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Wiener Index and It's Applications

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The undesigned here by certify that they have read and recommended to the College of Natural and Computational Sciences for acceptance of a project entitled **the Wiener Index and it's applications** by **Etaferahu Fekede** in partial fulfillment of the requirement for degree of master of science in mathematics.

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Abstract

The Wiener Index of a graph G is equal to the sum of distances between all pairs of vertices of G. It is known that the Wiener Index of a molecular graph correlates with certain physical and chemical properties of a molecule. In the mathematical literature, many good algorithms can be found to compute the distances in the graph, and these can easily be adapted for the calculation of the Wiener Index. An algorithm that calculates the Wiener Index of a tree in Linear Time is given. And also another algorithm that calculates Wiener Index for an arbitrary graph is given. Moreover, the application of Wiener Index is discussed.

Contents

Chapter 1

Introduction

The study of various molecular-graph based structure descriptors, so called ”topological indices”, has been undergoing rapid expansion in the last few years, without question, the wiener index is one of the best known and most examined among them [5].
Topological indices are numerical descriptors that are derived from molecular graphs of chemical compounds. Such indices based on the distances in a graph are widely used for establishing relationships between the structure of molecules and their physico-chemical properties. Chemical and other features of molecules can be modelled using topological indices [5].
The wiener index is a well-known distance-based topological index introduced originally for molecular graphs of alkanes. In 1947, chemist Harold Wiener introduced the Wiener index of a graph $G = (V, E)$, which is represented by $W(G)$. A number of books and reviews in the chemical and mathematical literature are devoted to the wiener index. In particular, the wiener index was used in the analysis of physico-chemical properties of benzenoid hydrocarbons. Various methods for calculation of wiener index were also put forward. In this project only simple connected graphs are considered. The vast majority of Wiener index investigations have a focus in one or more of the following directions:
(a) Computation of the Wiener index: This comprises determining W(G) or μ(G) algorithmically and getting closed-form equations for various graph classes of G.
(b) Relationship to other graph parameters
(c) Upper/lower bounds and asymptotes
(d) Characterization of extremal structures: Using one or more graph parameters, such as order and size, one can determine extremal graphs with the maximum and minimum possible W(G).
(e) Inverse Wiener index problem: The inverse problem is: does there exist

a graph G with $W(G) = n$ for a given integer n?

Some of the studies on wiener index and average distance are briefly summarized below. In this project, chapter two contains some preliminaries, in chapter three we will discuss about wiener index and it's relation with some topological indices, chapter four is about techniques of computing wiener index and the last chapter, chapter five, is about applications of wiener index. finally there is a summary.

Chapter 2

Preliminary

Definition 1. *Graph is a mathematical representation of a network and it describes the relationship between edges and vertices. A graph is made up of vertices with edges connecting them. It makes no difference how long the edges are or where the vertices are placed. A node is the name given to each object in a graph.*

Definition 2. *Path is a sequence of vertices with the property that each vertex in the sequence is adjacent to the vertex next to it.*

Definition 3. *A connected graph is a graph in which every pair of vertex has a path connecting them.*

Definition 4. *No loops or duplicate edges exist in a simple connected graph.*

Definition 5. *A tree is a graph G that is a connected and acyclic (contains no cycles).*

Definition 6. *let G be a simple connected graph with vertex set V(G) & edge set E(G).* $deg_G(v)$ *or deg(v), which is the degree of a vertex v in G, is the number of edges incident to v & the neighbourhoods of v, denoted by* $N_G(v)$*, is the set of vertices adjacent to v. Moreover if u,v*$\in$ *V(G) & uv* $\in$ *E(G), then we write* $u \sim v$*. Length of a path is just its number of edges.*

Definition 7. *Given a graph G, its line graph* $L(G)$ *is a graph such that:*
i. each vertex of $L(G)$ *represents an edge of G; and*
ii. two vertices of $L(G)$ *are adjacent if and only if their corresponding edges have a common end point in G.*

d_G(u,v) or d(u,v) denotes the distance between the vertices u & v of G which is defined as the length of a shortest path between u & v in G [5].
If edges in the graph have weights then the graph is said to be a weighted graph, if the edges do not have weights, the graph is said to be unweighted. A weight is a numerical value attached to each individual edge. In an unweighted graph the existence of a relationship is the subject of our interest.

A distance matrix is a square matrix(two-dimensional array) containing the distances, taken pairwise, between the elements of a set.

Chapter 3

Wiener index and its properties

Consider a simple and connected graph G which has a vertex set V(G) and an edge set E(G).

