Integrated Intelligent Research (IIR)
International Journal of Computing Algorithm
Volume: 01 Issue: 02 December 2012 Page No.35-37
ISSN: 2278-2397

Wiener Upper and Lower Sum of P_n^r - Tree

S. Rubanraj,[1] P. Rajkumar[2]
[1]Department of Mathematics, St. Joseph's College (Autonomous), Trichy, Tamilnadu, India
[2]Department of Mathematics, Srimad Andavan Arts and Science College, T.V. Koil, Trichy
Email : ruban946@gmail.com, journalrajkumar@gmail.com

Abstract- Given a simple connected undirected tree T, the Wiener index W(T) of T is defined as half the sum of the distances of all pairs of vertices of T. In practice, T corresponds to what is known as the molecular graph of an organic compound. We obtain the Wiener Lower Sum $W^L(T)$ and Wiener Upper Sum $W^U(L)$ of an arbitrary P_n^r - tree

Keywords: P_n^r - Tree, Wiener Lower Sum - Upper sum of P_n^r - Tree

I. INTRODUCTION

Given the structure of an organic compound, the corresponding (molecular) graph is obtained by replacing the atoms by vertices and covalent bonds by edges (double and triple bonds also correspond to single edges unless specified otherwise). The Wiener index is one of the oldest molecular-graph based structure-descriptors, first proposed by the Chemist Harold Wiener [7] as an aid to determining the boiling point of paraffins. The study of Wiener index is one of the current areas of research in Mathematical Chemistry [5, 8]. There are good correlations between Wiener index of molecular graphs and the Physico-Chemical properties of the underlying organic compounds.

II. PRELIMINARIES

A Tree is a connected graph without cycles. A connected graph without cycles is called acyclic graph or a forest. A path tree P_n is a connected acyclic graph with the vertex set $V(P_n) = \{u_1, u_2, u_3, \ldots u_n\}$ and edge set $E(P_n) = \{u_i u_{i+1} / 1 \leq i < n\}$.
Example

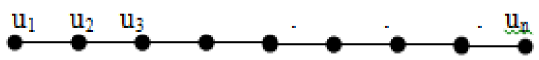

Figure – (i) Path Tree P_n

A F-tree is a graph obtained from a path graph, $n \geq 3$ by appending two pendent edges one to an end vertex and the other to vertex adjacent to the end vertex [9]. Let F_n be a F-tree with n vertices. Let $V(F_n) = \{u_1, u_2, \ldots, u_n, v_1, v_2\}$ and $E(F_n) = \{u_i u_{i+1} ; 1 \leq I < n\} \cup \{u_n v_1, u_{n-1} v_2\}$ be respectively vertex set and edge set of F_n.

A E-tree is a graph obtained from a path graph, $n \geq 3$ vertices by appending three pendent edges, first edge to an end vertex, second edge to last but one end vertex and third edge to last but two end vertices [9]. Let E_n be the E-tree with n vertices, let $V(E_n) = \{u_1, u_2, \ldots, u_n, v_1, v_2, v_3\}$ and $E(E_n) = \{u_i u_{i+1} ; 1 \leq i < n\} \cup \{u_n v_1, u_{n-1} v_2, u_{n-2} v_3\}$ be respectively vertex set and edge set of E_n.
Example

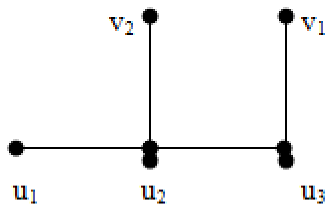

Figure – (ii) F_3-Tree

Example

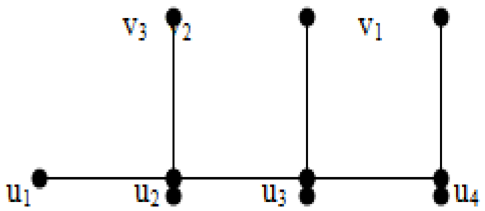

Figure – (ii) E_4-Tree

Given P_n is a path tree, let P_n^r tree be obtained by appending r pendant edges, $1 < r < n$ first edge to an end vertex, second edge to last but one end vertex and third edge to last but two end vertex and so on [9]. Let P_n^r be a tree with n vertices and r pendent vertices. Let $V(P_n^r) = \{u_1, u_2, \ldots u_n, v_1, v_2, v_3, \ldots v_r\}$ and $E(P_n^r) = \{u_i u_{i+1} ; 1 \leq i < n\} \cup \{u_n v_1, u_{n-1} v_2, \ldots u_{n-r+1} v_r\}$ be respectively the vertex set and the edge set of P_n^r.
Example

