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WIENER TYPE INDICES OF CERTAIN CLASSES OF TREES

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Abstract: The most acclaimed distance based topological index, Wiener index was introduced by the chemist H. Wiener in 1947 [20]. It is defined as the sum of the lengths of the shortest paths between all pairs of vertices of a graph G. In this paper, we have computed the Wiener and Terminal Wiener indices of certain classes of trees known as Gutman trees and Kragujevac trees.

Keywords and Phrases: Topological Indices, Wiener Index, Gutman Trees, Broom Graph, Kragujevac trees.

2020 Mathematics Subject Classification: 05C05, 05C07, 05C012, 05C35.

1. Introduction

Throught this paper, we consider finite, connected, undirected graphs without loops and multiple edges. For all further notations and terminology, see [13].

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The distance between two vertices u and v denoted by $d_G(u, v)$ or $d(u, v)$ is the length of shortest path between the vertices u and v in G. The degree $d_G(v)$ or $d(v)$ of a vertex v is the number of vertices adjacent to v and $N_G(v)$ is the set of vertices adjacent to v.

Chemical graph theory is a branch of Mathematical Chemistry which has an important effect on the development of chemical sciences. A single number used to characterize some property of the graph of the underlying molecule is called a topological index of that graph. There are numerous molecular descriptors also known as topological indices, that have found some applications in theoretical chemistry, especially in QSPR/QSAR research [2, 3, 4, 6, 7, 18].

Among those topological indices based on the topological distance matrix, the Wiener index is the most popular one both from a theoretical point of view and applications. Wiener basically studied the correlation between $W(G)$ and boiling points of paraffins based on the formula: Boiling point $= \alpha W(G) + \beta w(3) + \gamma$, where α, β, 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 three [19]. Wiener index of a graph G, denoted by $W(G)$, is defined as the sum of the lengths of the shortest paths between all pairs of vertices of G:

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

Terminal distance matrices were used for modeling amino acid sequences of proteins and of the genetic code, see [8, 12, 16]. Motivated by terminal distance matrix and its chemical applications, a distance–based molecular structure descriptor called terminal Wiener index was put forward by Gutman, Furtula and Petrović [10]. The Terminal Wiener index $TW(G)$ of a connected graph G is defined as the sum of the distances between all pairs of its pendent vertices. That is, if $V_T(G) = \{v_1, v_2, ...v_k\}$ is the set of all pendent vertices of G, then

$$TW(G) = \sum_{\{u,v\} \subseteq V_T(G)} d_G(u, v)$$

If the graph G has no pendent vertex or has only one pendent vertex, then $TW(G) = 0$. If G has at least two pendent vertices then $TW(G) \geq 1$ [15].

2. Wiener and Terminal Wiener indices of Gutman Trees

In this section, we compute the Wiener index and terminal Wiener index of Gutman trees and some of their subclasses.

When m_i vertices of degree one are added to i^{th} vertex of a path graph with p-vertices P_p, a *Gutman tree* or a *Benzenoid tree* or a *Caterpillar tree* is obtained and is denoted by $T_p(m_1, m_2, ..., m_p)$. This graph is shown in Figure 1. Since these trees can be made to generate resonance relations among the rings (hexagons) of unbranched benzenoid hydrocarbons, the name "Benzenoid Trees" has been suggested [1, 5, 17]. Clearly, $T_p(0, 0, ..., 0)$ is the path graph P_p.

Without loss of generality, here we label the vertices of the path P_p as v_1, v_2, v_3 and so on from left to right and m_i pendent vertices are attached to the vertex v_i of the path P_p resulting into a Gutman tree $T_p(m_1, m_2, ..., m_p)$. If $m_i \leq 2$ for each

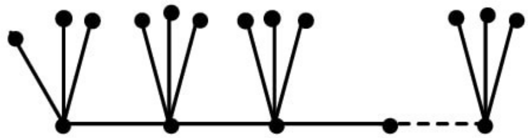

Figure 1: A Caterpillar Tree

$2 \le i \le p-1$ and $m_1 \le 3$ and $m_p \le 3$, then it is a chemical tree. In particular, let $T_p(a,b) = T_p(a,0,0,...,0,b)$ be a tree with n vertices and diameter d obtained by linking centers of two stars with a path P_p ($p \ge 2$). Clearly, $n = a+b+p$ and $d = p+1$. If $a = 0$ or $b = 0$, the tree $T_p(a,b)$ is called Broom graph $B_{n-a,\,p}$ of $n-a$ vertices which has a path P_p with p vertices. If $p = 2$, $d = 3$ and $a = b$, then $T_p(a,b)$ is called a Bistar denoted by $B_{a,\,a}$.