Definition 8. *The Wiener index W(G) is defined as the sum of distances between all pairs of vertices of a graph G [4]. In other way, wiener index is defined as half-sum of the elements of the distance matrix.*

$$W(G) = \sum_{\{u,v\} \subseteq V} d(u,v) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d_G(u,v) \tag{3.1}$$

where u and v are arbitrary vertices of G

Wiener index is also called Wiener number [7].
Given a vertex u ∈ V(G), we define $d^+(u,G)$ as

$$d^+(u,G) = \sum_{x \in V(G)} d(u,x) \tag{3.2}$$

This implies that

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} d^+(u,G)$$

Equation (3.1) can be shown to be equivalent to the expression for $W(T)$, if G≅ T, given by

$$W(T) = \sum_{e \in E(T)} n_1(e) n_2(e) \tag{3.3}$$

where, if $e = xy$ (x,y ∈ V(T)) then $n_1(e) = |s_1| \ \& \ n_2(e) = |s_2|$
where,$s_1 = \{w/w \in V(T) \ \& \ d_T(w,x) < d_T(w,y)\} \ \&$
$s_2 = \{w/w \in V(T) \ \& \ d_T(w,y) < d_T(w,x)\}$
Stated differently $n_1(e)n_2(e) = P(e)$, call, is the product of the orders of the two components of $T \setminus xy$. Also we can call $P(e)$ the path number of the edge e[8].
$W(G)$ is also known as transmission, total status & sum of all distances

[6][8]. A quantity related to $W(G)$ is the mean distance or the average distance μ(G) defined by

$$\mu(G) = \frac{W(G)}{\binom{|V(G)|}{2}}$$

Among all graphs of a given order n, the wiener index is the maximum for the path P_n and it is minimum for the complete graph K_n. That is, for any graph G_n (different from P_n and K_n) on n vertices $W(P_n) > W(G_n) > W(K_n)$.

Proof. Any two vertices in a connected graph are at distance at least one. This implies the wiener index for the minimum case is:

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\subseteq V} d(u,v) \\ &= \sum_{\{u,v\}\subseteq V} 1 \\ &= \binom{n}{2} \end{aligned}$$

And so we have the lower bound $\binom{n}{2} \leq W(G)$.
Let G have maximum wiener index among all graphs of order n. Since deletion of any edge increases the wiener index, G is a tree and has a vertex v of degree 1. Denote the sum of all distances between v and other vertices by $D(v)$.Then, $D(v) \leq 1+2+3+...+(n-1)$.
We have $W(G-v) \leq \binom{n}{3}$.
Hence we obtain

$$\begin{aligned} W(G) &= \sum_{w\in V-\{v\}} d_G(v,w) + \sum_{\{u,w\}\subseteq V-\{v\}} d_G(u,w) \\ &= D(v) + W(G-v) \\ &\leq 1+2+...+(n-1) + \binom{n}{3} \\ &= \binom{n+1}{3} \end{aligned}$$

Hence, equality in the lower bound holds if and only if every distance equals one, i.e., if G is complete.

Equality in the upper bound implies that D(v)=1+2+...+(n-1), and so G must be a path. □

This suggests that the Wiener index might be used to order isomers according to the extent of branching.
Every rational number $r \geq 1$ is the mean distance of some graph.
For K_n we have $W(K_n) = \frac{n(n-1)}{2}$ while for the star $K_{1,n-1}$ we have $W(K_{1,n-1}) = (n-1)^2$. Adding an edge to $K_{1,n-1}$ decreases the wiener index by 1 and this can be iteratively repeated till a complete graph is obtained. This gives a continuous interval of Wiener indices from $\frac{n(n-1)}{2}$ through $(n-1)^2$. The next interval, defined by $K_{1,n}$ and K_{n+1}, overlaps the previous interval, demonstrating that a graph G with $W(G) = n$ exists for any integer n.

3.1 The wiener index of a tree

The Wiener conjecture for trees says that every possible integer n is the wiener index of some tree, except for a finite collection (of integers).
This section's major result is an algorithm for computing $W(T)$ for an arbitrary tree T.
We used the following observations in our algorithm.

A. In a tree T, there is a unique shortest path between any pair vertices.

B. Let the number of shortest paths of T that pass through the specified edge e in $E(T)$ is denoted by $w(e)$. Then $W(T) = \sum_{e \in E(T)} w(e)$

C. If T is a tree and e in $E(T)$, let $n_1(e)$ and $n_2(e)$ denote the number of vertices in each of the two components of $T - \{e\}$, respectively. Then, $w(e) = n_1(e)n_2(e)$. Note also that for $i = 1, 2$: $n_i(e) = |V(T)| - n_{3-i}(e)$. (These results hold more generally in graphs that are not trees, as long as e is a bridge of a graph.)
A tree T on n vertices has $n-1$ edges. It's always possible to represent it as a rooted tree (and this will be assumed henceforth). This means that a vertex $v_0 \in V(T)$ is separated and called the root of T. (We can choose any vertex for the root.) All the remaining vertices are indexed as $v_1, v_2, \ldots, v_{n-1}$ in such a way that each $v_i (i \geq 1)$ has exactly one

neighbour among $v_0, v_1, \ldots, v_{i-1}$. This unique neighbour is denoted by T_i and called the predecessor of v_i.