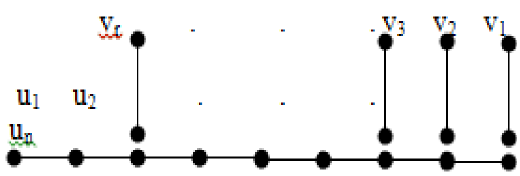

Figure – (iii) P_n^r Tree

A. Definition

Let G = (V(G), E(G)) be a connected undirected graph, any two vertices u, v of V(G), δ(u, v) denotes the minimum distance between u and v. Then the Wiener Lower Sum $W^L(G)$ of the graph is defined by

$$W^L(G) = \frac{1}{2} \sum_{u,v \in V(G)} \delta(u,v)$$

International Journal of Computing Algorithm
Volume: 01 Issue: 02 December 2012 Page No.35-37
ISSN: 2278-2397

where $\delta(u, v) = \min d(u,v)$

B. Definition

Let $G = (V(G), E(G))$ be a connected undirected graph, any two vertices u, v of V(G), $\Delta(u, v)$ denotes the maximum distance between u and v. Then the Wiener Upper Sum $W^U(G)$ of the graph is defined by

$$W^L(G) = \frac{1}{2}\sum_{u,v\in V(G)}\Delta(u,v)$$

where $\Delta(u, v) = \max d(u,v)$

Example

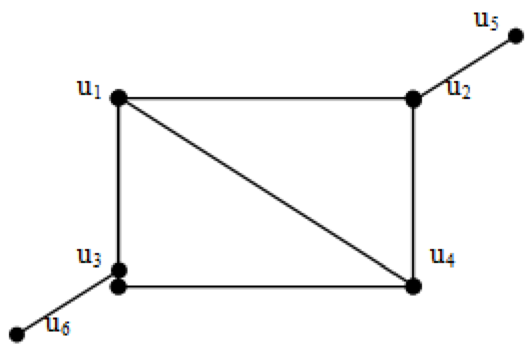

Figure – (iv) Graph

$$W^L(G) = 1 + 1 + 1 + 2 + 2 + 2 + 1 + 1 + 3 + 1 + 3 + 1 + 2 + 2 + 4 = 27$$

$$W^U(G) = 3 + 3 + 2 + 4 + 4 + 3 + 3 + 1 + 4 + 3 + 4 + 1 + 4 + 4 + 5 = 48$$

Our notation and terminologies are as in [1].

III. WIENER LOWER SUM OF THE P_N^R - TREE

A. Theorem

The Wiener Lower Sum of a P_n^r -tree is $W^L(P_n^r)$ =

$$\frac{n(n^2-1)+3r^3-3(n-2)r^2+3(n-1)(n+3)r}{6}$$

Proof

Let P_n be a path tree with n vertices then the Wiener Lower Sum of P_n is

$$W^L(P_n) = {}^{n+1}C_3$$

ie) $$W^L(P_n) = \frac{n(n^2-1)}{6}$$

Adding one pendant edge u_nv_1 to the end vertex then the Wiener Lower Sum is

$W^L(P_n^1) = W^L(P_n) + \sum \delta(v_1, u_i)$,

where

$1 \le i \le n$,

$\delta(v_1, u_i)$ – minimum distance between vertices v_1 and u_i

$$W^L(P_n^1) = W^L(P_n) + \frac{n(n+1)}{2}$$

Again adding another pendant edge $u_{n-1}v_2$ to the last but one end vertex then the Wiener Lower Sum is

$$W^L(P_n^2) = W^L(P_n^1) + \sum \delta(v_2, u_i) + \sum \delta(v_1, v_2),$$

where

$1 \le i \le n$,

$\delta(v_2, u_i)$ – minimum distance between vertex v_2 to all the vertices of P_n^1

$$W^L(P_n^2) = W^L(P_n^1) + \frac{(n-1)n}{2} + 2 + 3$$

Also, again adding one more pendant edge $u_{n-2}v_3$ to the last but two end vertices then the Wiener Lower Sum is

$$W^L(P_n^3) = W^L(P_n^2) + \sum \delta(v_3, u_i) + \sum \delta(v_3, v_k)$$

where

$1 \le i \le n$ and $1 \le k < 3$

$\delta(v_3, u_i)$ – minimum distance between vertex v_3 to all the vertices of P_n^2

$$W^L(P_n^3) = W^L(P_n^2) + \frac{(n-2)(n-1)}{2} + (2 + 3) + (3 + 4)$$

Continue the process of adding pendent edge until $1 < r < n$ then the Wiener Lower Sum of P_n^r is

$$W^L(P_n^r) = W^L(P_n^{r-1}) + \sum \delta(v_r, u_i) + \sum \delta(v_r, v_k)$$

where

$1 \le i \le n$, and $1 \le k < r$, Distance between vertex v_r to all the vertices of P_n^{r-1}

$$W^L(P_n^r) = W^L(P_n^{r-1}) + \frac{(n-r+1)(n-r+2)}{2} + \sum(2+3+\ldots r \text{ terms}) + \sum(3+4+\ldots r \text{ terms})$$

$$= \frac{n(n^2-1)}{6} + \frac{r^3-3(n+1)r^2+(3n^2+6n+2)r}{6} + \frac{r(r+1)(r+2)}{6} - r + \frac{(r+1)(r+2)(r+3)}{6} - (3r+1)$$

