 49 exceptions are [10]: 2, 3, 5, 6, 7, 8, 11, 12, 13, 14, 15, 17, 19, 21, 22, 23, 24, 26, 27, 30, 33, 34, 37, 38, 39, 41, 43, 45, 47, 51, 53, 55, 60, 61, 69, 73, 77, 78, 83, 85, 87, 89, 91, 99, 101, 106, 113, 147, 159. Based on these observations a stronger version of Conjecture 1.18 was proposed as follows.

Conjecture 1.19. *There are exactly 49 integers (listed above) that are not Wiener indices of any trees.*

The above conjecture was proved in [16] and [20]. The independent results were shown through entirely different approaches. In [16] it was proved that all but 49 integers are Wiener indices of trees with a diameter at most 4. The approach used in [20] showed that for every $n > 10^8$ there exists a caterpillar tree such that $W(G) = n$. Throughout these studies it was noted that the most interesting molecular graphs possess natural restrictions on their degrees or they have cycles with hexagonal or pentagonal structures. With this discovery of these characteristics, it has inspired the study of the inverse Wiener index problem for certain types of structures. The structures that are focused on are trees with a vertex degree ≤ 3 and types of graphs that possess hexagonal chains [18].

The inverse Steiner Wiener problem is of exactly the same nature, but apparently more complicated as it deals with Steiner distances. This was first proposed in [13] where some very useful observations were made.

1.5 OUTLINE OF OUR WORK

In Chapter 2 we will provide a solution for the inverse Wiener problem for general graphs. Although the result is already well-known, the presented proof will also shed some light on our approach to solve inverse Steiner k-Wiener problems.

In Chapter 3 we show our main result, stated as the following.

Theorem 1.20. *All but a finite number of positive integers are Steiner 3-Wiener indices of connected simple graphs.*

In Chapter 4 we provide some insights towards solving the inverse Steiner Wiener problem for general k. This includes some data from elementary analysis.

CHAPTER 2

THE INVERSE PROBLEM FOR THE WIENER INDEX

In this chapter we provide a solution to the inverse Wiener problem (or, equivalently, the Steiner 2-Wiener index) in general graphs. That is, we show a proof for the following previously established statement.

Theorem 2.1. *Every positive integer except for 2 and 5 is the Wiener index of some connected simple graph G.*

2.1 A KEY LEMMA

First we show that all integers between the Wiener index of a star and a complete graph on n vertices can be represented as the Wiener index of some graph of the same order.

Lemma 2.1.1. *All positive integers between $\binom{n}{2}$ and $(n-1)+\binom{n-1}{2}\cdot 2$ are Wiener indices of graphs of order n.*

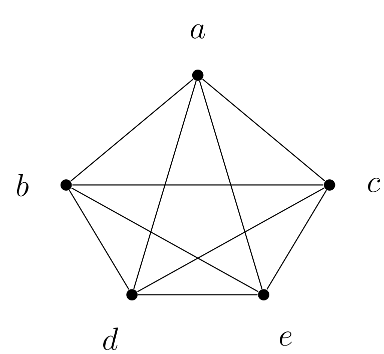


Figure 2.1: The complete graph K_5.

Proof. The Wiener index of the complete graph K_n is $W(K_n) = \binom{n}{2}$. The idea for our proof begins with taking a complete graph and removing edges from the graph until we transform the graph into a star.

In figure 1.6, we start with the complete graph of K_5 and we begin removing edges. Let c be our chosen vertex and then start removing edges from G that are not connected to the vertex c.

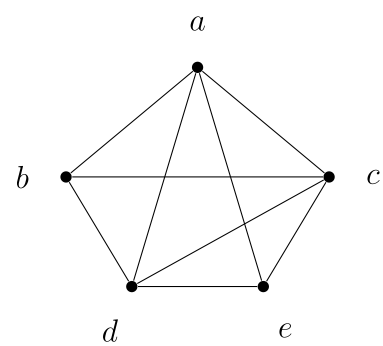


Figure 2.2: The graph G_1.

As shown in figure 1.7, we have removed the edge connecting vertices b and e and we get the graph G_1. The Wiener index of G_1 is $W(G_1) = \binom{n}{2} + 1$. Now, we continue removing edges from the remaining vertices of G.