The steps in the algorithm for computing $W(T)$ of an arbitrary tree T are as follows:

D. Linear time, LT, algorithm

1. The (rooted) tree is input as an array $T_i, i = 1, 2, \ldots, n-1$.
2. For each vertex compute (in linear time) its indegree $ind(v_i) = |j \mid v_i = T_j|$.
3. Form a queue of all leaves of T, the vertices with $ind(v_i) = 0$.
4. Delete all leaves one after another and compute $w(e)$ for the corresponding deleted edge.
5. Compute $W(T)$ using B.

Each of the preceding steps requires at most linear time, hence the algorithm as a whole is linear.

Example 1. *Let T be the tree of Fig2.1. It is the graph of the molecule of* $3,3-dimethyl-4-isopropyloctane$. *T has* $n = 13$ *vertices. For each edge e of T, we determine the number of vertices in the smaller of the two subtrees* $n_1(e)$ *and then add* $w(e) = n_1(e)(n - n_1(e))$ *for each e from* $E(T)$. *Then*

$$
\begin{aligned}
W(T) &= 6[1(13-1)] + 2[2(13-2)] + 2[3(13-3)] + 5(13-5) + 6(13-6) \\
&= 6 \times 12 + 2 \times 2 \times 11 + 2 \times 3 \times 10 + 5 \times 8 + 6 \times 7 \\
&= 258.
\end{aligned}
$$

This is a tree with W(T)=258

A Wiener Index Computation Algorithm that allows us to compute the Wiener index of any graph. The following algorithm is proposed for this purpose:

1. We assign one number to any vertex.
2. We determine all of adjacent vertices set of the vertex $i, i \in V(G)$ and this set denoted by $N(i)$.

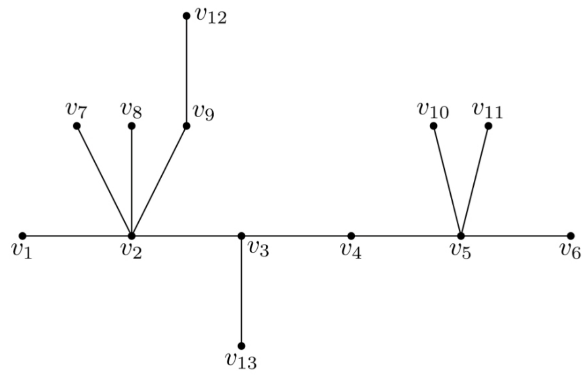

Figure 3.1: The graph of the molecule of 3,3,- dimethyl-4-isopropyloctane.

3. In the start of program, we set $w = 0$, and at the end of program, the value of $\frac{1}{2}w$ will be the Wiener index of graph G.

4. The set of vertices that their distance to vertex i is equal to $t(t \geq 0)$ is denoted by $D_{i,t}$ and consider $D_{i,0} = \{i\}$. We have the following relations:

$$V = \bigcup D_{i,t}, i \geq 0, i \in V(G) \tag{3.4}$$

$$W(G) = \frac{1}{2} \sum_{i \in V, t \geq 1} t \times |D_{i,t}| \tag{3.5}$$

We can get the Wiener index of the graph by determining these sets, according to 3.5. Because the distance between vertex i and its adjacent vertices is 1, $Di, 1 = N(i)$. For each $j \in D_{i,t} t \geq 1$, the distance between each vertex of set $N(j) \setminus (D_{i,t} \bigcup D_{i,t-1})$ and the vertex i is equal to $t + 1$, thus we have $D_{i,t+1} = Sj \in Di, t(N(j) \setminus (Di, tDi, t-1)t \geq 1$. According to above equation, we can obtain $D_{i,t}, t \geq 2$, for each $i \in V$. After determining each $D_{i,t}$, we add value $t \times |D_{i,t}|$ to w. Finally the Wiener index of the graph G is equal to $\frac{1}{2}w$.

3.1.1 Wiener index of complete binary trees

A binary tree T is defined on a finite set of vertices that either
a. contains no vertices or
b. is composed of three disjoint sets of vertices: a root vertex, a binary tree called the left subtree of T and a binary tree called the right subtree of T.

At depth 0, we define r as the root. At depth 1 are the vertices that are directly related to the root [8]. A vertex is generally k depth deep.
A complete binary tree of height k, often known as T_k, is a tree with vertices up to depth k and the maximum number of vertices at each depth.
The total number nT_k of vertices in T_k is given by [8]

$$nT_k = 2^{k+1} - 1 \tag{3.6}$$

Recalling the definition of $d^+(u, G)$ we get

$$d^+(r, T_k) = \sum_{i=0}^{k} iz^i = 2 + (k-1)2^{k+1} \tag{3.7}$$

Theorem 1. *The wiener index of a complete binary tree of height k is given by*

$$W(T_k) = (k+4)2^{k+1} + (k-2)2^{2(k+1)}$$

Proof. Let T_k be a complete binary tree with root r and a height of k. Let u , v be the children of r i.e., u *and* v are the roots of T_{k-1}. Then