Proposition 2.1. *The Wiener index of a Gutman tree $G = T_p(m_1, m_2, ..., m_p)$ is given by*

$$W(G) = \begin{cases} m_1^2 & if\ \ p=1 \\ (m_1+m_2)^2 + m_1m_2 + 2(m_1+m_2) + 1 & if\ \ p=2 \\ \sum_{i=1}^{3}(m_i^2 - m_i) + 3m_1m_2 + 4m_1m_3 & \\ +3m_2m_3 + 6(m_1+m_3) + 5m_2 + 4 & if\ \ p=3 \end{cases}$$

Proof. An easy computation yields the required result.

Theorem 2.1. *The Wiener index of a Gutman tree $G = T_p(m_1, m_2, ..., m_p)$ with $p > 3$ is given by*

$$\begin{aligned} W(G) &= \frac{p(p^2-1)}{6} + \frac{p(p+1)(m_1+m_p)}{2} + \sum_{i=1}^{p}(m_i^2 - m_i) \\ &\quad + \sum_{i=1}^{p-1}\sum_{r=3}^{p-i+2} r.m_i m_{i+r+2} + R. \end{aligned}$$

where the term R is given by

$$R = \begin{cases} \frac{1}{2}\sum_{s=2}^{p/2}(2s^2 - 2s - 2ps + p^2 + 3p)(m_s + m_{p-s+1}) & if\ \ p\ \ is\ \ even \\ & \\ \frac{1}{2}\sum_{s=2}^{(p-1)/2}(2s^2 - 2s - 2ps + p^2 + 3p)(m_s + m_{p-s+1}) & \\ +\frac{1}{4}m_{\left(\frac{p+1}{2}\right)}(p^2 + 4p - 1) & if\ \ p\ \ is\ \ odd \end{cases}$$

Proof. We have, $W(G) = \sum_{u \neq v} d_G(u, v)$.

Let the vertex set $V(G)$ of G be divided into vertex subsets A_i and B where $A_i = \{u_i \mid u_i \text{ is a pendent vertex at the vertex } v_i \; of \; P_p\}$, $\mid A_i \mid = m_i \, ; 1 \leq i \leq p$ and $B = \{u_i \mid u_i \text{ is a vertex of } P_p\}$, $\mid B \mid = p$, $p \geq 4$.
Following cases arise.

- Let $u_i, u_j \in A_i$. Clearly the distance between any two distinct vertices from the same A_i, $1 \leq i \leq p$ is 2. Then

$$\sum_{\{u_i, u_j\} \subseteq A_i} d_G(u_i, u_j) = \sum_{i=1}^{p} m_i^2 - m_i.$$

- Let $u_i \in A_i$ and $u_j \in A_j$ $(i \neq j)$. Then

$$\sum_{u_i \in A_i, u_j \in A_j} d_G(u_i, u_j) = \sum_{i=1}^{p-1} \sum_{r=3}^{p-i+2} r m_i m_{i+r-2}.$$

- Let $u_i \in A_i$ and $u_j \in B$. We have following two subcases.

  (i) If p is even,

$$\begin{aligned} \sum_{u_i \in A_i, u_j \in B} d_G(u_i, u_j) &= \frac{p(p+1)(m_1 + m_p)}{2} \\ &+ \frac{1}{2} \sum_{s=2}^{p/2} (2s^2 - 2s - 2ps + p^2 + 3p)(m_s + m_{p-s+1}) \end{aligned}$$

  (ii) If p is odd,

$$\begin{aligned} \sum_{u_i \in A_i, u_j \in B} d_G(u_i, u_j) = \frac{p(p+1)(m_1 + m_p)}{2} \\ + \frac{1}{2} \sum_{s=2}^{(p-1)/2} (2s^2 - 2s - 2ps + p^2 + 3p)(m_s + m_{p-s+1}) \\ + \frac{1}{4} m_{\left(\frac{p+1}{2}\right)} (p^2 + 4p - 1) \end{aligned}$$

- Let $u_i, u_j \in B$. Then $\sum_{\{u_i,u_j\}\subseteq B} d_G(u_i,u_j) = \frac{p(p^2-1)}{6}$

  From the above cases, the required result follows.

