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RESEARCH ARTICLE

WIENER INDEX OF GRAPH AMALGAMATION BY MATLAB

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ABSTRACT

The Wiener index is one of the oldest molecular-graph-based structure-descriptors. It was first proposed by American Chemist Harry Wiener in 1947 as an aid to determining the boiling point of paraffin. The study of Wiener index is one of the current areas of research in mathematical chemistry. It also gives good correspondence between Wiener index (of molecular graphs) and the physico-chemical properties of the underlying organic compounds. That is, the Wiener index of a molecular graph provides a rough measure of the compactness of the underlying molecule. The Wiener index W (G) of a connected graph G is the sum of the distances between all pairs (ordered) of vertices of G. $W(G) = \frac{1}{2}\sum_{u,v} d(u,v)$. In this paper, we give MATLAB program for computing theWiener index ofAmalgamation of cycles and paths with cycles and complete graphs.

Keywords: Distance, Wiener index, MATLAB

INTRODUCTION

A topological index is a unique value characteristic of the molecular graph and is mathematically known as the graph invariant. The topological index of a molecule is a non-empirical numerical quantity that quantifies the structure and thebranching pattern of the molecule. Therefore, the topological analysis of a molecule involves translating its molecular structure into a characteristic unique number (or index) that may be considered a descriptor of the molecule under examination. Usage of topological indices began in 1947 when chemist Harry Wiener [5] introduced Wiener index to demonstrate correlations between physicochemical properties of organic compounds and the index of their moleculargraphs. It is defined as the half sum of the distances between all pairs of vertices of G.

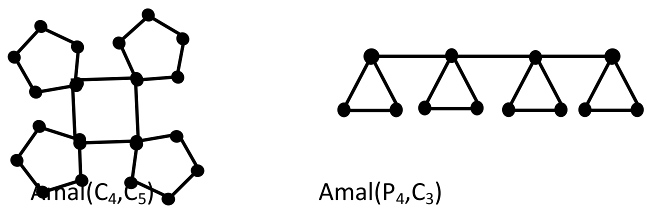
$$W(G) = \frac{1}{2}\sum_{u,v} d(u,v) = \sum_{u<v} d(u,v) = \sum_{i<j} d(u_i,u_j)$$

Where d(u,v) is the number of edges in a shortest path connecting the vertices u & v in G

2. Definition and preliminaries

In this paper, we consider finite, nontrivial, simple and undirected graphs. For a graph G, we denote by V(G) and E(G), its vertex and edge sets, respectively. Our notation is standard and mainly taken from standard books of graph theory[1]

Graph Amalgamation: Let H be a graph then graph Amalgamation G obtained by joining two or more copies of the same graph H either with common vertex or with common edge[3]. In other words, Let G and H are two graphs. Let $u \in V(G)$, $v \in V(H)$ then Amalgamation of (G, u)with(H,v) is the graph obtained by forming disjoint union of G and H and identifying u and v. It is denoted by Amal(G,H,(u,v))[2]. Let G and H are two graphs with $|V(G)| = m$ and $|V(H)| = n$. then Amalgamation of G and H is the graph obtained from taking one copyof G and n copies of H and attaching(identifying) the i^{th} vertex of G to i^{th} copy of H.



Amal(C_4,C_5) Amal(P_4,C_3)

Fig.1

Wiener index of a graph through MATLAB is given in [4] detail.Here, we find the Wiener index of Amalgamation of some standard graphs P_n and C_m,P_n and K_m , C_n and C_m , C_n and $K_m$with the extension of the earlier finding [4].

3. Wiener index of Amal(C_n, C_m)

The following program computes the Adjacency matrix of Amal(C_n, C_m) for arbitrary nand m.

```
%Adjacency matrix for Amal(Cn, Cm)
m= input('Cycle with vertices m=');
n= input('Cycle with vertices n=');
A=[];
for i=1:m:(m*n)-(2*m)+1
A(i,i+m)=1;A(i+m,i)=1;
end
for i=1:(m*n)-1
A(i,i+1)=1;A(i+1,i)=1;
if rem(i,m)==0
A(i,i+1)=0;A(i+1,i)=0;
end
end
for i=1:m:(m*n)-m+1
A(i,i+m-1)=1;A(i+m-1,i)=1;
A((m*n)-m+1,1)=1;A(1,(m*n)-m+1)=1;
end
A;
```

The following output illustrates Wiener index of Amal(C_4, C_5)