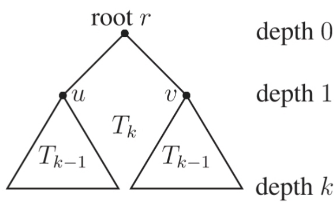

Figure 3.2: A complete binary tree T_k is subtree T_{k-1}

T_k can be formed using two subtrees T_{k-1} as shown in Fig.3.1.1. We first identify T_k as a tree of the type as shown in fig.3.1. We take T_a to be $T_{k-1} \bigcup (edge(u_r))$ and T_b to be $T_{k-1} \bigcup (edge(v_r))$ so that r is a cut-vertex of T_k with $T_a \bigcap T_b = \{r\}$. Then by (4.3) and (3.6) and noting that $T_b \cong T_a$, we have

$$W(T_k) = 2W(T_a) + (2^{k+1} - 2)d^+(u, T_a) \tag{3.8}$$

By invoking (4.3), it then follows that

$$W(T_a) = W(T_{k-1}) + (k-1)2^k + 1 \tag{3.9}$$

By using (3.7) it follows that

$$d^+(u, T_a) = (k-1)2^k + 1 \tag{3.10}$$

Substituting (3.9) and (3.10) in (3.8) gives us

$$W(T_k) = 2W(T_{k-1}) + 2^{2k+1}(k-1) + 2^{k+1}$$

Thus, the closed form of the above recurrence relation gives

$$W(T_k) = (k+4)2^{k+1} + (k-2)2^{2(k+1)}$$

□

Examples

Example 2. *1, Let G be the graph shown in figure A,* $d(V_4, V_6) = 2$ *using the path* (V_4, V_7, V_6) *and* $d(V_1) = 1+2+3+4+2+3+4 = 19$

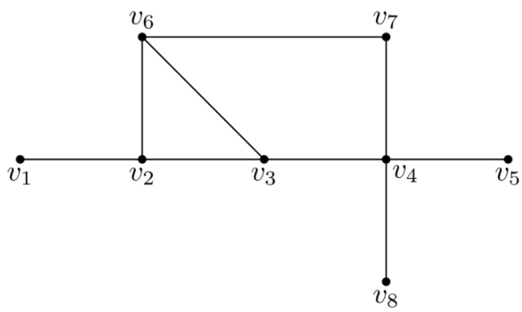

Figure 3.3: A

Then,

$$\begin{aligned} W(G) &= \sum_{i=1}^{7}\sum_{j=i+1}^{8} d(V_i, V_j) \\ &= 19 + 12 + 8 + 5 + 7 + 4 + 2 \\ &= 57 \end{aligned}$$

And the mean distance of G is

$$\mu(G) = \frac{57}{\binom{8}{2}} = \frac{57}{28}$$

2, Let T be a tree as shown in figure B, V_1 is a leaf and V_2 a branching point, but notice that V_9 is neither a leaf nor a branching point since $deg(V_9) = 2$

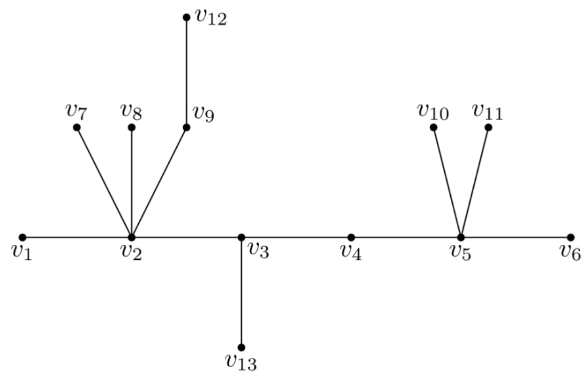

Figure 3.4: B

Then,

$$\begin{aligned}
W(G) &= \sum_{i=1}^{12} \sum_{j=i+1}^{13} d(V_i, V_j) \\
&= (1+2+3+4+5+2+2+2+3+3+5+5) \\
&\quad +(1+1+1+2+1+2+2+3+4+4+4) \\
&\quad +(1+2+3+3+3+1+2+2+2+3) \\
&\quad +(1+2+2+2+2+3+3+3+4) \\
&\quad +(1+1+1+3+4+4+4+5)+(2+2+4+5+5+6) \\
&\quad +(2+2+3+3+5+5)+(2+3+3+5+5) \\
&\quad +(1+3+5+5)+(2+4+6)+(4+6)+4 \\
&= 236
\end{aligned}$$