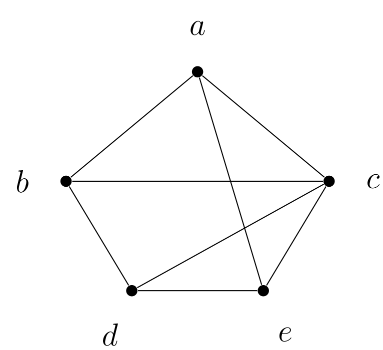


Figure 2.3: The graph G_2 with $W(G_2) = \binom{n}{2} + 2$.

$\square$

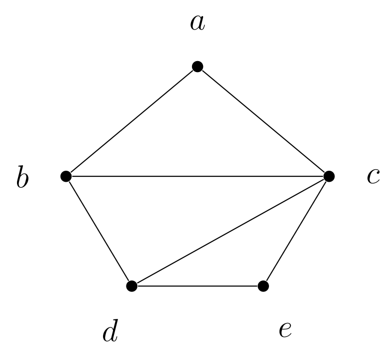


Figure 2.4: The graph G_3 with $W(G_3) = \binom{n}{2} + 3$.

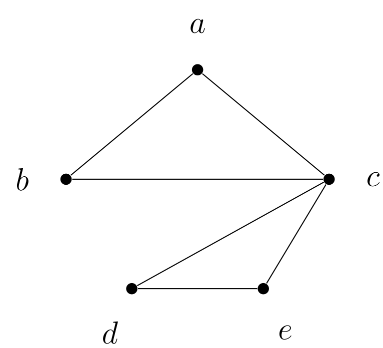


Figure 2.5: The graph G_4 with $W(G_4) = \binom{n}{2} + 4$.

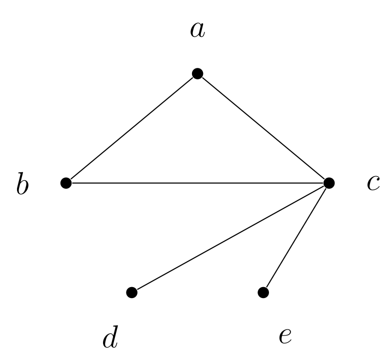


Figure 2.6: The graph G_5 with $W(G_5) = \binom{n}{2} + 5$.

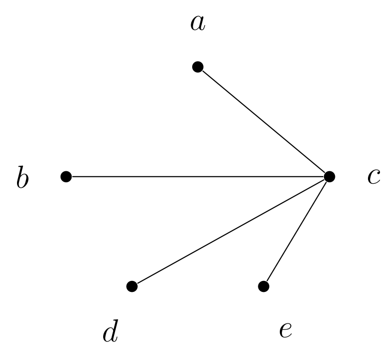


Figure 2.7: The star graph S_5 with $W(S_n) = (n-1) + \binom{n-1}{2} \cdot 2$.

2.2 Proof of Theorem 2.1

First note that from Lemma 2.1.1 we know that all integers in

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

are Wiener indices of some graph. We will now show that the union of such intervals contain all but two positive integers.

Lemma 2.2.1. *For any positive integer $x \neq 2, 5$,*

$$x \in \cup_{n=1}^{\infty} I_n.$$

Notice that we can simplify the upper bound of I_n

$$\begin{aligned}(n-1) + \binom{n-1}{2} \cdot 2 &= (n-1) + \frac{(n-1)(n-2)}{2} \cdot 2 \\ &= (n-1) + (n-1)(n-2) \\ &= (n-1)^2\end{aligned}$$

We now only need to show that the intervals I_{n-1} and I_n overlap, which follows from the following observation.

Claim 2.2. *When $n \geq 5$*

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

Proof. Note that

$$(n-1)^2 \geq \frac{1}{2}n(n+1)$$

is equivalent to

$$2(n-1)^2 \geq n(n+1)$$

and then simplified to

$$\begin{aligned} n^2 + n &\leq 2(n^2 - n - n + 1) \\ &= 2(n^2 - 2n + 1) \\ &= 2n^2 - 4n + 2 \end{aligned}$$

This is true if and only if

$$n^2 - 5n + 2 \geq 0,$$

which obviously holds when $n \geq 5$. $\square$

Now, together with Lemma 2.1.1, we have that every positive integer other than 2 and 5 is the Wiener index of some graph.

CHAPTER 3

THE INVERSE PROBLEM OF THE STEINER 3-WIENER INDEX

In this chapter we provide a solution to the inverse Steiner 3-Wiener problem. The main idea is similar to the regular case but the argument is much more technical.

