Abstract: The Wiener index is the one of the oldest and most commonly used topological indices in the quantitative structure-property relationships. It is defined by the sum of the distances between all (ordered) pairs of vertices of G. In this paper, we use MATLAB program for finding the Wiener index of the vertex weighted, edge weighted directed and undirected graphs

Keywords: Distance Sum, MATLAB, Sparse Matrix, Wiener Index

I. Introduction

The Wiener index $W(G)$ is a distance-based topological invariant, it much used in the study of the structure-property and the structure-activity relationships of several classes of biochemically interesting compounds introduced by Harold Wiener in 1947 for predicting boiling points (b,p) of alkanes based on the formula $b,p = \alpha W + \beta\omega(3) + \gamma$, where $\alpha, \beta, \gamma$ are empirical constants, and $\omega(3)$ is called path number. It was the first application of the Wiener index in 1947[11, 12]. In a sequence of the papers published in the following years, he pointed out the versatility of his index in structure property investigations. It is defined as the half sum of the distances between all pairs of vertices of G. $W(G) = \frac{1}{2} \sum_{u,v \in G} d(u,v)$. Various algorithms for the calculation of the Wiener index have been proposed in the chemical literature[5,6,7,8]. In this paper, we find $W(G)$ in minimum timewith the help of MATLAB through Adjacency matrix of a graph and existing formula of Wiener index. Especially it is convenient for the calculation of W of moderately large molecule. The Adjacency matrix of a graph G with n vertices and no parallel edges is an n by n matrix A(G) defined as

\[ a_{ij} = \begin{cases} 1, & \text{if there is an edge between } i \text{th and } j \text{th vertices and} \\ 0, & \text{if there is no edge between them} \end{cases} \]

Notation:[11, 12, 13]

\[ W(G) = \frac{1}{2} \sum_{u,v \in G} d(u,v) = \sum_{u,v} d(u,v) = \sum_{i,j} d(u_{ij}) \]

Let d(u, v) denote the length of a shortest path in G between u and v. If no such path exists, we defined(d(u, v) = $\infty$. Generally, the Floyd-Warshall algorithm and Johnson’s algorithm are the most well-known algorithms. In recent back, we have discussed the W(G) of undirected unweighted graph[10]. In this paper, we have determined Wiener index of a weighted graph and directed graph using Johnson’s algorithm through MATLAB. In MATLAB, N-by-N sparse matrix represents a graph. Where, sparse matrix is a matrix in which most of the elements are zero. By contrast, if most of the elements are nonzero, then the matrix is considered dense. The fraction of zero elements (non-zero elements) in a matrix is called the sparsity (density). Nonzero entries in matrix G represent the weights of the edges. By default, it gets weight of the edges for undirected graph as one. Johnson's algorithm has a time complexity of $O(N^{*}\log(N)+N^{*}E)$, where N and E are the number of nodes and edges respectively.

II. Algorithm For Finding Wiener Index Of Vertex Or Edge Weighted Directed / Undirected Graph

Let G be a given connected graph with n vertices.

**Input:** Adjacency list and Weights of vertices (edges) of a directed (undirected) graph G

**Step 1:** Determine sparse matrix G

**Step 2:** Determine Distance Matrix D of G

**Step 3:** Find Wiener index W of G

**Output:** Resulting Graph G and its Wiener Index
III. Finding The Wiener Index Of Weighted Undirected Graph

3.1 Wiener Index of Vertex–Weighted Graphs

A vertex–weighted graph \((G,w)\) is a graph \(G\) together with a function \(w : V(G) \rightarrow \mathbb{N}^*\). (Evidently, we could have chosen for vertex–weights (positive) real numbers. For the present considerations, however, weighting of the vertices with positive integers will suffice.) From now on vertex–weighted graphs in which all weights are positive integers will be called simply weighted graphs. The Wiener number \(W(G,w)\) of a weighted graph \((G,w)\) is defined as

\[
W(G,w) = \frac{1}{2} \sum_{u,v \in V(G)} w(u)w(v)d_G(u,v)
\]

Note that if \(w(u) = 1\) holds for all vertices \(u \in V(G)\), then \(W(G,w) = W(G)\). More generally, if \(w\) is a constant function, say \(w \equiv m\), then \(W(G,w) = m^2W(G)\). Observe also that if the distance matrix of a graph \(G\) is given, then it is no more difficult to compute \(W(G,w)\) than \(W(G)\). \([2,9]\)

The following Example illustrates finding \(W\) of weighted cycle graph through \(A(G)\) and \(w(u_i)\), \(i=1\) to \(n\).

