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Wiener Index of Some Graphs in the Context of Switching Operation

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Abstract. A topological representation of a molecule is called molecular graph. A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing the covalent bonds. These points are named vertices and the lines are named edges in graph theory language. One of the most widely known topological descriptors is Wiener index. It is named after chemist Harold Wiener who introduced in the year 1947. The Wiener index W (G) is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds. It is defined by the sum of the distances between all (ordered) pairs of vertices of G. In this paper, we find the Wiener index of switching the consecutive vertices in a cycle, path graphs.

Keywords: Adjacency Matrix, Wiener Index, MATLAB

AMS Mathematics Subject Classification (2010): 05C12, 05C85

1. Introduction

The Wiener index **W(G)** is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds introduced by Harold Wiener in 1947 for predicting boiling points **b.p** of alkanes based on the formula

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

where α, β, γ are empirical constants, and w(3) is called path number [1,9].

It is defined as the half sum of the distances between all pairs of vertices of G.

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

where d(u,v) is the number of edges in a shortest path connecting the vertices u and v in G.

Notation: [1,10] $W(G) = \frac{1}{2}\sum_{u,v\in G} d(u,v) = \sum_{u<v} d(u,v) = \sum_{i<j} d(u_i, u_j)$

2. Definitions and preliminaries

Ournotationisstandardandmainlytakenfromstandardbooksofgraphtheory.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 [2,3,4].

Let G = G(V;E) be a finite, simple graph. For a vertex $v \in V$, theoperation of switching at v transforms G to a new graph G_v by deleting alledges adjacent to v, and adding all potential edges from v to vertices notpreviously connected. This operation is known as **vertex switching, nodeswitching**, or **Seidel Switching**. It was originally introduced by J.H. van Lint and J.J. Seidel in 1966 as a tool to study equilateral point sets in elliptic spaces [5,8].

In 1973, J.J. Seidel was discussed about switching in 'A survey of two-graphs' as the operation of switching is an elegant example of a graph transformation, where the global transformation of a graph is achieved by applying local transformations to the vertices. The elegance stems from the fact that the local transformations are group actions, and hence basic techniques of group theory can be applied in developing the theory of switching. For a finite undirected graph G = (V;E) and a subset $\sigma \subseteq V$, the switch of G by σ is defined as the graph G σ = (V;E'), which is obtained from G by removing all edges between σ and its complement V - σ and adding as edges all non-edges between σ and V - σ. The switching class [G] determined (generated) by G consists of all switches G σ for subsets $\sigma \subseteq V$ [6].

In this paper, In particular we consider σbe the set of {1,2,….t} consecutive verticesand $\sigma \subset V$. In this article, we have given MATLAB Program for computing Adjacency matrix of switching the consecutive vertices in a Cycle C_n and Path P_n. This article is the continuation of the work [7] in which we had given MATLAB Program for computing Wiener index.

3. Switching the vertices in a cycle C_n

Lemma3.1. Let G be a cycle with n vertices and switching any one of its vertices then

$$\boldsymbol{W(G_v)} = \begin{cases} (n-1)^2 \; for \; n = 4,5 \\ n^2 - n - 3 \; for \; n \geq 6. \end{cases}$$

Proof: Let $v_1, v_2, \ldots, v_n$ be the successive vertices of C_n and G_v denotes graph obtained by switching one of the vertex v of G= C_n. Without loss of generality, let the switched vertex be v_1. We note that $|V(G_{v_1})|$= n and $|E(G_{v_1})|$ =2n-5.It follows immediately from the basic definition of W(G).

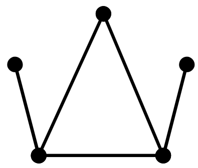

Figure 1: Switching a arbitrary vertex in C_5

Now we see, switching of t consecutive vertices in a cycle. We note that in a cycle with n vertices, maximum possibility of switching vertices be n-3. If it exceeds n-3, the graph becomes disconnected.Finding Wiener indices of the above switched graphs are very difficult when we switch the 't' consecutive vertices.

Theorem 3.2. Let G be a cycle with n vertices and switching t consecutive vertices then

$W(G_{v_i}) = n^2-(n-1)t+t^2-5$ for $1\leq t \leq n-5$, for all $n\geq6$

$= n^2-3n+6$ for $t = n-4$, for all $n\geq5$

$= (n-1)^2$ for $t = n-3$, for all $n\geq4$.