3.1 Some preliminaries

Let K_n be the complete graph on n vertices. There are $\binom{n}{3}$ choices for 3 vertices from K_n and the distance between the subset of vertices is 2. Hence

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

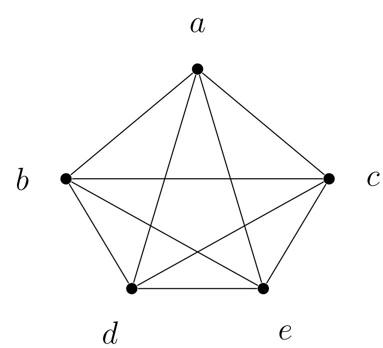


Figure 3.1: The complete graph K_5 with $SW_3(K_5) = 2\binom{5}{3}$

Let S_n represent the star graph on n vertices. To compute the Steiner 3-Wiener index of S_n, we have to consider two cases.

Case I Assume that our subset S of vertices contains the center vertex, then the distance of S is 2. It is easy to see that there are $\binom{n-1}{2}$ such sets of three vertices and so we have $2\binom{n-1}{2}$.

Case II Suppose that our subset S does not contain the center vertex of the star. Since S cannot contain the center vertex, then S consists of the vertices that represent the leafs of S_n. The distance of S is 3 and so we have $3\binom{n-1}{3}$.

Combining the two cases, we have

$$SW_3(S_n) = 2\binom{n-1}{2} + 3\binom{n-1}{3}$$

We can simplify this equation further. Observe that

$$2\binom{n-1}{2} = \frac{(n-1)(n-2)}{2} \cdot 2 = (n-1) \cdot (n-2)$$

and

$$3\binom{n-1}{3} = \frac{(n-1)(n-2)(n-3)}{6} \cdot 3 = \frac{(n-1)(n-2)(n-3)}{2} = \binom{n-1}{2} \cdot (n-3),$$

combining these two equations, we get the simplified expression

$$SW_3(S_n) = 2\binom{n-1}{2} + 3\binom{n-1}{3} = (n-1) \cdot \binom{n-1}{2}$$

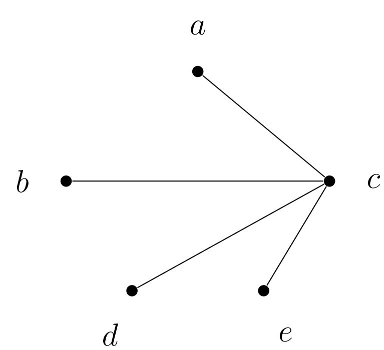


Figure 3.2: The star graph S_5.

Similar to before, we now claim the following.

Theorem 3.1. *There exist a connected graph G of order n such that*

$$SW_3(G) = x, \forall x \in \left[2\binom{n}{3}, (n-1)\binom{n-1}{2}\right]$$

In the rest of this chapter we first prove this statement by induction on n, which leads to the solution to the inverse Steiner 3-Wiener problem and a proof to Theorem 1.20.

3.2 THE INITIAL CASE

Consider the complete graph K_6 and the star graph S_6. The Steiner 3-Wiener value for K_n is

