WIENER INDEX OF SOME ACYCLIC GRAPHS

by

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ABSTRACT

In the field of chemical graph theory, a topological index (a.k.a.connectivity index) is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound[5]. In this thesis, we have studied one of the well-known topological indices called *Wiener*. It is obtained by adding all the geodesic distances (or shortest paths) of the graph. As the number of vertices grow for any graph, so does the Wiener number of that graph. We determine the Wiener values associated to several graphs, as functions of the number of vertices–We found that these infinite integer sequences have general formulae which include summations of triangular numbers. Further, we introduced new classes of trees and derived new infinite integer sequences that are not available in the largest online encyclopedia of integer sequences.

DEDICATION

This thesis work is dedicated to:

My two sons, Ralph H. Cole, III and Reginald G. Cole, my dad, Clifton M. Lewis, my family members and friends. Thank you for having patience with me as I dedicated the last two years to my studies.

My mother, Barbara Ann Wright Lewis Turner (who encouraged me at a young age to pursue math even when I couldn't see its value), my granddad, Roosevelt R. Wright, Sr, and my friends who transitioned while I was on this journey. I heard all of your silent whispers of encouragement those days I wanted to give up. Thank you my angels.

Dr. Herman Brown, who even as he lay ill, told me to go back to school and finish my degree in Math because the students need me.

E.C.S.U. administration, faculty, staff and my fellow students, I appreciate you for keeping me encouraged to persevere to the end.

The members of the committee: Dr. K. L. Jones, Dr. K. Kulkarni, and Dr. G. Del Villar. I appreciate you dedicating time to hear and evaluate my thesis defense.

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I would like to express my gratitude and appreciation to Dr. Julian A. D. Allagan, E.C.S.U. Associate Professor, Mathematics and Computer Science, for his patience and expertise in Graph Theory. You have opened my eyes to a new branch of math and exciting future research options.

Maenecia Lewis Cole, M.S. Ed.

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Chapter 1 Introduction

In this chapter, we introduce the reader to graph theory, its history, basic notions along with the structure of the thesis.

1.1 History

Graph theory began in 1736 when Leonard Euler published a paper that contained the solution to the 7 bridges of Konigsberg (see Figure 1.1 left) problem [2]. Is it possible to take a walk around town crossing each bridge exactly once and wind up at your starting point? A graph (vertices and links) is used to model or represent the Konigsberg problem (see Figure 1.1 right). The answer to this problem is "no". To help provide a solution to this problem, Euler used a drawing or a model that we call *graphs*, that reduces the problem down to its important elements, thus avoiding unnecessary details. We begin by introducing the basic information about graphs.

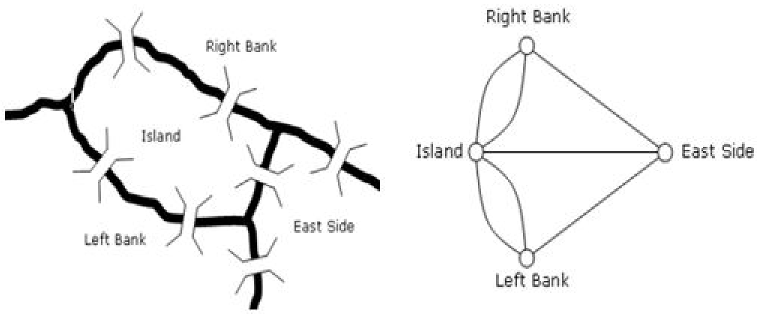


Figure 1.1: Konigsberg city and its corresponding graph model

James Sylvester of the 19^{th} century was said to be the first to use the word "graph" in the context of graph theory, who was one of many mathematicians that were intrigued with studying types of diagrams representing molecule [2]. Furthermore, in the mid-19^{th} century, Francis Guthrie presented the puzzle problem four-color problem led to the studies of graphs for theoretical and applied interests. The four-color problem seeks whether the countries on every map can be colored by using just four colors in a way that countries sharing an edge have different colors; however, this question can also be presented if the vertices of a planar graph can always be colored by using just four colors[8]. Although this problem would not be solved until more than a century later, it led to further studies within the broad field of graph theory. In 1862, De jaenish experimented to discover the minimum number of queens that can be placed on the chess board in such a way every square is either occupied by a queen or being attacked by at least one queen, which deals with domination. Through the work of solving practical problems in this time period, it made possible to obtain solutions important to graph theory such as Gustav Kirchhoff's complete set of equation for currents and voltages in electric circuits is summed up by representing his equations by a graph with skeleton tress and with the aid of these representations helped obtain linearly independent circuit systems. Arthur Cayley arrived at the situation of listing and describing trees with certain properties by starting from calculating the number of isomers of saturated hydrocarbons linking graphic theory and other sciences. At the start of the 20^{th} century, problems including graphs began to appear in physics, chemistry, electrical engineering, biology, economics, sociology and many other fields of study. Chemistry was a prominent field that would use lettered vertices to denote individual atoms while the lines denoted the chemical bonds with the degree of the vertices denoting the valence. The studies of connectivity properties, graph symmetry, and planarity are a few of several tools that helped direct the study of graph theory, which began to appear more frequently in the 1920s and 1930s, and soon extended throughout the 1940s and 1950s through the development of cybernetics and calculation techniques. As the range of problems that graph theory dealt with increased, so did the interest of graph theory; in addition, electronics computers became more useful with handling practical problems containing complex equations, leading to more discoveries using graphic theory. Methods were established to solve external problems, such as the construction of the maximum flow across a network, which could clearly be solved through graphs (tree and planar graphs) rather than arbitrary graphs. Problems in Graph theory could be less structured and free-flowing (combinatorial) while others were more (geometric) structured. Problems such as graph circuits and graph embedding were geometric in nature [6]. Other problems concerned with the modes of classification of graph such as classification by the properties of partitions of them. The results of these problems involving the existence of these graphs with certain properties can be shown by representing numbers by the degrees of the vertices of a given graph: "a collection of integers $0 < d_1 < \ldots < d_n$, the sum of which is even", can be understood by the degrees of the vertices of a graph not containing any loops and multiple edges. Problems questioning the enumeration of graphs with prescribed properties can be represented by problems of non-isomorphic graphs that contain the same number of vertices and/or edges. [8]

Graphic Theory can be used to deal with problems pertaining to the connectivity of graphs and to study the structure of graphs based off of the connectivity of graphs; Analysis of the reliability of electronic circuits or communication networks raise the problem of solving the amount of non-intersecting edges that connect vertices within a graph [8]. The result of this problem yielded that the least number of vertices separating two non-adjacent vertices are equal to the greatest number of non-intersecting simple edges that connect this pair of vertices. Algorithms were developed to establish the degree of connectivity of graphs. Other studies of graphs consisted of finding the number of edge progressions that include all the vertices or all the edges the graph; through multiple observations, the resulting criteria is that a connected graph a cycle containing all the edges and passing through each edge once and only once exists if and only if the degrees of all except two vertices of the graph are even. If the set of vertices of a graph is traversed, only some sufficient conditions for the existence of a cycle passing through each vertex once is available. [8] In all, results and methods of graph theory have been used extensively to aid in solving transportation problems, find optimal solutions for planning and control of project developments, establishing the best routes for the supply of goods, and modeling complex technological processes in the creation of wide varieties of discrete situations.

The term graph in this branch of mathematics does not concern data charts such as line graphs or bars graphs yet involves a set of points (vertex) that are joined by lines that can be called edges[2]. A graph containing at most one edge between any two points without any loops is called a simple graph; if stated otherwise, the term graph is to be assumed to be a simple graph. When two points are connected by two or more edges, the graph is described as a multigraph. A complete graph is a graph where every point contained in that graph is connected by and edge to every other point. In some cases, the direction can be assigned to each edge to produce a graph called a directed graph or digraph. Other important basic concepts of graph theory are a point's degree and the types of path [2]. Each vertex has a number associated with it called its degree, which is the number of edges that are connected to it; a loop contributes 2 to the degree of the vertex. The number of vertices in a complete graph classifies its nature, therefore complete graphs are commonly denoted by K_n, where n refers to the number of vertices, and all vertices of K_n have a degree of $n - 1$. With this information, Euler's theorem pertaining to Konigsberg bridge Problem could be translated in modern terms as: If there is a path along edges of a *multigraph*, that travels along each edge only once, then there exists at most two vertices of odd degree; additionally, if the path begins and ends at the same vertex, then no vertices will have an odd degree. A path is described as the route of the edges of the graph; a path can follow one edge between two points or follow multiple edges through multiple points. When a path connects any two vertices in a graph, the graph is connected; furthermore, when a path begins at a point and ends at that same point without crossing any edge more than once is called a *circuit*. In 1750 Euler discovered the polyhedral formula $V - E + F = 2$, where the equation relates to the number of vertices (V), edges (E), and Face (F) of a polyhedron; [2] the vertices and edges of this solid forms a graph leading to how graphs can be formulated on other surfaces.

Finally, graph theory and topology history are closely related and share common problems and techniques and the similarities between both topics led to a subsection named topological graph theory [2]. One problem in this area is called planar graphs, which are dotted graphs with edges on a plane no edges intersect.

1.2 Basic Definitions

A **simple graph** $G = (V, E)$ consists of $V = V(G)$, a nonempty set of objects called **vertices** (or nodes) and $E = E(G)$, a set of an unordered pair of distinct vertices called **edges**.

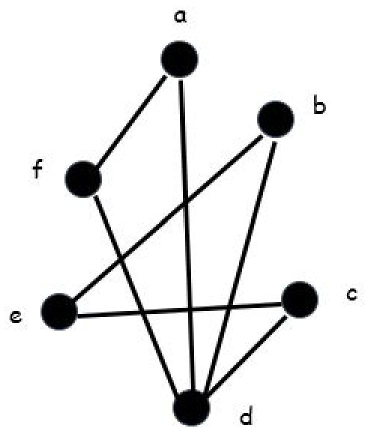


Figure 1.2: Example of a simple graph on 6 vertices

See Figure 1.2, for example. Vertices, say u and v that share an endpoint are said to be **adjacent**; u is also said to be a neighbor of v and vice-versa the edge denoted by uv is said to be incident to the vertices u and v. The **order** of the graph G is the size of its vertex set which we denote by $|V|$ and the size of the edge set, denoted by $|E|$, is called **size** of the graph G. The degree of vertex, v denoted by $deg(v)$, is the number of edges incident to v ; that is the size of its neighbor. A vertex of degree 0 is said to be **isolated** while a vertex of degree 1 is called a **leaf**. The **minimum degree** of G, denoted by $\delta(G)$, is its smallest vertex degree, and the **maximum degree** of G denoted by $\Delta(G)$ is the largest degree among its vertices. A vertex u is said to be connected to a vertex v, in a graph G, [9] if there exists a sequence of edges (or path) from u to v in G. A graph G is **connected** if there is a path that connects every two of its vertices. There are other types of graphs such as multigraphs (when multiple edges are allowed between vertices), pseudographs (when a vertex is allowed to be connected to itself, as in a loop) and directed graphs (when each edge is given an orientation, using an arrow). However, our thesis will focus only on simple graphs, as previously defined.