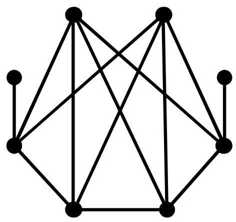

Figure 2: Switching two consecutive vertices in C_8

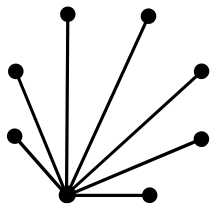

Figure 3: Switching five consecutive vertices in C_8

Switching of t consecutive vertices in a cycle C_n, where $4\leq n\leq15$ and $1\leq t\leq n-3$.

	n\t	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
	4	9											
	5	16	16										
	6	27	24	25									
	7	39	36	34	36								
	8	53	49	47	46	49							
$W(G_{v_i})$	**9**	69	64	61	60	60	64						
	10	87	81	77	75	75	76	81					
	11	107	100	95	92	91	92	94	100				
	12	129	121	115	111	109	109	111	114	121			
	13	153	144	137	132	129	128	129	132	136	144		
	14	179	169	161	155	151	149	149	151	155	160	169	
	15	207	196	187	180	175	172	171	172	175	180	186	196

Table 1: Programme for Finding Wiener index of a cycle C_n, by switching t consecutive vertices

MATLAB programme:

```
n= input('Cycle with vertices n=');
t= input('No. of consecutive  switching vertices t=');
A=[];
```

```
if n>=3&&t<=n-3
for j=t+2:n-1
for k=1:t
for i=t+1:n-1
A(i,i+1)=1;A(i+1,i)=1;
end
A(k,j)=1;A(j,k)=1;
end
end
A;
G = sparse(A);
disp('Distance matrix')
DM = graphallshortestpaths(G,'directed',false)
M=sum(sum(DM));
fprintf('Wiener index of switching, W = %d \n' , M/2)
elseif n==3||t>(n-3)
disp('Switching does not exist')
end
```

4. Switching the vertices in a path P_n

Lemma 4.1. Let G be a path with n vertices and switching one of its end vertices then
$W(G_v) = (n-1)^2$ for n = 3
= n(n-2) for n $\geq$ 4

Proof: Let $v_1, v_2, \ldots, v_n$ be the successive vertices of P_n and G_v denotes the graph obtained by switching of any one of its end vertex v of G= P_n. Without loss of generality, let the switched vertex be v_1.

We note that $|V(G_{v_1})|$= n and $|E(G_{v_1})|$=n+1. It follows immediately from the basic definition of W(G).

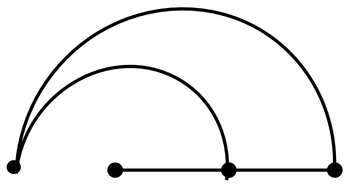

Figure 4: Switching a end vertex in P_4

Now we see, switching of t consecutive vertices in a Path.We note that in a Path with n vertices, maximum possibility of switching vertices be n-2. If it exceeds n-2, the graph tends to disconnected.

Theorem 4.1. Let G be a Path with n vertices and switching t consecutive vertices {1,2,…t} then

$W(G_{v_i}) = n^2 – n + t(1-n) + t^2 - 2, 1 \leq t \leq n-3, n \geq 5$

$= n(n-2)$ for $t = n-3$ for all $n=4$.

$= (n-1)^2$ for $t = n-2$ for all $n \geq 3$.

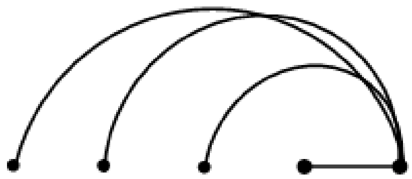

Figure 5: Switching 2 consecutive vertices in P_5,

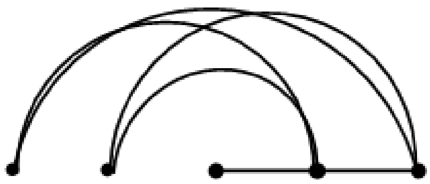

Figure 6: Switching 3 consecutive vertices in P_5

	n\t	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**
	3	4												
	4	8	9											
	5	15	14	16										
	6	24	22	22	25									
W(	**7**	35	32	31	32	36								
	8	48	44	42	42	44	49							
	9	63	58	55	54	55	58	64						
	10	80	74	70	68	68	70	74	81					
	11	99	92	87	84	83	84	87	92	100				
	12	120	112	106	102	100	100	102	106	112	121			
	13	143	134	127	122	119	118	119	122	127	134	144		
	14	168	158	150	144	140	138	138	140	144	150	158	169	
	15	195	184	175	168	163	160	159	160	163	168	175	184	196