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

and for S_n is

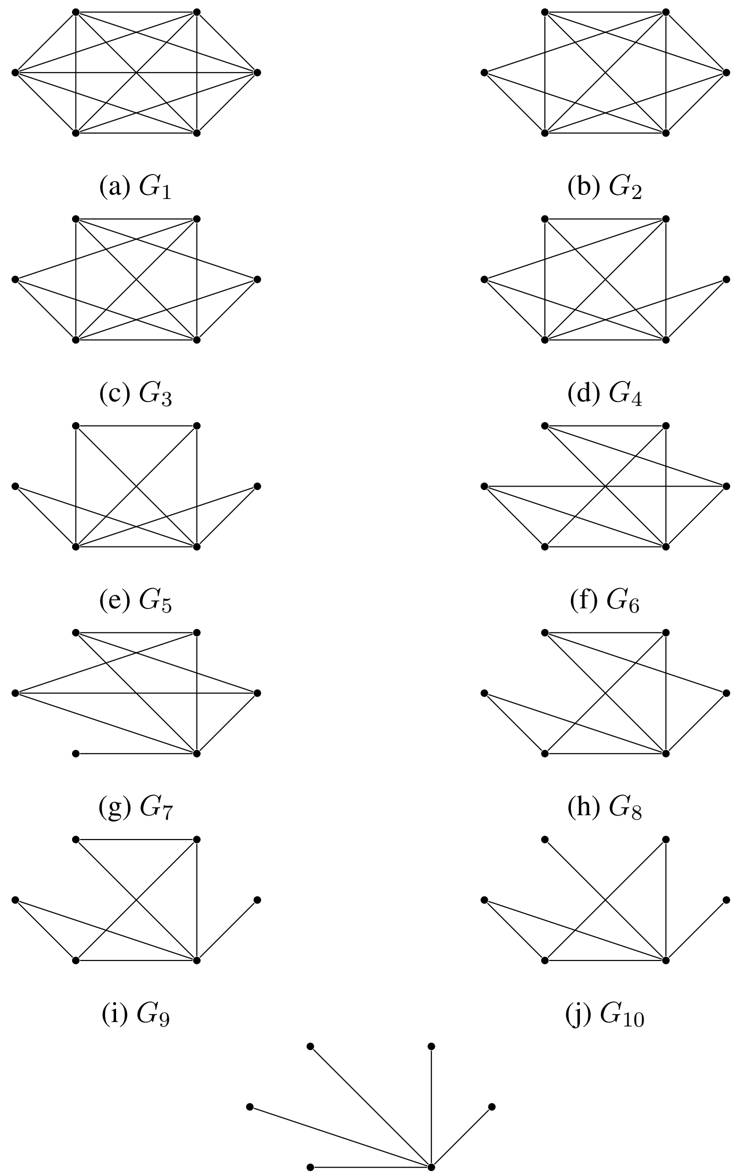
$$SW_3(S_n) = (n-1)\binom{n-1}{2}$$

When $n = 6$, we are interested in $x \in [40, 50]$ for the $SW_3(K_6)$ to $SW_3(S_6)$. For the complete graph K_6, the $SW_3(K_6) = 40$.

From Figure 3.3, we show that we can take the complete graph K_6 and transform K_6 into the star S_6 by removing some edges. In the process of removing edges, we obtain the graphs G_i for $i = 1, 2, ..., 11$ with exactly the desired values as their Steiner 3-Wiener indices.

G_i	$SW_3(G_i)$
1	40
2	41
3	42
4	43
5	44
6	45
7	46
8	47
9	48
10	49
11	50

Table 3.1: The graphs G_i and their Steiner 3-Wiener indices.



(a) G_1 (b) G_2

(c) G_3 (d) G_4

(e) G_5 (f) G_6

(g) G_7 (h) G_8

(i) G_9 (j) G_{10}

(k) G_{11}

Figure 3.3: Step 1: $n = 6$, and the values of $SW_3(G)$ are from 40 to 50.

3.3 PROOF OF THEOREM 3.1

Recall that $SW_3(K_n) = 2\binom{n}{3}$ because no matter which set of three vertices we select from the complete graph K_n, the distance between them is two. We now move on to the proof of Theorem 3.1.

Proof of Theorem 3.1. The initial case for $n = 6$ follows from the previous section. More specifically, we can observe that: Not only does there exist a connected graph G_i where $SW_3(G_i) = x$ for any $x \in [40, 50]$, this graph G can be obtained by adding edges to the star S_6 or by removing edges from the complete graph K_6.

Induction hypothesis: Let $n = m$, then

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

we have that $SW_3(G) = x$ for some G of order m. Since

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

we can get x by removing edges from K_m or adding edges to S_m, so we may represent x as

$$x = 2\binom{m}{3} + k_1 = (m-1)\binom{m-1}{2} - k_2$$

to indicate the removed or added edges.

Inductive step: Let $n = m + 1$, then we are interested in the values

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

For the inductive step, we will split the interval

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

into two cases.

Case I Let $x \in [2\binom{m+1}{3}, 2\binom{m+1}{3} + \binom{m-1}{3}]$

Suppose that $x = 2\binom{m+1}{3} + x_1$. Let

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

with $0 \leq x_1 \leq \binom{m-1}{3}$. By our induction hypothesis, we have a graph G' on m vertices where the $SW_3(G') = x'$. Suppose that we select a vertex w from the graph K_{m+1}. Suppose that we add w to the graph G' and note that w is adjacent to all of the vertices in G'. Once we add w to G', we get a graph G on $m+1$ vertices. See Figure 3.4.