Example 3. *a,*

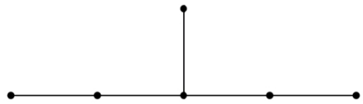

Figure 3.5: Tree with WI 31

b,

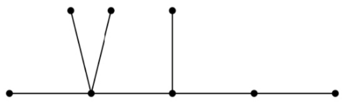

Figure 3.6: Tree with WI 63

c,

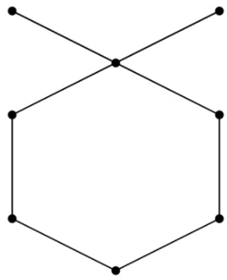

Figure 3.7: Bipartite graph with WI 59

d,

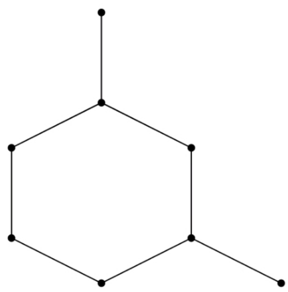

Figure 3.8: Bipartite graph with WI 61

3.2 Degree Distance(Schultz Index)

Definition 9. *The degree distance, DD(G), is defined by*

$$DD(G) = \sum_{\{u,v\} \subseteq V} (deg(u) + deg(v))d(u,v).$$

Dobrynin and Kochetova proposed the degree distance [4], a variant of the Wiener index, and Gutman independently proposed it under a different name (which is Schultz index). It appears that this quantity had also been mentioned in connection with certain chemical applications. In the mathematical literature, the degree distance has recently been studied in more depth. The degree distance can be considered a weighted version of the Wiener index.
Its definition encompasses both distance and degree. The Schultz index of the second kind [4] is a related index that uses the product rather than the sum of the degrees, but the name Gutman index has also been used.

Theorem 2. *For every tree T of order n,*

$$DD(T) = 4W(T) - n(n-1) \tag{3.-1}$$

Proof. Fix an edge uw of T and compare the contribution of this edge to the Wiener index and to the degree distance.
Let U and W be the vertex sets of the components of $T - uw$ containing u and w, respectively, and let
$n_{u,uw}$ and $n_{w,uw}$ be their respective cardinalities.

The Wiener index is the total length of shortest paths between the $\binom{n}{2}$ unordered pairs of vertices.

Clearly, $n_{u,uw}n_{w,uw}$ of these paths contain uw. Summing this over all edges we obtain

$$W(T) = \sum_{uw \in E(T)} n_{u,uw}n_{w,uw}.$$

The degree distance can be seen as the total lengths of shortest paths between all unordered pairs of vertices, where we have deg(x) + deg(y) shortest paths between x and y. The number of such paths containing uw is then

$$\begin{aligned}\sum_{x\in U, y\in W}(deg(x)+deg(y)) &= |W|\sum_{x\in U}deg(x)+|U|\sum_{y\in W}deg(y)\\ &= |W|(2|U|-1)+|U|(2|W|-1)\\ &= 4n_{u,uw}n_{w,uw}-n\end{aligned}$$

Summation over all edges now yields 3.-1. □

As a consequence of 3.-1 and the fact that the Wiener index is maximized for paths, and minimized for stars, we obtain sharp lower and upper bounds on the degree distance of a tree T of order n: $3n^2-7n+4 \leq DD(T) \leq \frac{n(n-1)(2n-1)}{3}$ with equality in the first or second inequality if and only if T is a star $K_{1,n-1}$ or a path P_n, respectively.

Definition 10. *A vertex v of a graph G is said to be pendant if deg(v)=1*

Lemma 1. *Let v be a pendant vertex of a graph G of order n and u be the vertex adjacent to v. Then,* $W(G) = W(G-v) + D_{G-v}(u) + n - 1$

Proof. By the definition of the Wiener index, we have

$$\begin{aligned}W(G) &= \sum_{x,y\in V(G)-v} d_G(x,y)\\ &= W(G-v)+D_{G-v}(u)+n-1\end{aligned}$$

□

3.3 Hyper-Wiener index

Because the Wiener and hyper-Wiener indices are based on the distances between pairs of vertices in a graph, similar ideas for distances between pairs of edges have been introduced under the names edge-Wiener index and edge-hyperWiener index, respectively. Let us say $f = xy$ and $g = uv$ are two edges of G. The distance between f and g is denoted by $de(f,g|G)$, and defined as the distance between the vertices f and g in the line graph of G. This distance is equal to $D(f,g)+1$, where $D(f,g) = min\{d(x,u),(x,v),(y,u),(y,v)\}$. For example, distance 1 means that the edges share a vertex and distance 2 means that at least two of the four end vertices of two edges are adjacent.

Definition 11. *The edge-Wiener index* $W_e(G) = \sum_{\{e_1,e_2\}\subseteq E(G)} d(e_1, e_2)$*, where the distance between two edges in a graph G is defined as the distance between their corresponding vertices in the line graph L(G) of G. Thus* $W_e(G) = W(L(G))$*.*

A modification of this index is the generalized Wiener index defined as $W_k(G) = \sum_{\{u,v\}\subseteq V(G)} d^k(u, v)$, where k is a real number.
In particular, it is known as the reciprocal Wiener index for $k = -1$ and the Harary index or Harary number for $k = -2$.
Following Wiener's discovery of a close relationship between the boiling points of certain alkanes and the sum of the distances between vertices in the graphs representing their molecular structures, it became clear that graph parameters, or topological indices, could be used to predict properties of chemical compounds. The Wiener index has been studied in the mathematical, chemical, and computer science literature under a variety of names and with slight differences in the definitions, and it is sometimes referred to as the graph's distance or total distance.