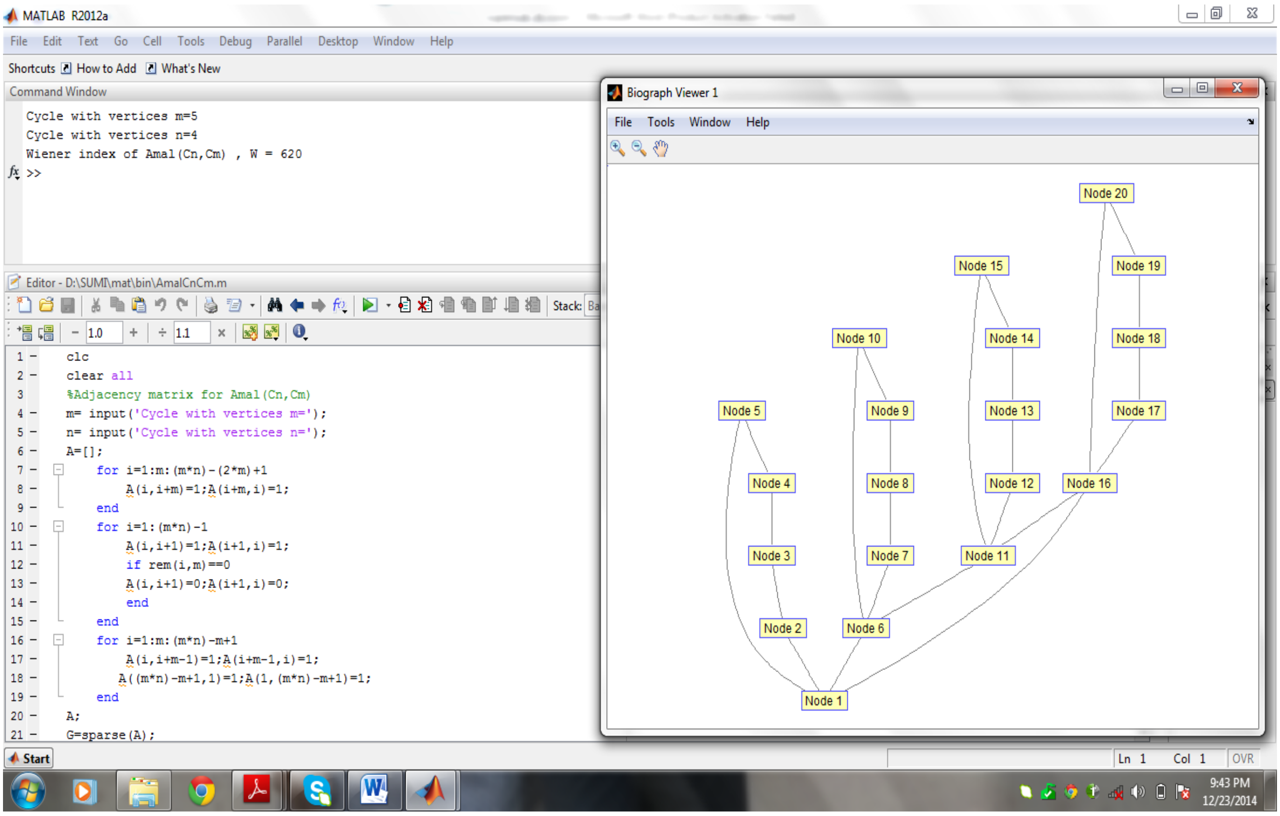


Fig.2

3.1. Wiener index of Amal(P_n, C_m)

When the symbol % is typed in the beginning of a line, the line is designated as a comment. This means that when the Enter key is pressed the line is not executed. Therefore, in the above program %A((m*n)-m+1,1)=1;A(1,(m*n)-m+1)=1;is not executed. We get aAdjacency matrix for Amal(P_n, C_m)

4. Wiener index of Amal(C_n, K_m)

The following program computes the Adjacency matrix of Amal(C_n, K_m) for arbitrary nand m.

```
%Adjacency matrix for Amal(Cn ,Km)
m= input('Complete graph with vertices m=');
n= input('Cycle with vertices n=');
A=[];
for i=1:m:(m*n)-(2*m)+1
A(i,i+m)=1;A(i+m,i)=1;
end
for i=1:(m*n)-1
A(i,i+1)=1;A(i+1,i)=1;
if rem(i,m)==0
A(i,i+1)=0;A(i+1,i)=0;
end
end
for i=1:m:(m*n)-m+1
A(i,i+m-1)=1;A(i+m-1,i)=1;
A((m*n)-m+1,1)=1;A(1,(m*n)-m+1)=1;
```

```
end
for k=1:n
for i=((k-1)*m)+1:k*m
for j=((k-1)*m)+1:k*m
if i==j
A(i,j)=0;A(j,i)=0;
else
A(i,j)=1;A(j,i)=1;
end
end
end
end
A;
```

4.1.Wiener index Amal(P_n, K_m)

The following outputillustrates Wiener index of Amal(P_3, K_4),in which program illustrates to find the Adjacency matrix of Amal(C_3, K_4).But %A((m*n)-m+1,1)=1; A(1,(m*n)-m+1)=1; is not executed. Therefore, We get a Adjacency matrix for Amal(P_3, K_4),.