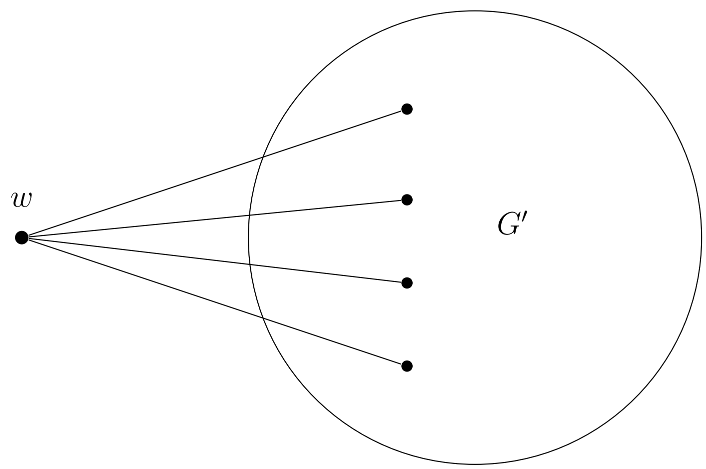


Figure 3.4: The graph G and G' in Case I.

Notice now, that

$$SW_3(G) = SW_3(G') + 2\binom{m}{2}$$

where

$$SW_3(G') = 2\binom{m}{3} + x_1$$

by the definition of G'. Then $2\binom{m}{2}$ is the contribution from choosing w and two other vertices in G' to be in the subset. Since w is adjacent to all vertices in G', each of the $\binom{n}{2}$ subsets will contribute 2 to $SW_3(G)$. When we combine these two parts, we have

$$SW_3(G) = (2\binom{m}{3} + x_1) + 2\binom{m}{2} = 2\binom{m+1}{3} + x_1 = x$$

from the claim below.

Claim 3.2.

$$2\binom{n}{3} + 2\binom{n}{2} = 2\binom{n+1}{3}$$

Proof of the Claim. The above statement is true by the identity

$$\binom{n+1}{k} = \binom{n}{k} + \binom{n}{k-1},$$

the proof of which we present below for completeness.

$$\begin{aligned}
\binom{n}{k} + \binom{n}{k-1} &= \frac{n!}{(n-k)!k!} + \frac{n!}{(n-(k-1))!(k-1)!} \\
&= \frac{n!}{(n-k)!k!} + \frac{n!}{(n-k+1)!(k-1)!} \\
&= \frac{(n-k+1)n!}{(n-k+1)(n-k)!k!} + \frac{n!k}{(n-k+1)!(k-1)!k} \\
&= \frac{(n-k+1)n! + n!k}{(n-k+1)!k!} \\
&= \frac{nn! - kn! + n! + n!k}{(n-k+1)!k!} \\
&= \frac{nn! + n!}{(n-k+1)!k!} \\
&= \frac{n!(n-1)}{(n-k+1)!k!} \\
&= \frac{(n+1)!}{((n+1)-k)!k!} \\
&= \binom{n+1}{k}
\end{aligned}$$

□

Case II Let $x \in [m\binom{m}{2} - \binom{m-1}{3}, m\binom{m}{2}]$.

Suppose that

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

with $0 \leq x_2 \leq \binom{m-1}{3}$. Now consider

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

By our inductive hypothesis, we know that there exists a graph G' on m vertices where the $SW_3(G') = x'$. We further know that G' may be taken to be a star graph plus some extra edges.

$$SW_3(G') = (m-1)\binom{m-1}{2} - x_2$$

Suppose that we have a vertex w that is adjacent to the center vertex of G', so G' with w gives the graph G on $m+1$ vertices. Then $G' \cup w$ is still a star graph with extra edges of order $m+1$. See Figure 3.5.

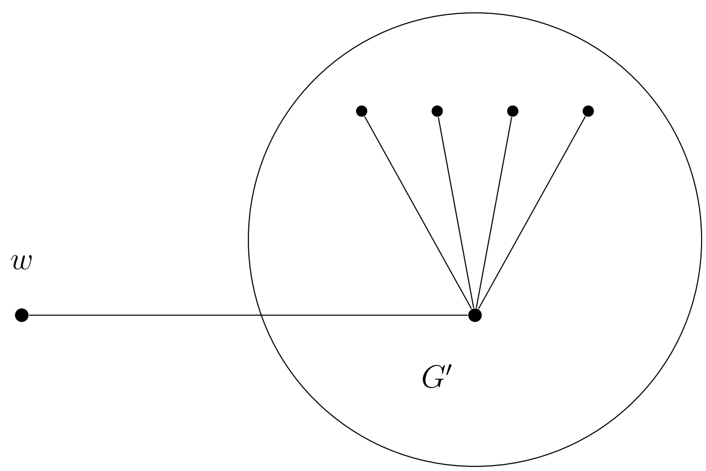


Figure 3.5: The graphs G and G' in Case II.