Definition 12. *The hyper-Wiener index of a graph G is defined as*
$WW(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u, v) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d^2(u, v)$

Definition 13. *the edge-hyper-Wiener index is*
$WWe(G) = \frac{1}{2}\sum_{e_1,e_2\subseteq E(G)} d(e_1, e_2) + \frac{1}{2}\sum_{e_1,e_2\subseteq E(G)} d^2(e_1, e_2)$.

3.4 Gutman index

Several Wiener index variants have been proposed and investigated. In this section, we look at a variant of the Wiener index, a quantity proposed by Gutman and named the Schultz index of the second kind, but now known as the Gutman index [4].

Definition 14. *The Gutman index of a graph G is defined as*
$Gut(G) = \sum_{\{u,v\}\subseteq V(G)} deg(u)deg(v)d(u, v)$.

The Gutman index is thus a kind of a vertex-degree-weighted sum of the distances between pairs of vertices in a graph, and it is closely linked to the Wiener index for trees.

Theorem 3. *Let T be a tree of order n. Then,*

$$Gut(T) = 8W(T) - 2(2n-1)(n-1)$$

Theoretical studies on the Gutman index with polycyclic compounds, according to Gutman, are more difficult. Since then, a number of researchers have investigated at the index and its relationship to other graph parameters. The edge-Wiener index $We(G)$ is a quantity that is closely analogous to the Wiener index and is related to the Gutman index. It is defined as the sum of the distances (in the line graph) between all pairs of edges of G.
For every tree T of order n, let us consider the degree distance, Gutman index, and edge-Wiener index,
i.$DD(T) = 4W(T) - n(n-1)$
ii.$Gut(T) = 4W(T) - (2n-1)(n-1) and$
iii.$W_e(T) = W(T) - \binom{n}{2}$

Chapter 4

Techniques for computing Wiener Index

Definition 15. *Given the graphs $G = (V, E)$ and $H = (V, E)$, where $V(G) = \{v_1, v_2, ...v_n\}$ and $V(H) = \{u_1, u_2, ...u_m\}$, their cartesian product $G \times H$ is a graph defined as:*

$$V(G \times H) = V(G) \times V(H) = \{(v_i, u_j) : (v_i \in V(G), u_j \in V(H)\} \ \ and$$

$$E(G \times H) = \{(a, x)(b, y)|a = b \ \ \& \ \ xy \in E(H) \ \ or \ \ ab \in E(G) \ \ and \ \ x = y\}$$

Example 4. *Let $G_1 = K_2$ and $G_2 = P_3$. Then*

$$V(G_1 \times G_2) = K_2 \times P_3$$

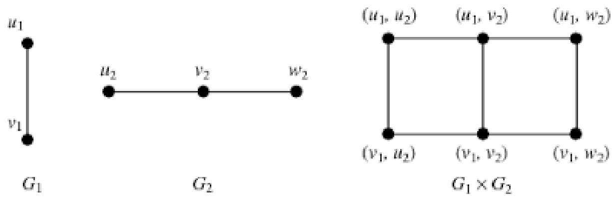

Figure 4.1:

$G \times H$ is associative and commutative.

Lemma 2. *The Wiener index of $G \times H$ is given by the formula[8]:*

$$W(G \times H) = |V(H)|^2 W(G) + |V(G)|^2 W(H) \tag{4.1}$$

Lemma 3. *(Cut vertex/edge lemma)*
Let T be a tree obtained from arbitrary trees T_a and T_b of orders n_1 and n_2 respectively and let $u \in V(T_a)$ and $v \in V(T_b)$. Then
(a) If u and v are fused together to form a single vertex, say u, then the vertex u

become a cut vertex in T [8], then

$$W(T) = W(T_a) + W(T_b) + (n_1 - 1)d^+(u, T_b) + (n_2 - 1)d^+(u, T_a) \quad (4.2)$$

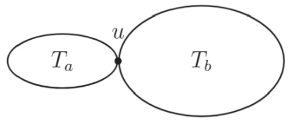

Figure 4.2: A tree T : assembled from trees T_a and T_b

(b) If an edge connects u and v, the edge uv in T becomes a cut-edge, then

$$W(T) = W(T_a) + W(T_b) + n_1 d^+(v, T_b) + n_2 d^+(u, T_a) + n_1 n_2 \quad (4.3)$$

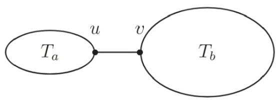

Figure 4.3: A tree T : assembled from trees T_a and T_b

4.1 Techniques

(a) Direct enumeration
i. $W(K_n) = \binom{n}{2}, (n \geq 2)$

Proof. $d(u, v) = 1$ for $u, v \in V$. Thus,

$$\begin{aligned} W(K_n) &= \sum_{\{u,v\} \subseteq V} d(u, v) \\ &= \sum_{\{u,v\} \subseteq V} 1 \\ &= \binom{n}{2} \end{aligned}$$