Table 2: The above table illustrates Switching of t consecutive vertices in a path $P_{n,}$ Where $3 \leq n \leq 15$ and $1 \leq t \leq n-2$

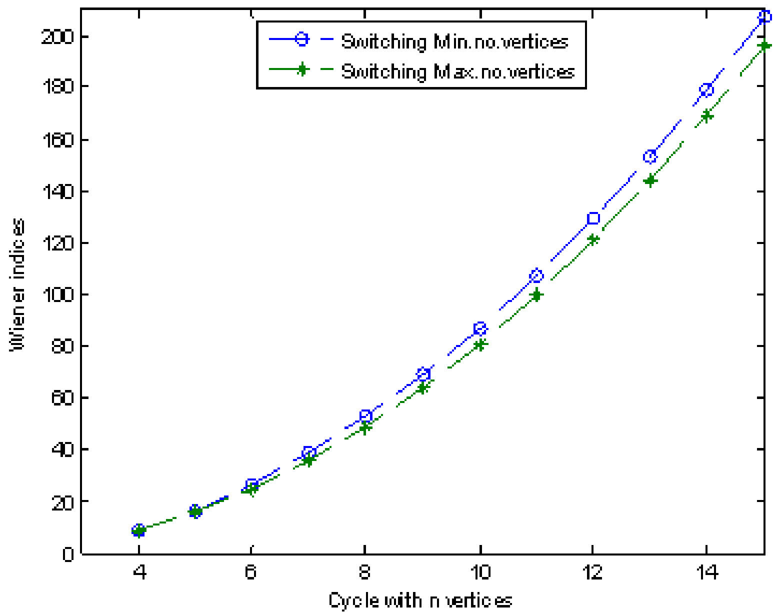

Figure 7: Comparison of Wiener index of cycle with respect to switching vertices

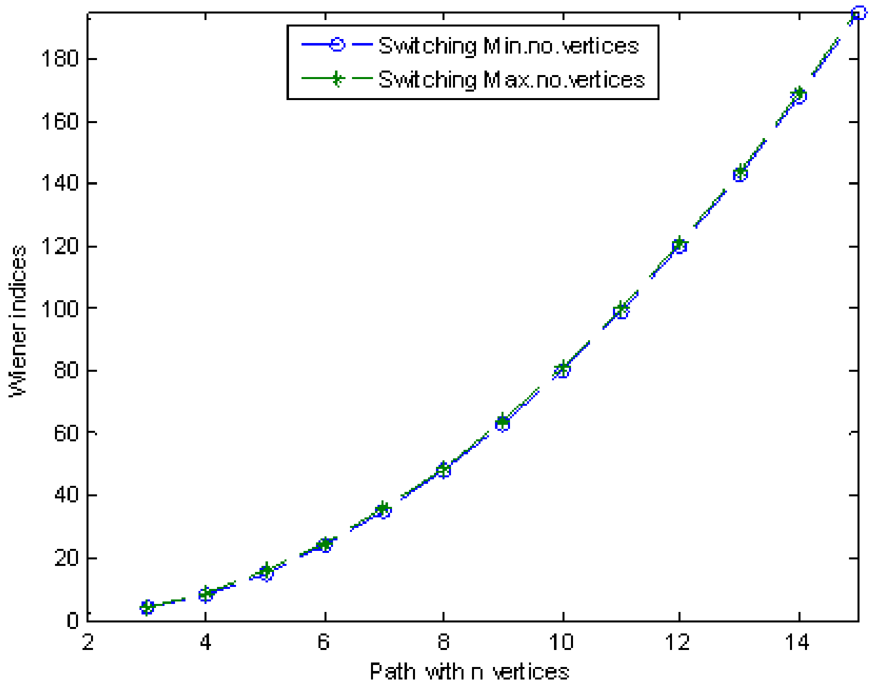

Figure 8: Comparison of Wiener index of path with respect to switching vertices

5. Conclusion

In this paper, we have determined the Wiener index of switching a particular vertex, consecutivevertices in a cycle, pathgraphsand compared the maximum and minimum Wiener indices with respect to the switching vertices in MATLAB Approach.

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