In Chapter 2, we define and introduce some fundamental properties of several graphs. These properties rely on the fundamentals of geodesics, the shortest path between any pair of vertices. nine graphs; one of them is new. Although not all of these properties are relevant to the core of our thesis, they are important in the context of computing the topological indices of graphs for future reference. Some graph operations were introduced; at least one of them was used later. In Chapter 3, we introduce the computational technique that is used to checking the validity of some of our results: Lagrange interpolating polynomial. We present several different polynomial interpolating techniques along with basic examples for the reader. Later, in Chapter 4, we introduce the reader to the notion of the Wiener index. We give basic examples and derive the Wiener index of several graphs such as Path, Star, Cartesian product of two paths. Further, in this chapter, we presented a new class of trees called Palms and some generalizations of these trees. Their Wiener indices were computed through strategic counting and verified using Lagrange Interpolating. We produced unknown integer sequences. We close this thesis with Chapter 5 where we present several useful research directions and open problems.

Chapter 2 Topological Properties of Some Graphs

In this chapter, we present some basic graph properties, after we define them. We give seven such properties for seven common graphs on $n \geq 2$ vertices.

2.1 Basic Definitions

Suppose G is a simple graph and $v \in V(G)$. The distance between two vertices $u, v \in V(G)$, often denoted by $d_G(u, v)$, is the length (number of edges) of their shortest path in G; this is also known as a **geodesic distance**. Given v, the **eccentricity** of v, written as $\epsilon(v)$ is the maximum of the distance to any vertex in the graph, i.e., $\epsilon(v) = \max_{u \in V}\{d_G(v, u)\}$. Further, the **diameter, d** of a graph is the maximum eccentricity of any vertex in the graph. In other words, the diameter is the longest distance between any two vertices in the graph. So, $d = \max_{v \in V} \epsilon(v)$. The **radius, r** of a graph is the minimum eccentricity among all vertices in the graph in which case $r = \min_{v \in V} \epsilon(v)$. These parameters are very useful in classifying acyclic (tree-like) graphs. Figure 2.1 shows two trees with the same radius but different diameters.

Likewise, for cyclic graphs, we define the following: the length of its shortest cycle is its **girth, g,** while the length of its longest cycle is its **circumference** which we denote by c. Note that, if a graph G is acyclic, then $g(G) = c(G) = \infty$ and if G is disconnected then $r(G) = \infty$.

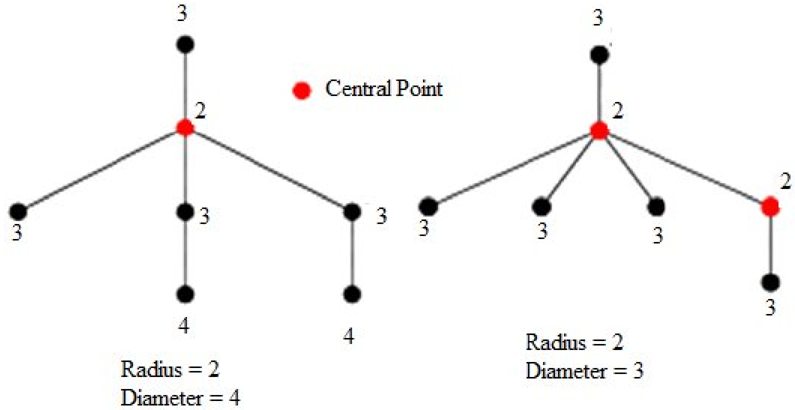


Figure 2.1: Diameters of two trees of radius 2

2.2 Topological Properties of Some Graphs

Here, we discuss nine different graphs, which come from well-known classes of graphs. For each graph, we present their seven (7) topological properties, after their definition. We list these properties as they obviously stem from the definition. Hence, no proof or additional statements is necessary.

2.2.1 Complete graphs

A **complete graph** also known as **cliques** on n vertices, denoted by K_n is a graph where every pair of vertices are adjacent. Below is a family of complete graphs, K_2, K_3, K_4, and K_5 (from left to right).

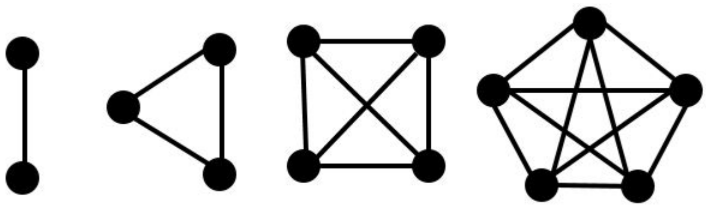


Figure 2.2: A family of four complete graphs

Topological Properties:

Given a complete graph on $n \geq 2$, we have

1. size (number of edges): $\binom{n}{2} = \frac{n(n-1)}{2}$, $n \geq 2$

2. δ (minimum degree): $n - 1$

3. Δ (maximum degree): $n-1$

4. r (radius): 1

5. d (diameter): 1

6. g (girth): 3

7. c (circumference): n

2.2.2 Cycles

A **cycle** on n vertices, denoted by C_n is a graph with exactly one closed path. Here is a C_5, a cycle on 5 vertices.

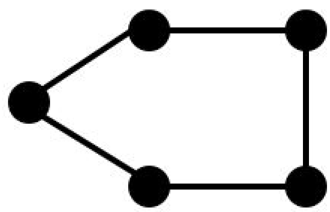


Figure 2.3: A Cycle on 5 vertices

Topological Properties:

For $n \geq 3$, we have

1. size (number of edges): n

2. δ (minimum degree): $n-1$

3. Δ (maximum degree): $n-1$

4. r (radius): $\lfloor \frac{n}{2} \rfloor$

5. d (diameter): $\lfloor \frac{n}{2} \rfloor$

6. g (girth): n

7. c (circumference): n

2.2.3 Trees

A **tree** also known as an **acyclic** graph on n vertices, denoted by T_n is a graph with no cycle. Figure 2.4 is an example of a tree on 6 vertices.

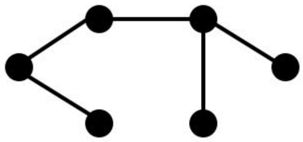


Figure 2.4: A tree on 6 vertices

Because trees are made of finitely many non-isomorphic members, we consider only one of its members: the stars. See Figure 2.5 as an example of a Star on 8 vertices. Thus, a star graph on n vertices is simply a central vertex that is connected to $n-1$ leaves.

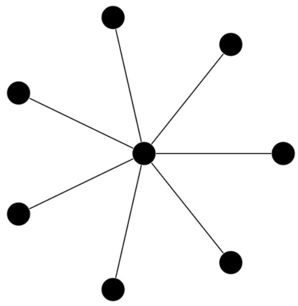


Figure 2.5: A Star on 8 vertices

Topological Properties:

Given a star graph on $n \geq 2$ vertices, we have

1. size (number of edges): $n-1$
2. δ (minimum degree): 1
3. Δ (maximum degree): $n-1$
4. r (radius): 2
5. d (diameter): 2
6. g (girth): ∞
7. c (circumference): ∞

2.2.4 2-trees

As a generalization of a tree, a *k-tree* is a graph that arises from a k-clique by 0 or more iterations of adding n new vertices, each joined to a k-clique in the old graph; This process generates finitely many non-isomorphic k-trees. $k \geq 2$ are shown to be useful in constructing reliable networks. [11] When $k = 2$, we consider a particular 2-tree is also known as a *Fan*. Figure 2.6 is an example of a Fan on 5 vertices.

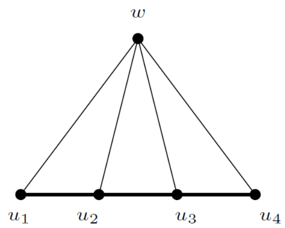


Figure 2.6: A Fan graph

Topological Properties:

Given a Fan on $n \geq 3$ vertices, we have

1. size (number of edges): $2(n-1) - 1 = 2n - 3$
2. δ (minimum degree): 2
3. Δ (maximum degree): $n - 1$
4. r (radius): 2
5. d (diameter): $n - 2$
6. g (girth): 3
7. c (circumference): n

2.2.5 Wheel

A Wheel on n vertices, denoted by W_n, is a cycle on $n - 1$ joined to a central vertex, say w, and every vertex of the cycle is connected to w. The vertex w is sometimes referred to as *hub*. Figure 2.7 is an example of a family of three Wheels.

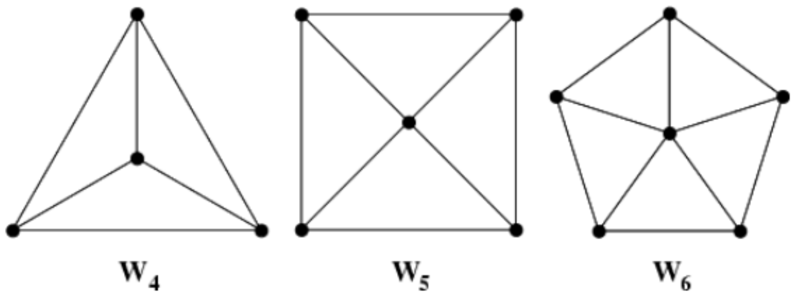


Figure 2.7: A family of three Wheels: W_4, W_5, W_6

Topological Properties:

Given a wheel on $n \geq 4$ vertices, we have

1. size (number of edges): $2(n-1)$
2. δ (minimum degree): 3
3. Δ (maximum degree): $n-1$
4. r (radius): 2
5. d (diameter): $\lfloor \frac{n}{2} \rfloor$
6. g (girth): 3
7. c (circumference): $n-1$

2.2.6 Barbell

The n-barbell graph is the simple graph obtained by connecting two copies of a complete graph K_n by a bridge. Figure 2.8 is an example of a 5-barbell on 10 vertices.