**Numerical Example:1**

```matlab
clear all
n = input('Cycle with vertices n=');
M = input('weights of the vertices in matrix form=');
A=[];
for i=1:n-1
    A(i,i+1)=1;A(i+1,i)=1;
end
A(1,n)=1;A(n,1)=1;
G=sparse(A);
D = graphallshortestpaths(G,'directed',false)
W =((M*D)*M')/2
fprintf('Wiener index of Cn, W = %d
', W);
```

Wiener indices of weighted graphs, as defined above, seem not to be previously studied (in either mathematical or chemical literature). Exceptionally, one of the present authors did some work \([4]\) on \(W(G,w)\), where the weight \(w(u)\) was set to be equal to the degree of the vertex \(u\).

The following Example illustrates finding \(W\) of weighted cycle graph through \(A(G)\) and defined \(w(u_i), i=1\) to \(n\).

**Numerical Example:2**

```matlab
clear all
n = input('Cycle with vertices n=');
A=[];
for i=1:n-1
    A(i,i+1)=1;A(i+1,i)=1;
end
A(1,n)=1;A(n,1)=1;
G=sparse(A);
D = graphallshortestpaths(G,'directed',false)
M=degree of u_i in matrix form
W =((M*D)*M')/2
fprintf('Wiener index of Cn, W = %d
', W);
```
Execution of the Example 2
For instance, the following is the execution of simple MATLAB Program in the command window for the vertex weighted cycle undirected graph with n=10

Note that in MATLAB, `toc` syntax stops a stopwatch timer started by the `tic` function, and displays the time elapsed in seconds. `toc(ticID)` syntax displays the time elapsed since the tic command corresponding to `ticID`. `elapsedTime = toc` syntax stores the elapsed time in a variable. `elapsedTime = toc(ticID)` syntax stores in a variable the time elapsed since the tic command corresponding to `ticID`. The output argument `elapsedTime` is the Scalar double, it represents the time elapsed between tic and toc commands, in seconds. [1, 14]

3.2 Wiener Index of Edge-Weighted Undirected Graph
In MATLAB, \( D = \text{graphallshortestpaths}(G) \) finds the shortest paths between every pair of nodes in the graph represented by matrix \( G \), using Johnson's algorithm. Nonzero entries in matrix \( G \) represent the weights of the edges. Elements in the diagonal of this matrix are always 0, indicating the source node and target node are the same. A 0 not in the diagonal indicates that the distance between the source node and target node is 0. An Inf indicates there is no path between the source node and the target node.

IV. Finding The Wiener Index Of Un Weighted/Weighted Directed Graph
A directed graph \( G \) is given by a set of vertices \( V = V(G) \) and a set of ordered pairs of vertices \( E = E(G) \) called directed edges or arcs. The number of vertices of \( G \) is denoted by \( n \) and the number of arcs is denoted by \( m \). A (directed) path in \( G \) is a sequence of vertices \( v_0, v_1, ..., v_n \) such that \( v_{i-1}, v_i \) is an arc of \( G \) for all \( i \). The distance \( d(u, v) \) is the length of a shortest path from \( u \) to \( v \). In digraphs, in general \( d(u, v) = d(v, u) \) does not hold. [3]
The following program illustrates finding \( W \) of directed graph

**Program 4.1**

```matlab
clc
clear all
n= input('Graph with vertices n=');
A=[ ];
for
    ....
    ....
end
A;
DG=sparse(A);
DM = graphallshortestpaths(DG,'directed',true)
W=sum(sum(DM));
fprintf('Wiener index of a Graph, W = %d
', W);
view(biograph(DG,[],'ShowArrows','on','ShowWeights','off'))
```

**Execution of the Numerical Example 4.2**

For instance, the following is the execution of simple MATLAB Program in the command window for the edge weighted cycle digraph with \( n=4 \). The program asks the user to enter the number of vertices of \( G \). Nonzero entries in the matrix of directed graph \( G \) represent the weights of the edges. Therefore we define the Adjacency matrix of some particular digraph \( G \) with weights.
V. Conclusion

With the help of above MATLAB program, we can easily find out the Wiener index of vertex weighted, edge weighted undirected and directed molecular graphs with large molecular size in shortest time.

VI. References

[9] Sandi Klavžar, Ivan Gutman ,Wiener number of vertex-weighted graphs and a chemical application