If we require w and the center vertex of G' for our selection of three vertices, then we get

$$2\binom{m-1}{1} = 2(m-1)$$

If we exclude the center vertex of G', then we get $3\binom{m-1}{2}$. Combining these steps, we have

$$SW_3(G) = (m-1)\binom{m-1}{2} - x_2 + 2(m-1) + 3\binom{m-1}{2} = m\binom{m}{2} - x_2 = x$$

by simple algebra as shown below.

Claim 3.3. $m\binom{m}{2} = (m-1)\binom{m-1}{2} + 2(m-1) + 3\binom{m-1}{2}$

Proof of the claim.

$$\begin{aligned}
&(m-1)\binom{m-1}{2} + 2(m-1) + 3\binom{m-1}{2} \\
&= (m-1)\frac{(m-1)(m-2)}{2} + 2m - 2 + 3 \cdot \frac{(m-1)(m-2)}{2} \\
&= \frac{(m-2)(m-1)^2}{2} + 2m - 2 + \frac{3(m-1)(m-2)}{2} \\
&= \frac{(m-2)(m-1)^2 + 3(m-1)(m-2)}{2} + 2m - 2 \\
&= \frac{m^3 - 4m^2 + 5m - 2 + 3m^2 - 9m + 6}{2} + 2m - 2 \\
&= \frac{m^3 - m^2 - 4m + 4}{2} + 2m - 2 = \frac{m^3 - m^2 - 4m + 4}{2} + \frac{2(2m-2)}{2} \\
&= \frac{m^3 - m^2 - 4m + 4 + 4m - 4}{2} = \frac{m^3 - m^2}{2} = \frac{m(m^2 - m)}{2} = \frac{1}{2}m^2(m-1) \\
&= m\binom{m}{2}
\end{aligned}$$

□

From case I, we have the interval

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

and from case II, we have the interval

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

We now claim that the two above mentioned intervals indeed overlap when m is large enough.

Claim 3.4. *When* $m \geq 6$

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

Proof. First note that each of the involved binomial coefficients can be expanded as follows

$$\begin{aligned} m\binom{m}{2} &= \frac{1}{2}m^2(m-1) \\ \binom{m-1}{3} &= \frac{(m-1)(m-2)(m-3)}{6} \\ 2\binom{m+1}{3} &= \frac{(m+1)(m)(m-1)}{3} \end{aligned}$$

We need to show

$$\frac{1}{2}m^2(m-1) - \frac{(m-1)(m-2)(m-3)}{6} \leq \frac{(m+1)(m)(m-1)}{3} + \frac{(m-1)(m-2)(m-3)}{6},$$

which is equivalent to

$$\frac{1}{2}m^2(m-1) - \frac{(m-1)(m-2)(m-3)}{3} - \frac{(m+1)(m)(m-1)}{3} \leq 0$$

The left side is

$$\begin{aligned} &\frac{m^3-m^2}{2} - \frac{-(m-1)(m-2)(m-3) - m(m+1)(m-1)}{3} \\ &= \frac{m^3-m^2}{2} + \frac{-2m^3+6m^2-10m+6}{3} \\ &= \frac{(m^3-m^2)\cdot 3}{6} + \frac{(-2m^3+6m^2-10m+6)\cdot 2}{6} \\ &= \frac{-m^3+9m^2-20m+12}{6} \\ &= \frac{-m^3}{6} + \frac{3m^2}{2} - \frac{10m}{3} + 2 \end{aligned}$$

This is obviously no more than zero when $m \geq 6$. □

Since we have shown that

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

the union of the intervals

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

and

$$\left[m\binom{m}{2} - \binom{m-1}{3}, m\binom{m}{2}\right]$$

contain all of the values for x under consideration. Therefore,

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

there exists a connected graph G where $x = SW_3(G)$.