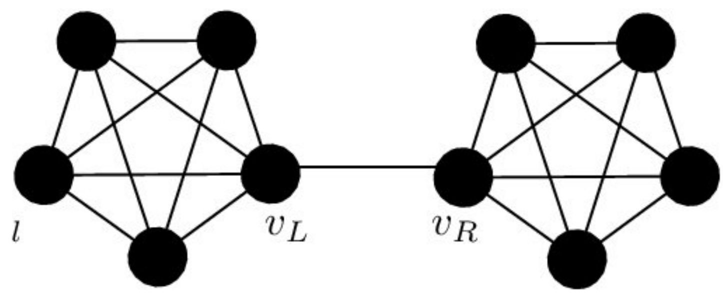


Figure 2.8: a 5-barbell

Topological Properties:

For $n \geq 2$, we have

1. size (number of edges): $2\binom{n}{2} + 1 = n(n-1) + 1$
2. δ (minimum degree): 1
3. Δ (maximum degree): $n - 1$
4. r (radius): 3
5. d (diameter): 3
6. g (girth): 3
7. c (circumference): n

2.2.7 Generalized Barbell

The (m, n)-barbell graph is a generalization of an n-barbell by connecting two complete graphs K_n and K_m by a bridge, for $m, g \geq 2$.

Topological Properties:

For $2 \leq n \leq m$, we have

1. size (number of edges): $\binom{n}{2} + \binom{m}{2}$
2. δ (minimum degree): 1
3. Δ (maximum degree): $n - 1$
4. r (radius): 3
5. d (diameter): 3
6. g (girth): 3
7. c (circumference): m

2.2.8 Complete bipartite graphs

A simple graph $G = (V, E)$ is called **bipartite** if its vertex set be divided into two disjoint groups, with edges connecting vertices from one group to the other; no edge connects vertices within the same group. We note that when each vertex from one group is connected to each vertex from the group, the resulting bipartite graph is said to **complete**; we write $K(m, n)$ where m, n, are the sizes of the two groups. Below is *complete bipartite* graph $K_{3,2}$ on $3 + 2 = 5$ vertices. We also note that $K(m, 1)$ is isomorphic a Star graph as discussed.

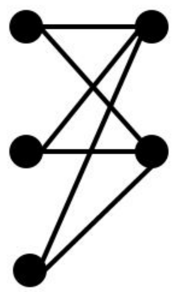


Figure 2.9: A complete bipartite graph with parts sizes 3 and 2

Topological Properties:

Given a complete bipartite graph $K(m, n)$ of order (number of vertices) $m + n$, with $1 \leq n \leq m$, we have

1. size (number of edges): mn

2. δ (minimum degree): n

3. Δ (maximum degree): m

4. r (radius): 1

5. d (diameter): 2

6. g (girth):

$$g = \begin{cases} \infty & n = 1, m \geq 2 \\ 4 & 2 \leq n \leq m \end{cases}$$

7. c (circumference):

$$c = \begin{cases} \infty & n = 1, m \geq 2 \\ n & 2 \leq n \leq m \end{cases}$$

2.2.9 Complete Multipartite graphs

A complete k-partite, $G = K(m_1, m_2, \ldots, m_k)$, is an extension of a complete bipartite with $k \geq 2$ disjoint parts, each of sizes $m_1, m_2, \ldots, m_k$. So, when $k = 2$, G is complete 2-partite also known as a complete bipartite graph and when $k = 3$, G is complete 3-partite also known as a complete tripartite. Figure 2.10 is a complete tripartite $K(5, 3, 2)$.

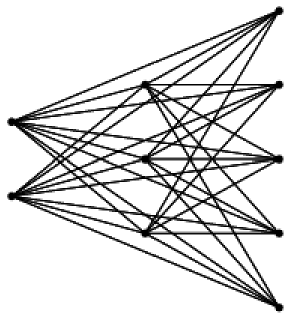


Figure 2.10: A complete 3-partite graph

Topological Properties:

For each $m_i \geq 1$, with $2 \leq i \leq k$, we have

1. size (number of edges): $\prod_{i=1}^{k} m_i$

2. δ (minimum degree): $\inf_i \{m_i\}$

3. Δ (maximum degree): $\sup_i \{m_i\}$

4. r (radius): 1

5. d (diameter): 1

6. g (girth):

$$g = \begin{cases} \infty & n = 1, m \geq 2 \\ 4 & 2 \leq n \leq m \end{cases}$$

7. c (circumference): varies

We think the last property (circumference) of complete multipartite graphs can simplified down to 3-4 cases, but it will require some proof which we are prepared to give in this thesis. For this reason, we leave it to the reader or future researchers to explore it. We close with some basic graph operations that the reader can find useful later.

2.2.10 Union of Graphs

Given two graphs G_1 and G_2, The union of G_1 and G_2 is the graph $G = G_1 \cup G_2$ i.e. the vertex set of G is the union of $V(G_1 \cup G_2) = V(G_1) \cup V(G_2)$; and the edge set is the union of E is $E(G_1 \cup G_2) = E(G_1) \cup E(G_2)$. An example in Figure 2.1 Union of Graphs, G_1 and G_2 is given.

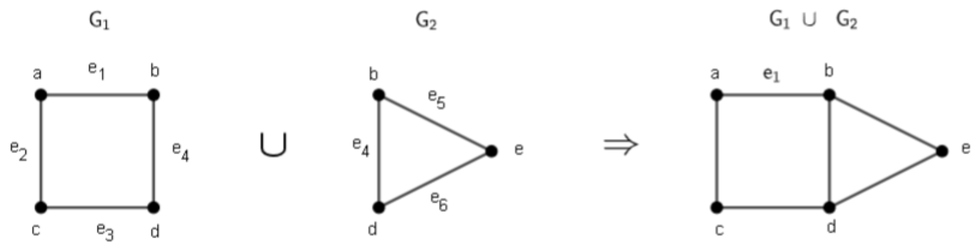


Figure 2.11: Union (∪) of Graphs

2.2.11 Intersection of Graphs

Given two graphs G_1 and G_2, The intersection of G_1 and G_2 is the graph $G = G_1 \cap G_2$ i.e. the vertex set of G is the union of $V(G_1 \cap G_2) = V(G_1) \cap V(G_2)$; and the edge set is the union of E is $E(G_1 \cap G_2) = E(G_1) \cap E(G_2)$. The vertex set of G has only those vertices present in both $V(G_1)$ and $V(G_2)$, and the edge set contains only those edges present in both $E(G_1)$ and $E(G_2)$ An example in Figure 2.2 Intersection of Graphs, G_1 and G_2 are given.

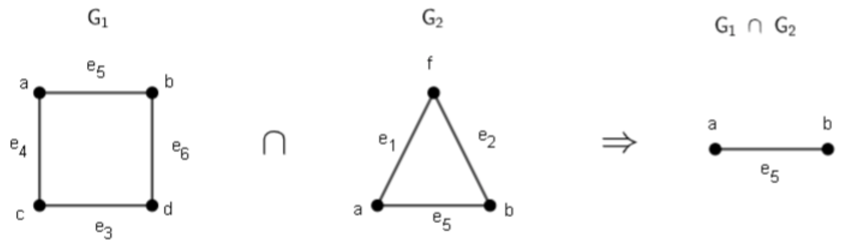


Figure 2.12: Intersection of Two Graphs

2.2.12 Join Graphs

Given two graphs G_1 and G_2, The **Join** of G_1 and G_2 is the graph $G = G_1 + G_2$. $V(G_1+G_2) = V(G_1)+V(G_2)$; and the edge set is the join of $E = E(G_1+G_2)$, where the edges, which are in G_1 and in G_2 edges obtained by joining each vertex of $V(G_1)$ with each vertex $V(G_2)$. An example in Figure 2.3 Join of Graphs, G_1 and G_2 is given

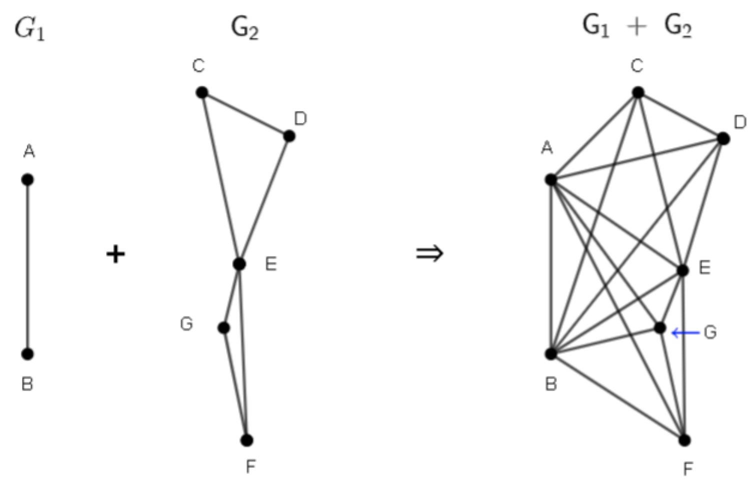


Figure 2.13: Join of Two Graphs

2.2.13 Ring Sum

Given two graphs G_1 and G_2, the **Ring Sum** of G_1 and G_2 is the graph $G = G_1 \oplus G_2$. $V(G)$ is equal to $V(G_1 \oplus G_2) = V(G_1) \cup V(G_2)$; and the edge set $E(G_1 \oplus G_2) = E(G_1) \cup E(G_2) - E(G_1) \cap E(G_2)$, edges, in G_1 or G_2, but not in both. An example in Figure 2.4 Ring Sum of Two Graphs, G_1 and G_2 is given.