$W^L(P_n^r)$ =

$$\frac{n(n^2-1)+3r^3-3(n-2)r^2+3(n-1)(n+3)r}{6}$$

B. Corollary

If r = 1 then the Wiener Lower Sum of P_n^1 – tree is

$$W^L(P_n^1) = \frac{n(n^2-1)}{6} + \frac{n(n+1)}{2}$$

C. Corollary

If r = 2 then the Wiener Lower Sum of P_n^2 – tree is

$$W^L(P_n^2) = \frac{n^3 + 6n^2 - n + 30}{6}$$

D. Corollary

If r = 3 then the Wiener Lower Sum of P_n^3 – tree is

$$W^L(P_n^2) = \frac{n^3 + 9n^2 - 10n + 108}{6}$$

Properties:

- The Wiener Lower Sum of P_n^1-tree same as the Wiener Lower Sum of Path tree P_{n+1}
- ie) $W^L(P_n^1) = W^L(P_{n+1})$
  $= {}^{n+2}C_3$
- The Wiener Lower Sum of P_n^2-tree is same as the Wiener Lower Sum of F-Tree
  ie) $W^L(P_n^2) = W^L(F_n)$
- The Wiener Lower Sum of P_n^3-tree is same as the Wiener Lower Sum of E-Tree
  ie) $W^L(P_n^3) = W^L(E_n)$
- In any tree the Wiener Lower Sum and Wiener Upper Sum are equal, since there is only one path between any pair of vertices in a tre

ie) $W^L(P_n^r) = W^U(P_n^r)$

IV. PROGRAM

/*Wiener Lower Sum of P_n^r – Tree*/

```
#include<stdio.h>
#include<conio.h>
void main()
  {
    int i,j,k,n,s=0,r,c;
    clrscr();
    printf("\nNo of Vertices in G :N - \t");
    scanf("%d",&n);
    printf("\nNo of Pendent in G : r - \t");
    scanf("%d",&r);
    for(i=1;i<n;i++)
           {
             for(j=i;j<n;j++)
               s=s+i;
           }
    for(i=1,c=1;i<=r;i++,c=1)
           {
             for(j=i;j<=n;j++,c++)
                s=s+c;
           }
    for(i=2,c=2;i<=r;i++,c=2)
           {
             for(j=1;j<i;j++,c++)
                s=s+c;
           }
    for(i=2,c=3;i<=r;i++,c=3)
           {
             for(j=1;j<i;j++,c++)
                s=s+c;
           }
    printf("\nWL(Pn) = \t%d",s);
    getch();
  }
```

Output

No of Vertices in G :N - 5
No of Pendent in G : r - 3
WL(Pn) = 68

V. CONCLUSION

The Wiener Lower and Upper Sum of P_n^r -Tree are useful for systems like radar tracking, remote control, communication networks and radio-astronomy etc. Estimation of the Wiener Lower Sum and the Upper sum for other graph or tree is under investigation

REFERENCES

[1] R. Balakrishnan and K. Ranganathan, “A Text book of Graph Theory”, Springer, New York, 2000
[2] A.A. Dobrynin, R. Entringer, and I. Gutman, Wiener Index of Trees: Theory and Applications, Acta appl. Math. 66 (2001), 211-249
[3] A.A. Dobrynin, I. Gutman, S.Klavzar and P. Zigert, Wiener Index of Hexagonal Systems, Acta appl. Math. 72 (2002), 247-294
[4] E. Estrada and E. Uriarte, Recent Advances on the Role of Topological Indices in drug Discovery Research, Cur.Med.Chem. 8 (2001), 1573-1588
[5] I. Gutman and O. Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin, 1986
[6] M. Miller and J. Siran, Moore Graphs and Beyond: A Survey of the Degree/Diameter Problem, The Elec. J. Combin. DS14 (2005), 1-61
[7] H. Wiener, Structural Determination of Paraffin Boiling Points, J. Amer. Chem. Soc. 69 (1947), 17-20
[8] L. Xn and X. Guo, Catacondensed Hexagonal Systems with Large Wiener Numbers, MATCH Commun. Math. Comput. Chem. 55 (2006), 137-158
[9] Wiener Index of F-Tree and E-Tree, S. Rubanraj, P. Rajkumar, International Conference in Stella Maris Colege at Chennai. Pg 216-217, 2012
[10] [Bruce E. Sagan, Yeong-Nan Yeh, “The Wiener Polynomial of a Graph”, MI 48824-1027, U.S.A.