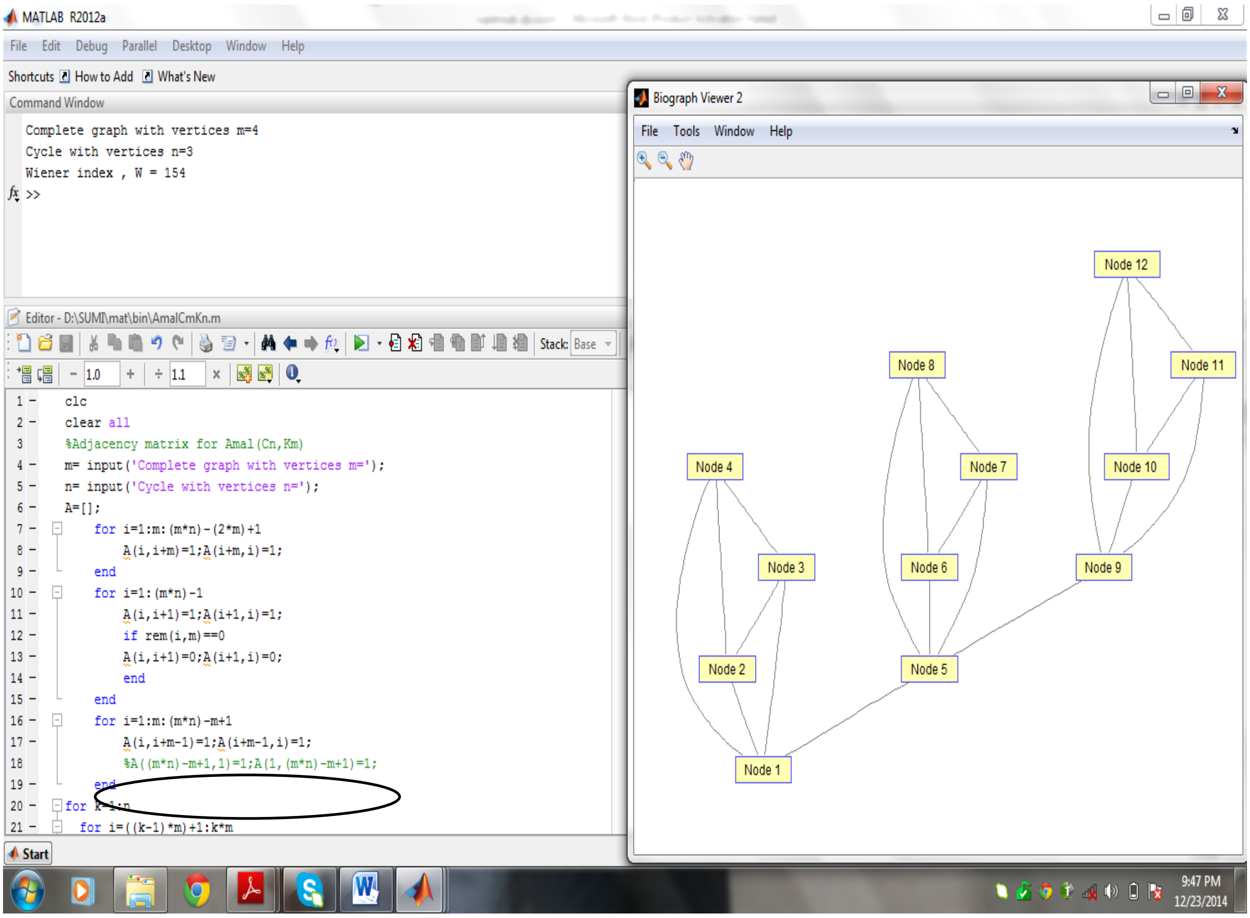


Fig.3

Table 1: **Wiener index of Amalgamation (G,H)**

S.No.	Amal(G,H)	Wiener index
1	Amal(C_{100}, C_{50})	623437500
2	Amal(C_{25}, K_{60})	9188250
3	Amal(P_{60}, C_{40})	114704000
4	Amal(P_{35}, K_{75})	46864125

CONCLUSIONS

In this paper,MATLAB Program has been presented for computing the Wiener index of Amalgamation of cycles and paths with cycles and complete graphs for arbitrary values of m,n.

REFERENCES

[1]. Balakrishnan R &Renganathan K , A Text book of graph theory, springer – verlag New York, (2000)

[2]. Murugesan .Nand Uma .R, A Conjecture on Amalgamation of Graceful Graphs with Star Graphs**,** Int. J. Contemp. Math. Sciences, Vol. 7, 2012, no. 39, 1909 – 1919.

[3]. Shigehalli V. S, Misale D. N. and ShanmukhKuchabal, On the Hyper-Wiener Index of Graph Amalgamation,Journal of computer and mathematical sciences, 2014, Vol.5(4): Pg.352-356

[4]. Thilakam K, Sumathi A, How to Compute the Wiener index of a graph using MATLAB, International Journal of Applied Mathematics& Statistical Sciences ISSN: 2319-3972; Vol. 2, Issue 5, Nov 2013, 143-148.

[5]. Wiener H, Structural determination of paraffin boiling points- J.Am chem. Soc.6 (1947) 17-20.