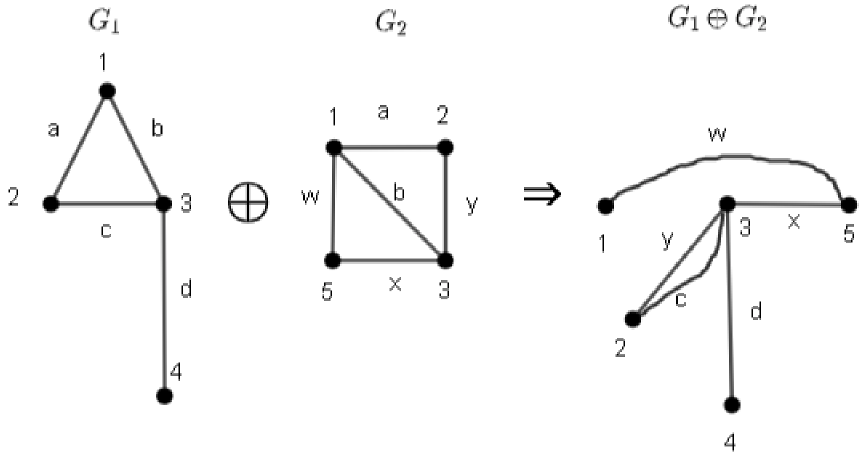


Figure 2.14: Ring Sum of Two Graphs

2.2.14 Cartesian Product

Given two graphs G_1 and G_2, the **Cartesian Product** of G_1 and G_2, denoted by $G_1 \times G_2$ is the set of all ordered pairs of $v(G_1), u(G_2)$ such that $v \in V(G_1)$ and $u \in V(G_2)$, $G_1 \times G_2 = \{\{(v,u)\}\,|v \in V(G_1), u \in V(G_2)\}$. in which vertices (u, v) and (u', v') are adjacent iff either

(1) $u = u'$ and v, v' are adjacent in G_1, or

(2) $v = v'$ and u, u' are adjacent in G_2

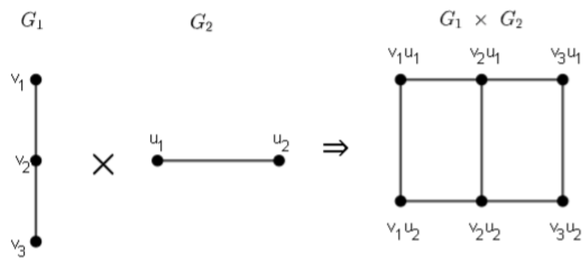


Figure 2.15: Cartesian Product of Two Graphs

2.3 Graph Complement

Given a graph G_1, the **Complement** of G_1, denoted by and $\overline{G}$ is a graph with the same vertex set, such that an edge $e(G_1)$ exists in G, but $e(G_1)$ does not exist in $\overline{G}$.

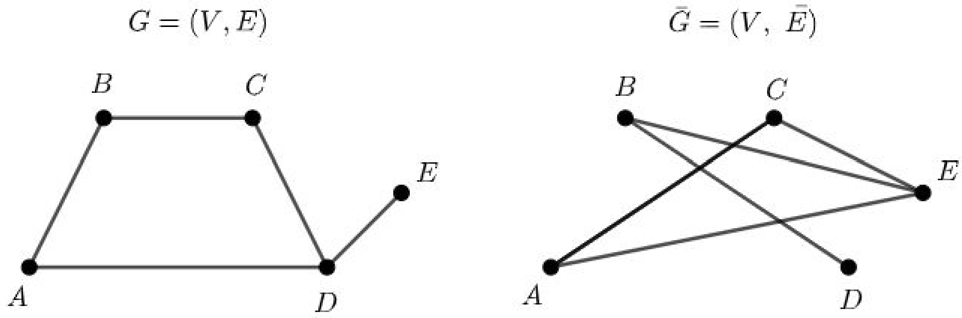


Figure 2.16: Complement of a Graph

Chapter 3 Methodology: Polynomial Interpolation

3.1 Polynomial Interpolations

Polynomial interpolation is the procedure of fitting a polynomial of degree n to a set of $n+1$ data points. For example, if we have two data points, then we can fit a polynomial of degree 1 (i.e., a linear function) between the two points. If we have three data points, then we can fit a polynomial of the second degree (a parabola) that passes through the three points.[1]

Polynomial interpolation relies on the fact that for every n+1 data points, there is a unique polynomial of degree n that passes through these n+1 data points. This fact relies on the Fundamental Theorem of Algebra that states that every degree n polynomial has exactly n roots. So, if two degree n polynomials p_1 and p_2 agree on $n+1$ points, then, their difference $z = p_1 - p_2$ is a polynomial of degree n but has $n+1$ roots which implies that $z = 0$.

To find the unique polynomial of degree n that passes through $n+1$ data points, we need to solve a linear set of $n+1$ equations with the coefficients of the polynomial being the unknowns. Let (x_i, y_i) be the i^{th} data point where $i \leq n+1$. Then, we have:

$$
\begin{aligned}
a_0 + a_1 x_1 + a_2 x_1^2 + \cdots + a_n x_1^n &= y_1 \\
a_0 + a_1 x_2 + a_2 x_2^2 + \cdots + a_n x_2^n &= y_2 \\
&\vdots \\
a_0 + a_1 x_{n+1} + a_2 x_{n+1}^2 + \cdots + a_n x_{n+1}^n &= y_{n+1}
\end{aligned}
$$

Which can be written as follows in matrix form:

$$\begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^n \\ 1 & x_3 & x_3^2 & \cdots & x_3^n \\ \vdots & \vdots & \vdots & \vdots & \\ 1 & x_{n+1} & x_{n+1}^2 & \cdots & x_{n+1}^n \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{n+1} \end{pmatrix}$$

The above system can be solved to find the values of the coefficients $a_0, a_1, a_2, \cdots, a_n$ which would ensure that the polynomial curve $y = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n$ passes through the $n+1$ data points[1].

Example 3.1.1. *Find an interpolating polynomial that would fit the data points* $(1, 1.1), (2, 2.1), (3, 5), (3.4, 7)$.

Solution

There are four data points, so, we can fit a third degree polynomial whose coefficients can be found by solving the following system of four linear equations:

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2^2 & 2^3 \\ 1 & 3 & 3^2 & 3^3 \\ 1 & 3.4 & 3.4^2 & 3.4^3 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 1.1 \\ 2.1 \\ 5 \\ 7 \end{pmatrix}$$

Solving the above system yields:

$$a_0 = 0.625 \qquad a_1 = 0.670833 \qquad a_2 = -0.425 \qquad a_3 = 0.229167$$

Therefore, the interpolating polynomial that would pass through all four data points is:

$$y = 0.625 + 0.670833x - 0.425x^2 + 0.229167x^3$$

It is important to note that Mathematica also has a built-in program "**InterpolatingPolynomial[Data,x]**" function that would automatically form and solve the above equation as shown below. Simply provide the data points as a list and Mathematica would produce the interpolating polynomial as a function of "x".

The following **Mathematica** code was used to solve the above equations and produce the plot below:

```
M = {{1, 1, 1, 1}, {1, 2, 4, 2^3}, {1, 3, 9, 27}, {1, 3.4, 3.4^2, 3.4^3}};
yv = {1.1, 2.1, 5, 7}
a = Inverse[M].yv
y = a[[1]] + a[[2]]*x + a[[3]]*x^2 + a[[4]]*x^3
Plot[y, {x, 0, 4}, Epilog -> {PointSize[Large],
Point[{{1, 1.1}, {2, 2.1}, {3, 5}, {3.4, 7}}]},
AxesLabel -> {"x", "y"}, ImageSize -> Medium, PlotLabel -> "y" == Expand[y]]
```

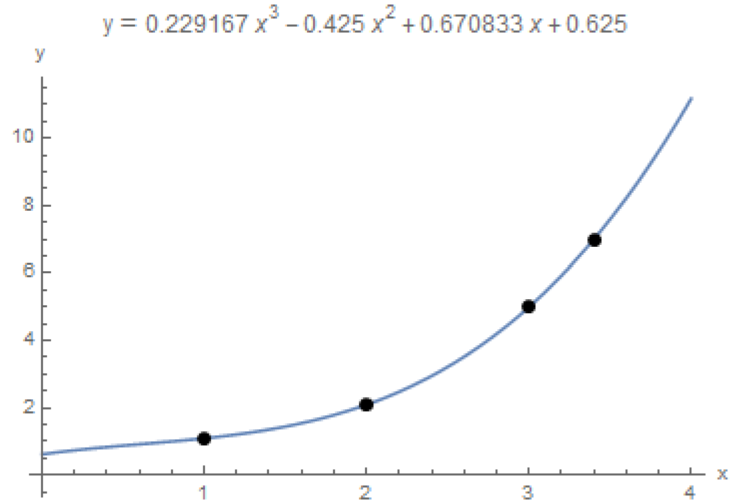


Figure 3.1: Polynomial Interpolation on four data points

Unfortunately, in general, the matrix formed in the previous Equation can be so difficult to solve and its inverse may not exist. A relatively simpler method can be used to find the interpolating polynomial using **Newton's Interpolating Polynomials** formula for fitting a polynomial of degree n through $n+1$ data points (x_i, y_i) with $1 \leq i \leq n+1$.

3.1.1 Newton Interpolating Polynomials

The **Newton polynomial** also known as **Newton's divided differences interpolation polynomial** is given by

$$f_n(x) = b_1 + b_2(x - x_1) + b_3(x - x_1)(x - x_2) + \cdots + b_{n+1}(x - x_1)(x - x_2) \cdots (x - x_n)$$

where the coefficients b_i are defined recursively using the "divided differences" as follows:

$$\begin{aligned}
b_1 &= y_1 \\
b_2 &= [y_1, y_2] = \frac{y_2 - y_1}{x_2 - x_1} \\
b_3 &= [y_1, y_2, y_3] = \frac{[y_2, y_3] - [y_1, y_2]}{x_3 - x_1} = \frac{\frac{y_3 - y_2}{x_3 - x_2} - \frac{y_2 - y_1}{x_2 - x_1}}{x_3 - x_1} \\
&\vdots \\
b_{n+1} &= [y_1, y_2, y_3, \cdots, y_{n+1}] = \frac{[y_2, y_3, \cdots, y_{n+1}] - [y_1, y_2, y_3, \cdots, y_n]}{x_{n+1} - x_1}
\end{aligned}$$

This formula for generating an interpolating polynomial is similar to that of a Taylor's polynomial but its coefficients $b_i's$ are computed using finite differences rather than the derivatives.

Example 3.1.2. *Using Newton's interpolating polynomials, find the interpolating polynomial to the data:* $(1, 1), (2, 5)$.

Solution We have two data points, so, we will create a polynomial of the first degree. Therefore:

$$b_1 = y_1 = 1 \qquad b_2 = \frac{5 - 1}{2 - 1} = 4$$

Therefore, the interpolating polynomial has the form:

$$y = 1 + 4(x - 1) = 1 + 4x - 4 = -3 + 4x$$

Example 3.1.3. *Using Newton's interpolating polynomials, find the interpolating polynomial to the data:* $(1, 1), (2, 5), (3, 2)$.