Corollary 2.1. *The Wiener index of path graph P_p is $W(P_p) = \frac{p(p^2-1)}{6}$.*
Proof. When $m_i = 0$ for $1 \leq i \leq p$, Gutman tree reduces to a path graph P_p. Hence the result follows.

Theorem 2.2. *The Wiener index of $T_p(a,b)$ is*

$$W(T_p(a,b)) = a(a-1) + b(b-1) + abd + \frac{p(p+1)}{6}[3a+3b+p-1]$$

Proof. Let the vertex set $V[T_p(a,b)]$ of $T_p(a,b)$ be divided into three subsets A, B and C as follows:
$A = \{u_i \mid u_i \text{ is a pendent vertex at left end of } P_p\}, \mid A \mid = a$
$B = \{u_i \mid u_i \text{ is a pendent vertex at right end of } P_p\}, \mid B \mid = b$
$C = \{u_i \mid u_i \text{ is a vertex of } P_p\}, \mid C \mid = p$
Following cases arise.

- If $u_i,\ u_j \in A$, $\sum d_{T_p(a,\ b)}(u_i,u_j) = a(a-1)$.
- If $u_i,\ u_j \in B$, $\sum d_{T_p(a,\ b)}(u_i,u_j) = b(b-1)$.
- If $u_i \in A,\ u_j \in B$, $\sum d_{T_p(a,\ b)}(u_i,u_j) = abd$.
- If $u_i \in A,\ u_j \in C$, $\sum d_{T_p(a,\ b)}(u_i,u_j) = \frac{ap(p+1)}{2}$.
- If $u_i \in B,\ u_j \in C$, $\sum d_{T_p(a,\ b)}(u_i,u_j) = \frac{bp(p+1)}{2}$.
- If $u_i,\ u_j \in C$, $\sum d_{T_p(a,\ b)}(u_i,u_j) = \frac{p(p^2-1)}{6}$.

From these cases, it follows that
$W(T_p(a,b)) = a(a-1) + b(b-1) + abd + \frac{p(p+1)}{6}[3a+3b+p-1]$.

Corollary 2.2. *The Wiener index of Broom graph $B_{n-a,\ p}$ is given by*

$$W(B_{n-a,\ p}) = b(b-1) + \frac{p(p+1)}{6}[3b+p-1].$$

Corollary 2.3. *The Wiener index of Bistar graph $B_{a,\ a}$ is given by*

$$W(B_{a,\ a}) = 5a^2 + 4a + 1.$$

Theorem 2.3. *The Terminal Wiener indices of a Gutman tree G, $T_p(a,\ b)$, Broom graph $B_{n-a,\ p}$ and Bistar graph $B_{a,\ a}$ are given by* *(i)* $TW(G) = \sum_{i=1}^{p}(m_i^2 - m_i) + \sum_{i=1}^{p-1}\sum_{r=3}^{p-i+2} r.m_i m_{i+r+2}$, *if* $m_1 \geq 1$ *and* $m_p \geq 1$

(ii) $TW(T_P(a,b)) = a(a-1) + b(b-1) + ab(p+1)$

(iii) $TW(B_{n-a,\ p}) = b^2 + b(p-1)$

(iv) $TW(B_{a,\ a}) = 5a^2 - 2a$

Proof. The proof directly follows from the proofs of Theorem 2.1, Theorem 2.2, Corollaries 2.2 and 2.3.

3. Wiener and Terminal Wiener indices of Kragujevac Trees

Let P_3 be the 3-vertex tree rooted at one of its terminal vertices. For k = 2, 3,... construct the rooted tree B_k by identifying the roots of k copies of P_3. The vertex obtained by identifying the roots of P_3-trees is the root of B_k. See Figure 2.

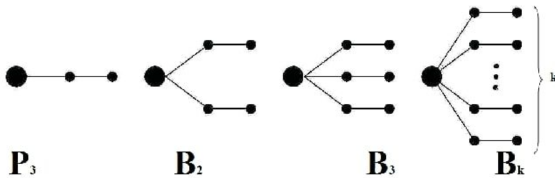

Figure 2: Branches of Kragujevac trees

A kragujevac tree is a tree possessing a central vertex of degree atleast 2 to which branches of the form B_1 and (or) B_2 and (or) B_3 and (or)...and (or) B_k are attached as shown in Figure 3. A typical Kragujevac tree is denoted by $Kg_{t,k}$, where $t \geq 2$ is the degree of the central vertex and $k \geq 2$ [9, 14].