□

ii. $W(K_{m,n}) = (m+n)^2 - (m+n) - mn, (m, n \geq 1)$

(b) Use of recurrence relations

Example 5. *i. Let P_n denote a path on $n(n \geq 2)$ vertices. Then it follows that $W(P_n) = W(P_{n-1}) + \frac{1}{2}n(n-1), (n > 2)$ with $W(P_2) = 1$ Thus, $W(P_n) = \binom{n+1}{3}$*
ii. Let G be the tree T_n formed by taking the path P_{n+2} and adding two vertices to each non-pendant vertex of P_{n+2}. It follows that $W(T_n)$ satisfies the following recurrence:

$$W(T_n) = W(T_{n-1}) + \frac{9}{2}n^2 + \frac{27}{2}n - 3 \;\; n > 1 \;\; with \;\; W(T_1) = 16$$

It then follows that

$$W(T_n) = 1 + \frac{3}{2}(n^2 + 6n + 3)$$

iii. Let G be the ladder graph L_n,$(n \geq 1)$i.e.,L_n resembles a ladder with $n+1$ rungs. Note that $L_n \cong P_n \times P_2$, $n \geq 1$. It then follows that

$$W(L_n) = W(L_{n-1}) + 2(n+1)^2 - 1, \;\; (n > 1) \;\; \& \;\; W(L_1) = 8$$

Thus we get

$$W(L_n) = \frac{1}{3}(n+1)(n+3)(2n+1)$$

(c) Use of graph product

Example 6. *i. Let P denote the graph of a prism obtained by the Cartesian product of C_3 and K_2 i.e.,$P \cong C_3 \times K_2$. It then follows from (4.1) that $W(P) = 21$.*
ii. For $m, n \geq 2$, let G be the $m \times n$ grid i.e.,$G \cong P_m \times P_n$. Then by (4.1), we get

$$W(P_m \times P_n) = \frac{1}{6}(m+n)mn(mn-1)$$

The special case for the ladder graph is found by taking m to be $n+1$ and n to be 2 from the expression for $W(P_m \times P_n)$.

(d) Use of Cut-vertex/Cut-edge lemma
(e) Use of combinatorial techniques

4.2 A decomposition algorithm

Let $G = (V, E)$ with $|V| = n$ and $|E| = m$. We first use the concept of a clique-separator to extend the cut-vertex/cut-edge lemma. A clique-separator(or a clique-cut set) in G is a clique $G[S]$, where $S \subset V$ such that $G[V \backslash S]$ has more connected components than G. If $G[S]$ is a clique-separator in G, then we can decompose G into two subgraphs $G_1 = G[V_1]$ and $G_2 = G[V_2]$ where $V(G) = V_1 \cup V_2$ and $S = V_1 \cap V_2$. Let $|G_1| = n_1$, $|G_2| = n_2$ and $|S| = k$. Let DIST denote the sum of all distances $d(u, v)$ where $u \in G_1 \backslash S$ and $v \in G_2 \backslash S$. Then it follows that

$$W(G) = W(G_1) + W(G_2) - \binom{k}{2} + DIST \tag{4.4}$$

In reality, the extension with a clique-separator is beneficial in determining the wiener index of various molecular graphs whose underlying components consist of ring systems (i.e.,containing more than one benzene ring structurally). A clique-separator with two vertices can be found in these situations.

Chapter 5

Application of Wiener Index

The wiener index is most significant in chemical graph theory. It's also important in the study of graph distance and the possible related applications.

5.1 Applications in graph theory

For a tree T, it is known that $W(L(T)) = W(T) - \binom{n}{2}$
where $L(T)$ denotes the line graph of T.
The iterated line graph $L_k(G)$ is defined as $L_k(G) = L(L^{k-1}(G))$, where $k \geq 1$ and $L_0(G) = G$.
For a tree T, the size of $L_k(T)$ rapidly increases as k tends to infinity. Therefore, for sufficiently large k, we have $W(T) < W(L_k(T))$, except for paths and $k_{1,3}$.

Definition 16. *A spanning tree T is a tree that is subgraph of a connected graph G and contains all vertices of G.*

Among all spanning trees, trees with smallest Wiener index are of great practical importance in the design of economical networks.[2]
Wiener index is applicable in finding optimal spanning tree of a connected graph G.
Wiener index uses to distinguish between non-isomorphic n-vertex trees (chemical trees) depends on n in an alternative manner for $n \leq 11 (n \leq 15, resp.)$: it increases for even values of n and decreases for odd values of n.