Solution We have three data points, so, we will create a polynomial of the second degree. Therefore:

$$b_1 = y_1 = 1 \qquad b_2 = \frac{5-1}{2-1} = 4 \qquad b_3 = \frac{\frac{2-5}{3-2} - \frac{5-1}{2-1}}{3-1} = -3.5$$

Therefore, the interpolating polynomial has the form:

$$y = 1 + 4(x-1) - 3.5(x-1)(x-2) = -3.5x^2 + 14.5x - 10$$

Unfortunately, we found no Mathematica code or procedure that would allow such computations to be carried out, so for practical purposes of this thesis, we opted for another similar method which is computationally feasible in Mathematica: Lagrange Interpolation. In fact, the Lagrange interpolating polynomials produce the same polynomial as the general method of the Newton's interpolating polynomials.

3.2 Lagrange Interpolating Polynomials

Lagrange Polynomials technique is another equivalent method to find the interpolating polynomials. Given $n+1$ data points: $(x_1, y_1), (x_2, y_2), \cdots, (x_{n+1}, y_{n+1})$, then the Lagrange polynomial of degree n that fits through the $n+1$ data points has the form:

$$f_n(x) = L_1 y_1 + L_2 y_2 + L_3 y_3 + \cdots + L_{n+1} y_{n+1} = \sum_{i=1}^{n+1} L_i y_i$$

where

$$L_i = \prod_{j=1, j \neq i}^{n+1} \frac{x - x_j}{x_i - x_j}$$

Example 3.2.1. *Using Lagrange interpolating polynomials, find the interpolating polynomial to the data:* $(1, 1), (2, 5)$.

Solution. We have two data points, so, we will create a polynomial of the first degree. Therefore, the interpolating polynomial has the form:

$$
\begin{aligned}
y = L_1 y_1 + L_2 y_2 &= \left(\frac{x - x_2}{x_1 - x_2}\right) y_1 + \left(\frac{x - x_1}{x_2 - x_1}\right) y_2 \\
&= \left(\frac{x-2}{1-2}\right) \times 1 + \left(\frac{x-1}{2-1}\right) \times 5 \\
&= 4x - 3
\end{aligned}
$$

Example 3.2.2. *Using Lagrange interpolating polynomials, find the interpolating polynomial to the data:* $(1,1),(2,5),(3,2)$.

Solution. We have three data points, so, we will create a polynomial of the second degree. Using Lagrange polynomials:

$$
\begin{aligned}
y &= L_1 y_1 + L_2 y_2 + L_3 y_3 \\
&= \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} y_1 + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} y_2 + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} y_3 \\
&= \frac{(x-2)(x-3)}{(1-2)(1-3)}(1) + \frac{(x-1)(x-3)}{(2-1)(2-3)}(5) + \frac{(x-1)(x-2)}{(3-1)(3-2)}(2) \\
&= -3.5x^2 + 14.5x - 10
\end{aligned}
$$

Example 3.2.3. *Using Lagrange polynomials, find the interpolating polynomial to the data:* $(1,1),(2,5),(3,2),(3.2,7),(3.9,4)$.

Solution. A fourth order polynomial would be needed to pass through five data points. Using Lagrange polynomials, the required function has the form:

$$
\begin{aligned}
y =& \frac{(x-x_2)(x-x_3)(x-x_4)(x-x_5)}{(x_1-x_2)(x_1-x_3)(x_1-x_4)(x_1-x_5)} y_1 + \frac{(x-x_1)(x-x_3)(x-x_4)(x-x_5)}{(x_2-x_1)(x_2-x_3)(x_2-x_4)(x_2-x_5)} y_2 \\
&+ \frac{(x-x_1)(x-x_2)(x-x_4)(x-x_5)}{(x_3-x_1)(x_3-x_2)(x_3-x_4)(x_3-x_5)} y_3 + \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_5)}{(x_4-x_1)(x_4-x_2)(x_4-x_3)(x_4-x_5)} y_4 \\
&+ \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(x_5-x_1)(x_5-x_2)(x_5-x_3)(x_5-x_4)} y_5 \\
=& -14.3461x^4 + 144.181x^3 - 509.935x^2 + 739.728x - 358.628
\end{aligned}
$$

The following **Mathematica** code was used to confirm the result:

```
Expand[InterpolatingPolynomial[{{1, 1}, {2, 5}, {3, 2}, {3.2, 7}, {3.9, 4}}, x]]
```

and we get the output function which is plotted in Figure 3.2

```
-358.628 + 739.728 x - 509.935 x^2 + 144.182 x^3 - 14.3461 x^4
```

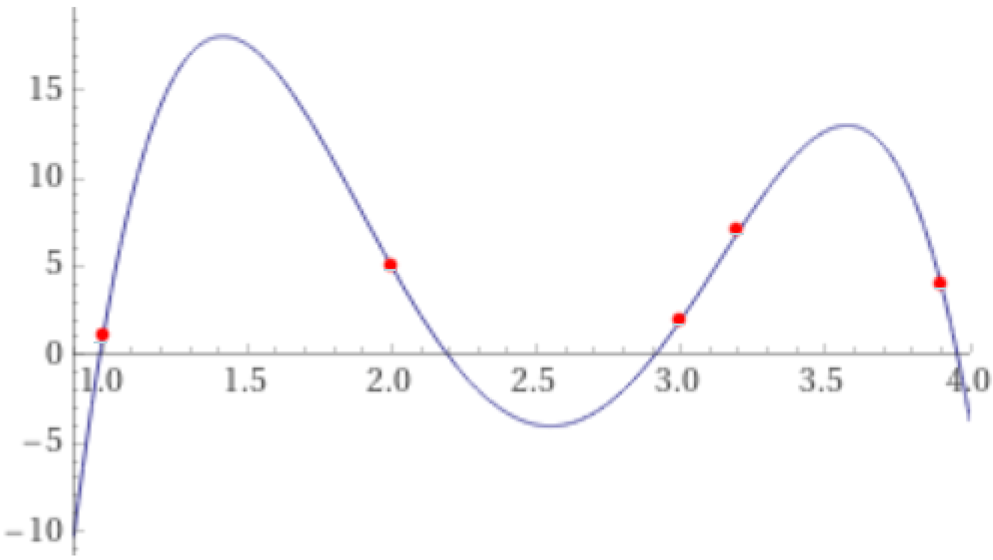


Figure 3.2: Lagrange Interpolating Polynomial on five data points

Chapter 4 Wiener Index of Some Graphs

4.1 Definitions and Background

Topological Indices, also known as the connectivity index, are best described as the invariants of a molecular graph which are used for structure-property or structure-activity correlations (Lokesha, 2020). These molecular graphs are correlated with chemical structures that have different appearances, physically, and are given a numerical value, topological index. The topological index describes the molecular structure in the fields of chemical graph theory, molecular topology and mathematical chemistry. The visualization of the structure of an atom was one of the most important discoveries in the world of Chemistry. The modern atomic theory is based on evidence that all atoms are made up of subatomic units called neutrons, protons, and electrons thereby creating matter. The periodic table lists each of the 118 elements, their chemical symbols, atomic weight, and masses. The final step of communicating the structure of the atom would involve a method for plotting integral snapshots of the complex particles orbiting in space. The way that we are able to plot this snapshot is through calculations of the numerical values based on the molecular structure descriptor (identifier). Just as in graph-theory, topological indices have similar definitions. We describe the structure by the number of vertices, or cardinality, and the degree by the number of edges connected to a vertex.

There are various types of topological indices in the many fields of science and math. Some common names are the Wiener Index (1947), also known as the Path Number, The Hosoya Index (1971) or the Index Z, the Randic Index (1975), or Connectivity Index, Branching Index or Product Connectivity Index, the Zagreb Index(1980), the Hyper-Wiener (1993), Estrada Index (2007) or Atom-bond Connectivity Index

(ABC), Narumi-Katayana Index, Szeged Index, Padmakar-Ivan Index and many others waiting to be discovered.

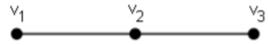
The Wiener topological index (W), introduced around 1947 by Harry Wiener, is the representation of data through a network of vertices (nodes) and edges (connections) which construct shapes to interpret patterns and relationship properties. It is one of the first of many graph theory indices introduced in chemistry and the most commonly used topological index (Knor, Skrekovski, & Tepeh, 2016). The original definition, as defined by Wiener, is "the path number W as the sum of the geodesics (short distances) between any two carbon atoms in the molecule (alkane), in terms of carbon bonds." In graph theory, we define a simple connected graph, G, with vertices, V and edges, E as $G = (V, E)$. For $u, v \in V$, the length of the shortest edge from u to v is represented as the distance, $d(u, v)$. The Wiener Index, $W(G)$, is the sum with respect to (u, v) of the subsets of G.

4.2 Examples of Computing the Wiener Index of a Path

Example 4.2.1. *Given a Path graph $G = P_n$, we determine its Wiener Index for various values of n.*

(1) Find the Wiener Index of $G = P_n$ when:

(a) $n = 3$ vertices, i.e., P_3



Answer: Since the Wiener Index of P_3 is the sum of the geodesics (short distances) between every pair of vertices of G, we compute such values: $d(v_1, v_2) = 1$. We continue to count the number of edges from v_1 to v_3, giving $d(v_1, v_3) = 2$. Further, we count the number of edges from v_2 to v_3, giving $d(v_2, v_3) = 1$. Together, we have

$$\begin{aligned} W(P_3) &= d(v_1, v_2) + d(v_1, v_3) + d(v_2, v_3) \\ &= 1 + 2 + 1 \\ &= 4 \end{aligned}$$

(b) $n = 4$ vertices, i.e., P_4

Answer: Since the Wiener Index of P_4 is the sum of the geodesics (short distances) between every pair of vertices of G, we compute such values: $d(v_1, v_2) = 1$. We continue to count the number of edges from v_1 to v_3, giving $d(v_1, v_3) = 2$, and v_1 to v_4, giving $d(v_1, v_4) = 3$. Since we have previously computed the $W(P_3)$ in (a), we can add the sum of the diameter of P_4 to the $W(P_3)$.Together, we have

$$\begin{aligned} W(P_4) &= d(v_1, v_2) + d(v_1, v_2) + d(v_1, v_3) + d(v_1, v_4) + W(P_3) \\ &= 1 + 2 + 3 + W(P_3) \\ &= 6 + 4 \\ &= 10 \end{aligned}$$

(2) In general, we have the following:

Path Graph with 1 vertex

$W(P_1) = 0$

Path Graph with 2 Vertices

$W(P_2) = 1$

Path Graph with 3 Vertices

$W(P_3) = 3 + 1 = 4$ *(or* $3 + W(P_2)$*)*

Path Graph with 4 Vertices

$W(P_4) = 6 + 3 + 1 = 10$ *(or* $6 + W(P_3)$*)*

Path Graph with 5 Vertices

$W(P_5) = 10 + 6 + 3 + 1 = 20$ *(or* $10 + W(P_4)$*)*

Number of Vertices, n	1	2	3	4	5
Wiener Index $W(P_n)$	0	1	4	10	20

Table 4.1: Wiener Index of a Path Graph, $W(P_n)$, $n \geq 1$

4.3 Wiener Index of a Path

We obtain from the table the following sequence of values $0, 1, 4, 10, 20, 35, 56, 84, \ldots$. This values correspond to the following series $n + (n-1) + (n-2) + \ldots + 3 + 2 + 1$ as we prove later. Using Lagrange Interpolation, we found that it corresponds to the function:

$$f(x) = \frac{x^3 - x}{6} = \frac{1}{6}x(x-1)(x+1)$$

as plotted below.