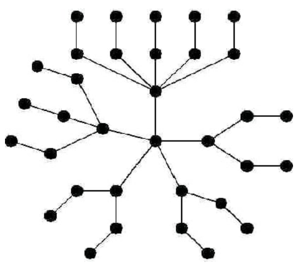

Figure 3: A Kragujevac tree with $t = 5$

Theorem 3.1. *Let* $Kg_{t,k}$ *be a Kragujevac tree with* $t \geq 2$, *then Wiener index of*

$Kg_{t,k}$ is given by

$$W(Kg_{t,k}) = t^2 + \frac{1}{2}\sum_{i=1}^{t}\left(3m_i^2 + 2m_i + 5\right) + \sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2}\left[5m_i m_{i+r-2} - \frac{3}{2}\left(m_i + m_{i+r-2}\right) - 2\right]$$

Proof. By definition, we have $W(G) = \sum_{u\neq v} d_G(u,v)$. Let $|B_i| = m_i$. Following cases arise.

- If $u_i, u_j \in B_i$, then

$$\sum_{\{u_i,u_j\}\subseteq B_i} d_G(u_i,u_j) = \sum_{i=1}^{t}\left\{\left(\frac{(m_i-1)}{2}\right)(1+2) + \left[\left(\frac{(m_i-3)(m_i-1)}{8}\right)(3+4)\right]\right\}$$
$$+ \sum_{i=1}^{t}\left\{\left(\frac{m_i-1}{2}\right)(1) + \left[\left(\frac{(m_i-3)(m_i-1)}{8}\right)(2+3)\right]\right\}$$
$$= \frac{1}{2}\sum_{i=1}^{t}(m_i-1)(3m_i-5)$$

- If $u_i \in B_i$ and $u_j \in B_j$ $(i \neq j)$, then

$$\sum_{u_i\in B_i, u_j\in B_j} d_G(u_i,u_j) = t(t-1) + \sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2}\frac{(m_i + m_{i+r-2} - 2)}{2}(3+4)$$
$$+ \sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2}\frac{(m_i-1)}{2}\frac{(m_{i+r-2}-1)}{2}(4+2(5)+6)$$
$$= t(t-1) + \sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2}\left[5m_i m_{i+r-2} - \frac{3}{2}\left(m_i + m_{i+r-2}\right) - 2\right]$$

- If $u_i \in B_i$, w is the central vertex, then

$$\sum_{u_i\in B_i, vi=w} d_G(u_i,w) = t + \sum_{i=1}^{t} m_i\,(2+3)\,.$$

From above three cases, the result follows.

Theorem 3.2. *Let $Kg_{t,k}$ be a Kragujevac tree with $t \geq 2$, then the Terminal Wiener index of $Kg_{t,k}$ is given by*

$$TW(Kg_{t,k}) = \frac{1}{2}\sum_{i=1}^{t}\left(m_i^2 - 4m_i + 3\right) + \frac{3}{2}\sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2}\left[m_i m_{i+r-2} - (m_i + m_{i+r-2}) + 1\right]$$

Proof. As the distance between every pair of pendent vertices belonging to the same B_i is 4 and there are $\frac{(m_i-3)(m_i-1)}{8}$ such pairs in each B_i, we have

$$\sum_{\{u_i,u_j\}\subseteq B_i} d_G(u_i,u_j) = \sum_{i=1}^{t}\frac{(m_i-3)(m_i-1)}{8}(4)$$

If $u_i \in B_i$, $u_j \in B_j$ $(i \neq j)$, then $d_G(u_i,u_j) = 6$
Therefore,

$$\sum_{u_i\in B_i, u_j\in B_j} d_G(u_i,u_j) = \sum_{i=1}^{t-1}\sum_{r=3}^{t-i+2}\frac{(m_i-1)}{2}\frac{(m_{i+r-2}-1)}{2}(6)$$

From the above two cases, the required result follows.

4. Conclusion

It is very surprising to note that caterpillar trees are of great importance for understanding and simplifying combinatorial properties of much more complicated graphs. Three main areas which involve the use of these trees are computational methods, ordering and data reduction. Moreover, studying Wiener type indices of Gutman trees and their possible usage in the study of quantitative structure activity relations to correlate certain biological activities of benzenoid hydrocarbons might be of very significant in chemical graph theory.

The class of Kragujevac trees emerged in several studies addressed to solve the problem of characterizing a tree with minimal atom-bond connectivity index [11]. Therefore, there is a scope for further research by using these indices in QSPR/QSAR modeling.

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