5.2 Application in networks

Definition 17. *A computer network is a group of computers that are linked together to allow one computer to communicate with another to share resources, data, and applications.*

Wiener index is applicable in the study of optimal distributed processing in networks.Using it some researchers showed that, given a network with a tree topology, choosing a centroid vertex and then routing all the information through it is the best possible strategy, in terms of worst-case number of messages sent during any execution of any distributed sorting algorithm. The quantity $\mu(G)$ is useful for various types of networks that arise in computer architecture since it is a course measure of the mean distance between each pair of vertices in G. In turn, this implies that $\mu(G)$ is a measure of the average distance traversed by messages transmitted by processes comprising a parallel computation within the processer-interconnection network and thus the average communication delay of the network for an application.
In other words, if we can estimate the amount of messages exchanged when running a parallel algorithm on a specific architecture as specified by a graph, we may predict the algorithm's average communication delay for an application.

5.3 Applications in chemistry

Chemical graph theory, with in valence bond theory, depicts organic compounds or, equivalently, their molecular structures as graphs, called molecular graphs[8], in which atoms are represented by vertices and covalent chemical bonds by edges. If there are any double or triple bonds, they are approximated by a single edge when generating the molecular graph.

The quantity $W(G)$ is named after Harold Wiener, a chemist who seems to have been the first to investigate the relationship between $W(G)$ and paraffin physicochemical properties. Having a molecule, when we represent atoms as vertices and bonds as edges in a molecule, we get a molecular graph. Topological indices are graph theoretic invariants of molecular graphs that predict properties of the corresponding molecule. The Wiener index, often known as the path number, is the oldest topological index. It was first introduced in 1947. Initially, the Wiener index was used to estimate the boiling points of paraffins, but later, a strong correlation between the Wiener index and a compound's chemical properties was discovered. This index is now utilized for preliminary drug molecule screening. In a preliminary stage, the Wiener index also predicts the binding energy of a protein-ligand complex.

For alkanes, Wiener defined W as the total of all carbon-carbon bonds between all pairs of carbon atoms[7].

The first application of the wiener number was for predicting the boiling points (b.p) of alkanes based on the formula:

$$b.p. = \alpha W + \beta w(3) + \gamma$$

where α, β and γ are empirical constants and $w(3)$ is the so-called "path number", namely, the number of pairs of vertices whose distance is equal to 3. Wiener emphasized the versatility of his index in structural-property investigations in a series of papers published in 1947 and 1948. He calculated boiling points, molar volumes, refractive indices, isomerization heats, and vaporization heats of alkanes using W.
It is nowadays well understood that the wiener number measures the extent of branching of the carbon-atom skeleton and consequently, the compactness of a given molecule. Therefore, W reflects the molecular surface-to-volume ratio. In connection with this, W was claimed to be related to the intermolecular forces, especially in the case of non-polar molecules like hydrocarbons.
Those physical and chemical properties of substances which are expected to depend on the volume-to-surface ratio of their molecules and/or on the level of branching of the molecular carbon-atom skeleton, are typically well correlated with W.
The prediction of organic substances in gas chromatography is of particular practical importance. For instance, the chromatographic retention times (CRT) of monoalkyl- and o-dialkylbenzenes were shown to obey the following functional dependence on W:

$$CRT = \alpha W^{\beta} + \gamma$$

where α, β and γ are empirically determined parameters (different, of course, from those in wiener's formula for b.p.).
A somewhat less standard result along the same line is the connection between W and the velocity of ultra-sound in alkanes and alcohols.

Example 7. *Butane(C_4H_{10}) has two different structural isomers: n-butane, which has a four-carbon linear structure, and isobutane, which has a branched structure. The molecular graph of n-butane is a four-vertex path graph, while that of isobutane is a tree with one central vertex connected to three leaves.*

Figure 5.1: n-butane

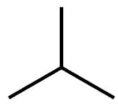

Figure 5.2: isobutane

The n-butane molecule has three pairs of vertices that are one distance apart, two pairs that are two distances apart, and one pair that is three distances apart. Therefore its wiener index is

$$3 \times 1 + 2 \times 2 + 1 \times 3 = 10$$

The isobutane molecule has three pairs of vertices that are one distance apart from each other and three pairs that are two distances apart, so its wiener index is

$$3 \times 1 + 3 \times 2 = 9$$

Therefore, despite the fact that these two molecules have the same chemical formula and the same number of carbon-carbon and hydrogen-carbon bonds, they have different Wiener indices due to their differing structures.
Equation(3.1) is a natural variant suggested as a possible generalization for graphs that need not be trees.
The study of Wiener index appears to be limited to acyclic molecular graphs for the vast majority of chemical applications.

Summary

The Wiener index W(G) is defined as the sum of distances between all pairs of vertices of G. It has maximum and minimum value in a given order. It might be used to order isomers according to the extent of branching. The degree distance can be considered a weighted version of the Weiner Index and the gutman index is closely linked to the Wiener Index for trees.There are many techniques to compute Wiener Index and it is applicable in many areas, such as, graph theory, network, chemistry, and so on.

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