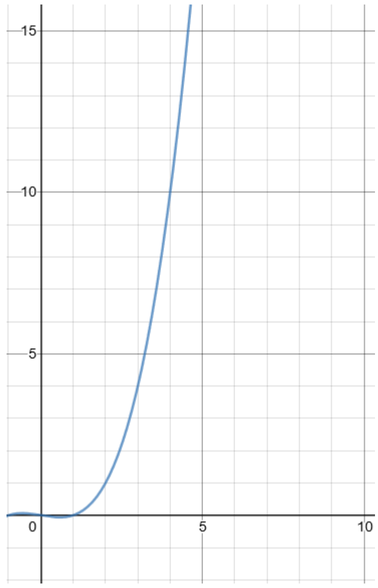


Figure 4.1: Plot of Wiener index of a path on $n > 1$ vertices

We found that, the sequence clearly includes another related number called **triangular number** By definition, a number T_n is called **triangular number** if it can be represented in the form of triangular grid of points such that the points form an equilateral triangle and each row contains as many points as the row number, i.e., the first row has one point, second row has two points, third row has three points and so on. The first four triangular numbers are 1, 3 (1+2), 6 (1+2+3), 10 (1+2+3+4), giving $\frac{n(n+1)}{2}$. It is important to note that these are the partial sums of the series $1+2+3+4+5+6+\ldots$, which are $1, 3, 6, 10, 15, \ldots$ and the n^{th} partial sum is the same formula. Here, we state some essential series that not only in the computation of Wiener numbers but also in string theory, quantum mechanics, and complex numbers.

(a) $\sum_{i=1}^{n} k = k + \ldots + k = kn$

(b) $\sum_{i=1}^{n} i = 1 + 2 + \ldots + n = \frac{n(n+1)}{2} = T_n$ (n^{th} triangular number)

(c) $\sum_{i=1}^{n} i^2 = 1^2 + 2^2 + \ldots + n^2 = \frac{n(n+1)(2n+1)}{6}$

(d) $\sum_{i=1}^{n} i^3 = 1^3 + 2^3 + \ldots + n^3 = \frac{n^2(n+1)^2}{4}$

(e) $\sum_{i=1}^{n}(a_i \pm b_i) = \sum_{i=1}^{n}(a_i) \pm \sum_{i=1}^{n}(b_i)$

Theorem 4.3.1. *The Wiener Index of a path of n vertices is given by* $W(P_n) = \binom{n+2}{3}$

Proof. Consider the **distance matrix**, presented in the form of Table 4.2. It is clear that $d(v_i, v_i) = 0$ and $d(v_i, v_j) = d(v_j, v_i)$, by symmetry. Thus, considering all distances between distinct pairs (v_i, v_j) gives the result from the table.

	v_1	v_2	v_3	v_4	$\dots$	v_n
v_1	0	1	2	3	$\dots$	$n-1$
v_2		0	1	2	$\vdots$	$n-2$
v_3			0	1		$n-3$
v_4				0	$\dots$	$n-4$
$\vdots$					$\ddots$	$\vdots$
v_n						0

Table 4.2: Distance Matrix of a Path on $n \geq 1$

Now, consider the sum of each row as shown in Table 4.3.

	v_1	v_2	v_3	v_4	$\dots$	v_n	T_n
v_1	0	1	2	3	$\dots$	$n-1$	$\frac{n(n-1)}{2}$
v_2		0	1	2	$\vdots$	$n-2$	$\frac{(n-1)(n-2)}{2}$
v_3			0	1		$n-3$	$\frac{(n-2)(n-3)}{2}$
v_4				0	$\dots$	$n-4$	$\frac{(n-3)(n-4)}{2}$
$\vdots$					$\ddots$	$\vdots$	$\vdots$
v_n						0	0

Table 4.3: Distance Matrix of a Path on $n \geq 1$ with i row sum, T_i, $1 \leq i \leq n$

It follows from the definition, that $W(P_n)$ is the value obtained by adding all entries of the matrix, in which case,

$$
\begin{aligned}
W(P_n) = \sum_{k=0}^{n-1} T_k = \sum_{k=1}^{n} T_k = \sum_{k=1}^{n} \frac{k(k+1)}{2} \\
&= \sum_{k=1}^{n}\left(\sum_{i=1}^{k} i\right) \\
&= \frac{n(n+1)(n+2)}{6} \\
&= \frac{n^{\overline{3}}}{3!} \\
&= \binom{n+2}{3},
\end{aligned}
$$

when written in a *binomial form*. □

Remark.

1. Observe that $x^{\overline{n}}$ is called the n^{th} **rising factorial** and it is equivalent to $x^{\overline{n}} = x(x+1)(x+2)\cdots(x+n-1) = \prod_{k=1}^{n}(x+k-1) = \prod_{k=0}^{n-1}(x+k)$.

   Further, the n^{th} **tetrahedral number**, Te_n commonly known as the sum of the first n triangular numbers is also given by $Te_n = \frac{n^{\overline{3}}}{3!}$. Very recently (Jan 2021) Enrique Navarrete has suggested that Te_n also corresponds to the number of binary strings of length $n+2$ with exactly three $0's$.

2. We note that while using the Interpolating polynomials, we have $W(P_x) := f(x) = \dfrac{x^3 - x}{6} = \dfrac{1}{6}x(x-1)(x+1)$ and yet, using enumeration (counting) as previously described we obtain $W(P_n) := g(n) = \dfrac{n(n+1)(n+2)}{6}$. Clearly setting $x = n+1$ in $f(x)$ gives $g(n)$; one is simply a horizontal shift of the other, as shown in Figure 4.2.

For the rest of the thesis, we rely primarily on enumeration while using Lagrange interpolation to support our results, whenever possible.

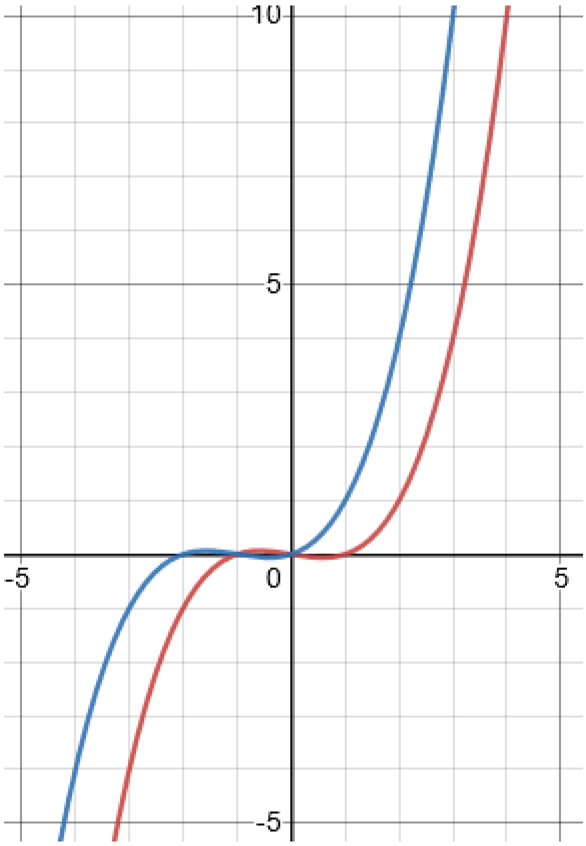


Figure 4.2: Plot of Wiener index of a path P_x using Lagrange interpolation (Red) and Enumeration (Blue)

4.3.1 Wiener Index of the Cartesian product of two paths

We repeatedly determine the Wiener Index of the graph as we increase the value of $n \geq 0$, we generate the sequence $0, 8, 72, 320, 1000, 2520, 5488, \ldots$. Using Lagrange Interpolation, we found that it corresponds to the function:

$$f(x) = \frac{x^5 - x^3}{3} = \frac{1}{3}x^3(x-1)(x+1)$$

as plotted below.

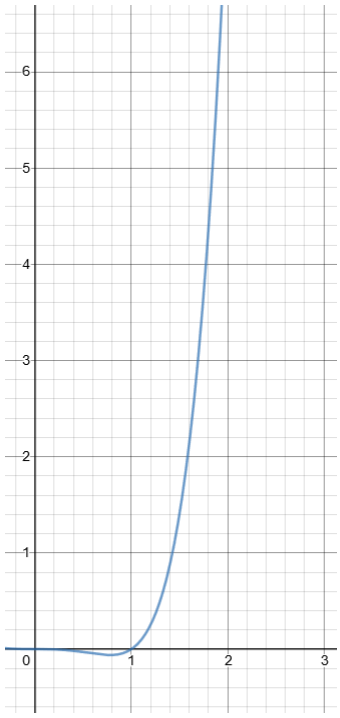


Figure 4.3: Plot of Wiener index of a $P_n \times P_n$ on $n > 1$ vertices

Using the result from Lagrange Interpolation, we conclude that

$$W(P_n \times P_n) = \frac{1}{3}n^3(n-1)(n+1)$$

for all $n \geq 2$.

We note that the results from Lagrange Interpolations only give estimates of the Wiener Index of these graphs, and yet, these estimates are exactly the same as computing or counting the Wiener Index. For the upcoming results, we focus more on the counting arguments to generate the formulae.

4.4 Wiener Index of a Star

We repeatedly determine the Wiener Index of the graph as we increase the value of $n \geq 0$, giving sequence whose values are $0, 1, 4, 9, 16, 25, 36, 49, 64, \ldots$. Here, it is very clear that by a simple inspection that the sequence is

$$f(x) = x^2$$

as plotted below.