$\square$

3.4 Proof of Theorem 1.20

With Theorem 3.1, we only need to show that the collection of the intervals

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

contain all but finitely many positive integers. This is true by noting that the upper bound of the n-th interval,

$$(n-1)\binom{n-1}{2}$$

is larger than the lower bound of the $(n+1)$-th interval,

$$2\binom{n+1}{3},$$

when n is sufficiently large.

Claim 3.5. *When* $n \geq 11$

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

Proof. Observe that

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

can be simplified to

$$\frac{(n-1)^2(n-2)}{2} \geq 2\frac{(n+1)n(n-1)}{6}$$

$$3(n-1)(n-2) \geq 2n(n+1)$$

$$3(n^2-3n+2) \geq 2(n^2+n)$$

$$n^2-11n+6 \geq 0$$

This is true when $n > 10$ □

We have a number of possible exceptions and they are:

$$2 \leq n \leq 8$$

$$9 \leq n \leq 20$$

$$24 \leq n \leq 40$$

$$50 \leq n \leq 70$$

$$90 \leq n \leq 112$$

$$147 \leq n \leq 168$$

$$224 \leq n \leq 240$$

$$324 \leq n \leq 330$$

CHAPTER 4

GENERAL INVERSE PROBLEMS AND CONCLUDING REMARKS

To deal with the inverse Steiner k-Wiener problem for general k, we first note that the argument in our inductive step for the $k = 3$ case is still valid.

However, to show a general initial case appears to be very difficult. Through the help of computer analysis the $k = 4$ and $k = 5$ cases can be verified. To deal with higher values of k one needs to consider some "initial set" of graphs that can potentially generate as many values for the Steiner Wiener index as possible, through as simple operations as possible.

As an example, starting from all graphs on five vertices, the first table below shows the Steiner 4-Wiener indices of them.

Now by adding a pendant edge at different vertices in the graphs, we have a variety of values for the Steiner 4-Wiener indices of some graphs on six vertices. We conclude this thesis with a table of this data.

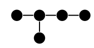
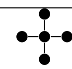
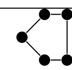
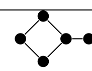
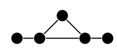
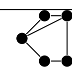
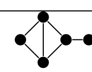
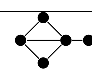
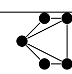
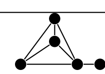
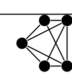
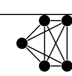
G_i	$SW_4(G_i)$	G
1	18	
2	17	
3	16	
4	15	
5	16	
6	17	
7	15	
8	16	
9	16	
10	15	
11	16	
12	15	
13	15	

Table 4.1: Steiner 4-Wiener indices of graphs on five vertices.

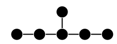
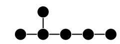
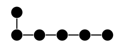
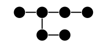
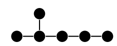
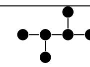
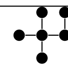
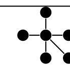
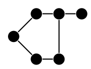
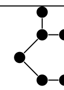
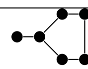
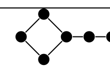
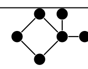
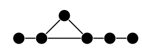
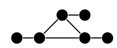
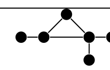
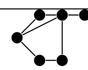
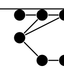
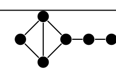
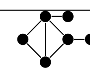
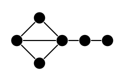
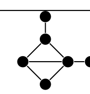
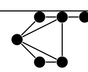
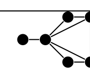
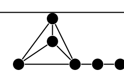
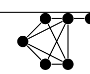
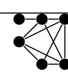
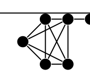
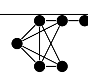
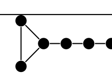
$G_{i,j}$	$SW_4(G_i)$	G	$G_{i,j}$	$SW_4(G_i)$	G
1,1	58		1,2	59	
1,3	63		2,1	58	
2,2	59		2,3	56	
3,1	54		3,2	50	
4,1	53		4,2	52	
4,3	52		5,1	55	
5,2	51		6,1	58	
6,2	57		6,3	54	
7,1	49		7,2	52	
8,1	56		8,2	53	
9,1	54		9,2	52	
10,1	50		10,2	49	
11,1	54		12,1	49	
12,2	49		13,1	49	
14,1	49		15,1	59	

Table 4.2: Steiner 4-Wiener indices of “some” graphs on six vertices.

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