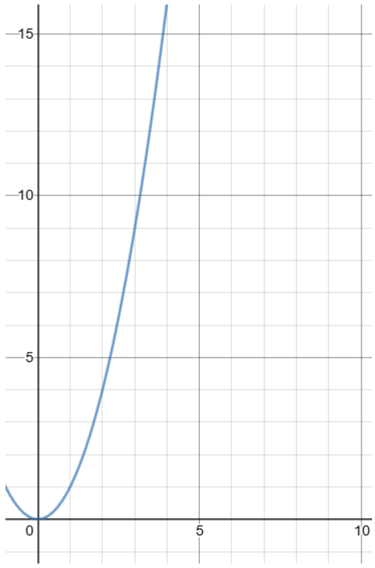


Figure 4.4: Plot of Wiener index of a Star on $n \geq 1$ vertices

Using the result from Lagrange Interpolation, we conclude that

$$W(S_n) = (n-1)^2$$

for all $n \geq 2$, although we provide a more formal proof later in Corollary 4.5.3.

4.5 Wiener Index of Palm Leaf graphs

Here, we introduce a new family of graphs called **Palm Tree**. Suppose $P_n := v_1 - v_2 - \ldots - v_{n-1} - v_n$, denotes a path on $n \geq 3$ vertices. By sequentially adding some pendant vertices to some v_i, $2 \leq i \leq n-1$, we obtain a **Palm Leaf**. A **Palm tree** is naturally defined as a Path with Palm leaves (making it a general tree). It is obvious that there are infinitely many such non-isomorphic trees. For the purpose of this thesis, we focus on some special family members. A Palm Leaf graph, obtained by adding $k \geq 1$ pendant vertices to $v_2 \in P_n$ is often called a **Broom**. We denote it as B_n^k. The special case when $k = 1$ is called a **Sling** (see Figure 4.4) and the resulting graph when $k = 2$ is called **Tridon**. (see Figure 4.5)

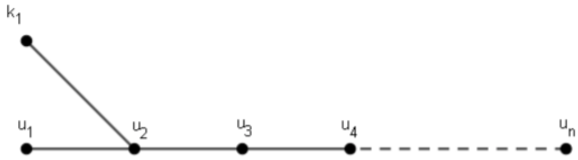


Figure 4.5: Palm Leaf Graph Special Case - Sling

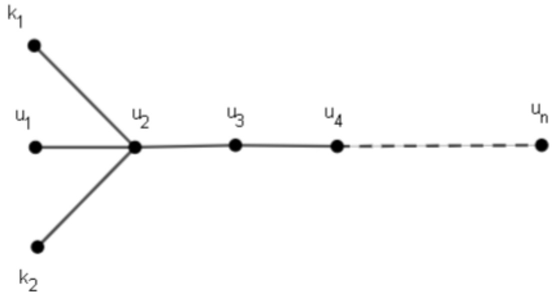


Figure 4.6: Palm Leaf Graph Special Case - Tridon

We note that a Broom obtained from P_n by adding $k \geq 2$ vertices to v_1 or v_{n-1} is isomorphic to a Broom obtained from P_{n-1} by adding $k-1 \geq 1$ vertices to v_2 or v_{n-2}. (see Figure 4.6) This is the main reason we choose to add the pendant vertices to the $v_i' s$ with $2 \leq i \leq n-1$.

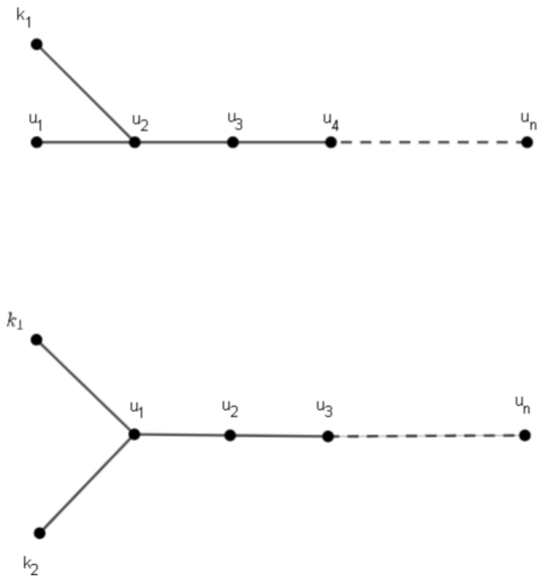


Figure 4.7: Isomorphic Brooms

Theorem 4.5.1. *Suppose B_n^k denotes a Broom on $n+k$ vertices. Then $W(B_n^k) = 2T_k + kT_{n-1} + W(P_n)$ for all $n \geq 3$, $k \geq 1$.*

Proof. Let T_n denote the n^{th} triangular number and u_i, $i = 1\dots, k$, the pendant vertices. Consider the P_n, $n \geq 3$, giving $W(P_n)$. With each additional pendant vertex, u_i connected to $v_2 \in P_n$, we have $d(u_i, v) = T_{n-1}$, for each $v \in P_n$ and $v \neq v_1$. This gives $\sum_{j=1}^{k} T_{n-1}$ for each u_i, $i = 1, \dots, k$. Finally $d(u_i, v_1) = 2 = d(u_i, u_j)$ with $i \neq j$, giving $\sum_{j=1}^{k} 2j$. Together, we have

$$\begin{aligned} W(B_n^k) &= \sum_{j=1}^{k} 2j + \sum_{j=1}^{k} T_{n-1} + W(P_n) \\ &= 2\sum_{j=1}^{k} j + \sum_{j=1}^{k} T_{n-1} + W(P_n) \\ &= 2T_k + kT_{n-1} + W(P_n), \end{aligned}$$

giving the result. □

It is very tempting to consider this alternative proof: Observe that the k pendant vertices joined to v_2 together with v_1 form a Star on $k+2$ vertices and $W(S_{k+2})$ is its Wiener value. Further, the Wiener of each $(k+1)$ path, P_n', with a starting or pendant vertex u_i or v_1 is $W(P_n') = W(P_n)$. Now, it is clear that we have double counted $d(u_i, v_2) = 1$, for each $i = 1, \dots k$, and $d(v_1, v_2) = 1$ as part of $W(S_{k+2})$ and $W(P_n)$. Hence we have

$$W(B_n^k) = W(S_{k+1}) + \sum_{j=1}^{k+1} W(P_n) - (k+1)$$

The problem is this argument is that, each $W(P_n)$, after the first count, repeats for all vertices from v_i, $i \geq 2$.

Corollary 4.5.1. *Suppose B_n^1 denotes a Sling graph on $n \geq 4$ vertices. Then,* $W(B_n^1) = \dfrac{n^3}{6} + n^2 - \dfrac{n}{6} + 2$

Proof. By definition, a Sling is a Broom on $k = 1$ pendant vertex. So, when $k = 1$, the result in Theorem 4.5.2 becomes

$$\begin{aligned} W(B_n^1) &= 2T_1 + T_{n-1} + W(P_n) \\ &= 2 + \frac{(n-1)n}{2} + W(P_n) \\ &= 2 + \frac{n(n-1)}{2} + \frac{n(n+1)(n+2)}{6} \\ &= \frac{n^3}{6} + n^2 - \frac{n}{6} + 2. \end{aligned}$$

□

n	4	5	6	7	8	9	10	11	12	13
$\frac{n^3}{6} + n^2 - \frac{n}{6} + 2$	28	47	73	107	150	203	267	343	432	535

Table 4.4: The first ten values of Wiener of a Sling graph on $n \geq 4$

In Table 4.6, we compute the first ten values of such function. We found that there is no such sequence in the On-Line Encyclopedia of Integer Sequences (OEIS) databank, and we hope to submit this formula, for their record. Further, using the first 10 ordered pair we derive a similar function from a Lagrange Interpolation.

```
Expand[InterpolatingPolynomial[{{4, 28}, {5, 47}, {6, 73}, {7, 107},
{8, 150}, {9, 203}, {10, 267}, {11, 343}, {12, 432}, {13, 535}}, x]]
```

Corollary 4.5.2. *Suppose B_n^2 denotes a Tridon graph on $n \geq 5$ vertices. Then,* $W(B_n^2) = \frac{n^3}{6} + \frac{3n^2}{2} - \frac{2n}{3} + 6$

Proof. By definition we obtain the Wiener value of a Tridon on $n \geq 5$ from Theorem 4.5.2, when $k = 2$. In which we have

$$\begin{aligned} W(B_n^2) &= 2T_2 + 2T_{n-1} + W(P_n) \\ &= 6 + 2\frac{(n-1)n}{2} + W(P_n) \\ &= 6 + n(n-1) + \frac{n(n+1)(n+2)}{6} \\ &= \frac{n^3}{6} + \frac{3n^2}{2} - \frac{2n}{3} + 6 \end{aligned}$$

after an expansion. $\square$

Once again, we found that there is no such sequence in the On-Line Encyclopedia of Integer Sequences (OEIS) databank, and we hope to submit this formula, for their record.

Corollary 4.5.3. *Suppose S_n denotes a Star graph on $n \geq 2$ vertices. Then, $W(S_n) = (n-1)^2$*

Proof. Without loss, we assume $n \geq 3$ and consider Theorem 4.5.2. It follows that when $n = 3$, it is clear that, a Broom B_3^k is isomorphic to S_{k+3}. Thus, it suffices to prove that $W(B_3^k) = (k+2)^2$, to establish the result for all $n \geq 2$. In which case, we have

$$
\begin{aligned}
W(B_3^k) &= 2T_k + kT_2 + W(P_3) \\
&= 2T_k + k(3) + 4,
\end{aligned}
$$

since $T_2 = 3$ and $W(P_3) = 4$. Further, since $T_k = \dfrac{k(k+1)}{2}$, we have

$$
\begin{aligned}
W(B_3^k) &= 2\frac{k(k+1)}{2} + 3k + 4 \\
&= k(k+1) + 3k + 4 \\
&= k^2 + 4k + 4 \\
&= (k+2)^2.
\end{aligned}
$$

$\square$

4.5.1 Wiener Index of Comb graph

Given a path, say, P_n, instead of adding several pendant vertices to say, $v_2 \in P_n$, here we are adding n pendant vertices, one to each vertex $v \in P_n$. The resulting graph is called a Comb. Below is a Figure

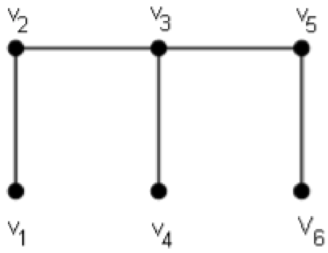


Figure 4.8: Comb Graph with 3 pendant vertices

Theorem 4.5.2. *Suppose G denotes a Comb on $n \geq 4$ vertices. Then* $W(G) = \dfrac{n(2n^2+6n-5)}{3}$ *for all $n \geq 4$.*

Proof. Let P_n be the graph to which vertices, we are adding k pendant vertices. It is clear that the size of G is $n + k = 2n$ and when $n = 2$ G is isomorphic to P_4, and $W(G) = 10$. For $n \geq 2$, each additional path brings in two new vertices, say u_1 and u_2 where u_1 is a leaf. Then, we count the distance from each of these vertices to any vertex $v \in G'$ where $G = G' \cup \{u_1, u_2\}$. It follows that we obtain, recursively

$$\begin{aligned}
W(G) &= 10 + \sum_{k=1}^{n-2} (9 + 4(T_{k+2} - 3)) \\
&= 10 + \sum_{k=1}^{n-2} (4T_{k+2} - 3) \\
&= 10 + \sum_{k=1}^{n-2} (4T_{k+2}) - 3(n-2) \\
&= 10 + 4\sum_{k=1}^{n-2} \left(\frac{(k+2)(k+3)}{2}\right) - 3(n-2) \\
&= 2\sum_{k=1}^{n-2}(k+2)(k+3) - 3n + 16
\end{aligned}$$

□

4.6 Wiener Index of Generalized Palms

We extend the results concerning Palm leaves to a family of graphs called **Generalized Palm Tree**. Suppose $P_n := v_1 - v_2 - \ldots - v_{n-1} - v_n$, denotes a path on $n \geq 3$ vertices. By sequentially adding some path graph P'_m, on $m \geq 1$ vertices to some v_i,

$2 \le i \le n-1$, we obtain a *generalized Palm Leaf*. Once again, there are infinitely many such non-isomorphic trees. Here, we discuss two special families. A generalized palm tree that is obtained by connecting sequentially $k \ge 1$ paths, P_2's, to $v_2 \in P_n$ will be referred to as **Level 2 generalized Palm Leaf**. The case where we connect sequentially $k \ge 1$ paths, P_2's, to $v_3 \in P_n$ will be referred to as **Level 3 generalized Palm Leaf**. Clearly, a Level 1 generalization only extends the path, as it remains a path. We note that symmetry in levels along P_n will produce isomorphic graphs.

4.6.1 Generalized Level 2 Wiener Index of Palms

Let G^k denotes a Level 2 generalized path leaf, obtained by adding $k \ge 1$ 2-paths, $P'_k := u_{1k} - u_{2k}$, for $k \ge 1$ to v_2. When $k = 2$, is shown in Figure 4.9

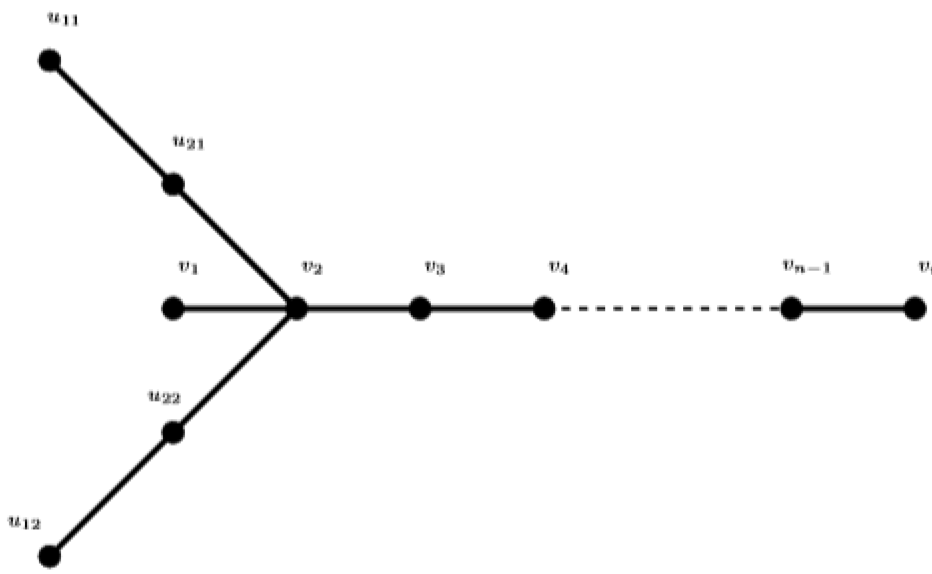


Figure 4.9: Level 2 Wiener Index of Palm

Theorem 4.6.1. *The Wiener Index of a generalized Palm Tree G^k is given by* $W(G^k) = \dfrac{n(n+1)(n+2)}{6} + kn^2 + \dfrac{5}{2}k(k+1) + 7k - 7$ *with $n \ge 3$ and $k \ge 1$*

Proof. It is clear that Wiener index of the path $P_n := v_1 - v_2 \ldots - v_n$ is $W(P_n) = \frac{1}{6}n(n+1)(n+2)$. Now, it suffices to add the values of $d(u_{1k}, v)$ and $d(u_{2k}, v)$, for each $v \in P_n$ and $k \ge 1$.

Observe that $\sum_{x_k} d(u_{1k}, x_k) = T_n$ and $\sum_{y} d(u_{2k}, y) = T_{n-1}$ for every $x_k \in \{u_{2k}, v_2, v_3, \ldots, v_n\}$ and $y \in \{v_2, v_3, \ldots, v_n\}$. Further, $d(u_{1k}, v_1) = 3$ and

$d(u_{2k}, v_1) = 2$.

Thus, when $k = 1$, we have

$$W(G^1) = W(P_n) + \sum_{x_1} d(u_{11}, x_1) + \sum_{y} d(u_{21}, y) + d(u_{11}, v_1) + d(u_{21}, v_1)$$

$$= W(P_n) + T_n + T_{n-1} + 2(1) + 3(1)$$

When $k = 2$. We have $d(u_{12}, v_1) = 3 = d(u_{12}, u_{21})$, $d(u_{22}, v_1) = 2 = d(u_{22}, u_{21})$, and $d(u_{12}, u_{11}) = 4$, $d(u_{22}, u_{11}) = 3$. Together, with $\sum_{x_2} d(u_{12}, x_2) + \sum_{y} d(u_{22}, y)$ for every $x_2 \in \{u_{22}, v_2, v_3, \ldots, v_n\}$ and $y \in \{v_2, v_3, \ldots, v_n\}$, we have

$$W(G^2) = W(G^1) + \sum_{x_2} d(u_{12}, x_2) + \sum_{y} d(u_{22}, y) + 2(2) + 2(3) + 1(3 + 4)$$

Similarly, when $k = 3$, we obtain

$$W(G^3) = W(G^1) + W(G^2) + \sum_{x_3} d(u_{13}, x_3) + \sum_{y} d(u_{23}, y) + 2(3) + 3(3) + 2(3 + 4)$$

Thus, for all $k \geq 1$, we obtain recursively that,

$$W(G^k) = \sum_{i=1}^{k-1} W(G^i) + \sum_{x_k} d(u_{1k}, x_k) + \sum_{y} d(u_{2k}, y) + 2\left(\sum_{i=1}^{k} i\right) + 3\left(\sum_{i=1}^{k} i\right)$$
$$+(3 + 4)\left(\sum_{i=1}^{k-1} i\right)$$

$$= W(P_n) + kT_n + kT_{n-1} + 2T_k + 3T_k + 7(k - 1)$$

$$= W(P_n) + k(T_n + T_{n-1}) + 5T_k + 7(k - 1)$$

$$= \frac{n(n + 1)(n + 2)}{6} + 2kT_{n-1} + kn + 5T_k + 7(k - 1),$$

Because $W(P_n) = \dfrac{n(n + 1)(n + 2)}{6}$ and $T_n + T_{n-1} = 2T_{n-1} + n = n^2$, with $T_r = \dfrac{r(r + 1)}{2}$, we obtain that

$$W(G^k) = \frac{n(n + 1)(n + 2)}{6} + kn^2 + \frac{5}{2}k(k + 1) + 7k - 7, k \geq 1.$$

□

In the next two Corollaries, we present two special cases; the case case when $k = n$ in which case we connect exactly $n \geq 3$ 2-paths to $v_2 \in P_n$, the main path and the case when $k = 1$ in which case we connect exactly one 2-path to $v_2 \in P_n$. Both cases follow directly from the previous theorem, after an expansion.

Corollary 4.6.1. *The Wiener Index of a generalized Palm Tree G^n is given by $W(G^n) = \frac{7}{6}n^3 + 3n^2 + \frac{59}{6}n - 7$ with $n \geq 3$ and $k \geq 1$.*

Here are some of the values of G^n:

n	3	4	5	6	7	8	9	10	11	12
$\frac{n^3}{6} + \frac{3n^2}{2} - \frac{2n}{3} + 2$	81	155	263	412	609	861	1175	1558	2017	2559

Table 4.5: The first ten values of Level 2 generalized Wiener Palm Tree with $n \geq 3$ 2-Paths

Corollary 4.6.2. *The Wiener Index of a generalized Palm Tree G^1 is given by $W(G^1) = \frac{1}{6}n^3 + \frac{3}{2}n^2 + \frac{1}{3}n + 5$ with $n \geq 3$.*

Here are some of the values of G^1:

n	3	4	5	6	7	8	9	10	11	12
$\frac{1}{6}n^3 + \frac{3}{2}n^2 + \frac{1}{3}n + 5$	24	41	65	97	138	189	251	325	412	629

Table 4.6: The first ten values of Level 2 generalized Wiener Palm Tree with one 2-Path

Chapter 5 Conclusion and Future Research

In this research, we visit an important graph topological index, Wiener Index (Harold Wiener 1947), as we attempt to classify several non-isomorphic trees. The results obtained are established using both Lagrange Interpolating polynomials (with at least 10 data points) and rigorous counting techniques. These results produce several sequences some of which are known, others are new and have not yet appeared in the On-Line Encyclopedia of Integer Sequences (OEIS) databank. For instance, there is no record of the integer sequence produced by the Wiener Index of a Sling or Tridon, two newly defined graphs that we introduced. We plan to submit these results. Moreover, we introduced a new class of trees, known as Palms, along with some variants of their generalizations on two levels. The results of one of the levels (Level 2-generalization) is presented. Our work can easily be extended to Level 3 or higher in future research. Further, the results can serve as a model for computing other graph topological indices such as Hosoya Index (Haruo Hosoya 1971) Zagreb Index and Randić Index.

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