International Journal of Applied Mathematics
& Statistical Sciences (IJAMSS)
ISSN(P): 2319-3972; ISSN(E): 2319-3980
Vol. 2, Issue 5, Nov 2013, 143-148

International Academy of Science, Engineering and Technology
Connecting Researchers; Nurturing Innovations

HOW TO COMPUTE THE WIENER INDEX OF A GRAPH USING MATLAB

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ABSTRACT

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. It is defined by the sum of the distances between all (ordered) pairs of vertices of G. In this paper, we give MATLAB Algorithm for finding the Wiener index of the graph (molecular graph)

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

1. INTRODUCTION

Graph theory is the study of graphs, mathematical structures used to model pair wise relations between objects from a certain collection. A "graph" in this context refers to a collection of vertices or 'nodes' and a collection of *edges* that connect pairs of vertices.

In chemical graph theory, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. A chemical graph is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Its vertices are labeled with the kinds of the corresponding atoms and edges are labeled with the types of bonds.[7]

A hydrogen-depleted molecular graph or hydrogen-suppressed molecular graph is the molecular graph with hydrogen vertices deleted.

A representation of an object giving information only about the number of elements composing it and their connectivity is named as topological representation of an object. 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. The advantage of topological indices is in that they may be used directly as simple numerical descriptors in a comparison with physical, chemical or biological parameters of molecules in Quantitative Structure Property Relationships (QSPR) and in Quantitative Structure. Activity Relationships (QSAR).One of the most widely known topological descriptor is the Wiener index named after chemist Harold Wiener.[14] Wiener index correlates well with many physico-chemical properties of organic compounds and as such has been well studied over the last quarter of a century.[11]

Molecular descriptor is a final result of a logic and mathematical procedure which transforms chemical information encoded with in a symbolic representation of a molecule into a useful number or the result of some standardized experiment.[4] [10][13]

This approach is especially used in computer processing of molecular structures, ranging from chemical editors to database searching. The shortest path problem can be defined for graphs whether undirected, directed, or mixed. All graphs considered in this paper are undirected and un weighted.

The most important existing algorithms for solving this problem are:

- Dijkstra's algorithm solves the single-source shortest path problems.
- Bellman–Ford algorithm solves the single-source problem if edge weights may be negative.
- A* search algorithm solves for single pair shortest path using heuristics to try to speed up the search.
- Floyd– War shall algorithm solves all pairs shortest paths.
- Johnson's algorithm solves all pairs shortest paths, and may be faster than Floyd–War shall on sparse graphs.

Like the above distance algorithms, many software languages are also used to solve the shortest path problem in graph theory. In a similar way, apart from this, more researchers use the methods like SEMS Method through labeling, Matching, Embedding, Cut method, Minimum spanning tree method for finding Wiener indices.[2] [3] [12] [15] Here we have attempted with the help of MATLAB.

1.1. About MATLAB

It is a high-level language and interactive environment for numerical computation, visualization, and programming. Using MATLAB, we can analyze data, develop algorithms, and create models and applications. The language, tools, and built-in math functions enable us to explore multiple approaches and reach a solution faster than with spreadsheets or traditional programming languages, such as C/C++ or Java.[8]

1.2. Definition

Our notation is standard and mainly taken from standard books of graph theory. All graphs considered in this paper are simple and connected. The vertex and edge sets of a graph Garede noted by V (G) and E (G) respectively.

The **distance** d (u,v) between the vertices u and v of the graph G is equal to length of the shortest path that connects u and v.

The Wiener index **W(G)** is a distance-based topological invariant is also a molecular descriptor, it 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 ($\boldsymbol{b.p}$) of alkanes based on the formula

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

where$\boldsymbol{\alpha, \beta, \gamma}$ are empirical constants, and **w(3)** is called path number. It is defined as the half sum of the distances between all pairs of vertices of G.[1] [5] [6] [9]

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

Notation

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

2. ALGORITHM FOR FINDING WIENER INDEX

Let G be a given connected graph with n vertices.

Input: Adjacency Matrix of G.

Step 1: Define adjacency matrix A of G

Step 2: Determine sparse matrix G

Step 3: Determine Distance Matrix D of G

Step 4: Find Wiener index W of G

Output: Resulting Graph G and its Wiener Index of G

3. PROGRAM FOR FINDING WIENER INDEX

```
%This MATLAB Program calculates the Wiener index of G

clc

clearall

A = input ('Adjacency Matrix');

G = sparse(A);

D = graphallshortestpaths(G, 'directed', false)

M = sum(sum(D));

fprintf ('Wiener index W = %d \n' , M/2);

UG = tril(G + G');

view (biograph(UG,[],'Show Arrows', 'off',' Show Weights', 'off'))
```

Note

We must predefine the Adjacency Matrix ‘A’ of the graph, before coding the program, as adjacency matrix is not common for all the graphs. If we have Adjacency Matrix of G, then we can immediately run the Program.

The only complexity of this program is that, for any graph G, it is very hard to give the adjacency list as an input if the order of G is large. To overcome this complexity, we must add the coding for finding the adjacency list.

3.1. Advantages

- It takes less execution time than the other algorithms.
- We can see the resulting(Output) graph with the corresponding Wiener Index
- It is also used to find the Wiener Index for directed, weighted graph having some modifications

Note: If any value in i or j is larger than 2^31-1 for 32-bit platforms, or 2^48-1 on 64-bit platforms, then the sparse matrix cannot be constructed.

4. EXECUTION OF THE PROGRAM

For instance, the following is the execution of simple MATLAB Program in the command window for ‘cycle with four nodes’

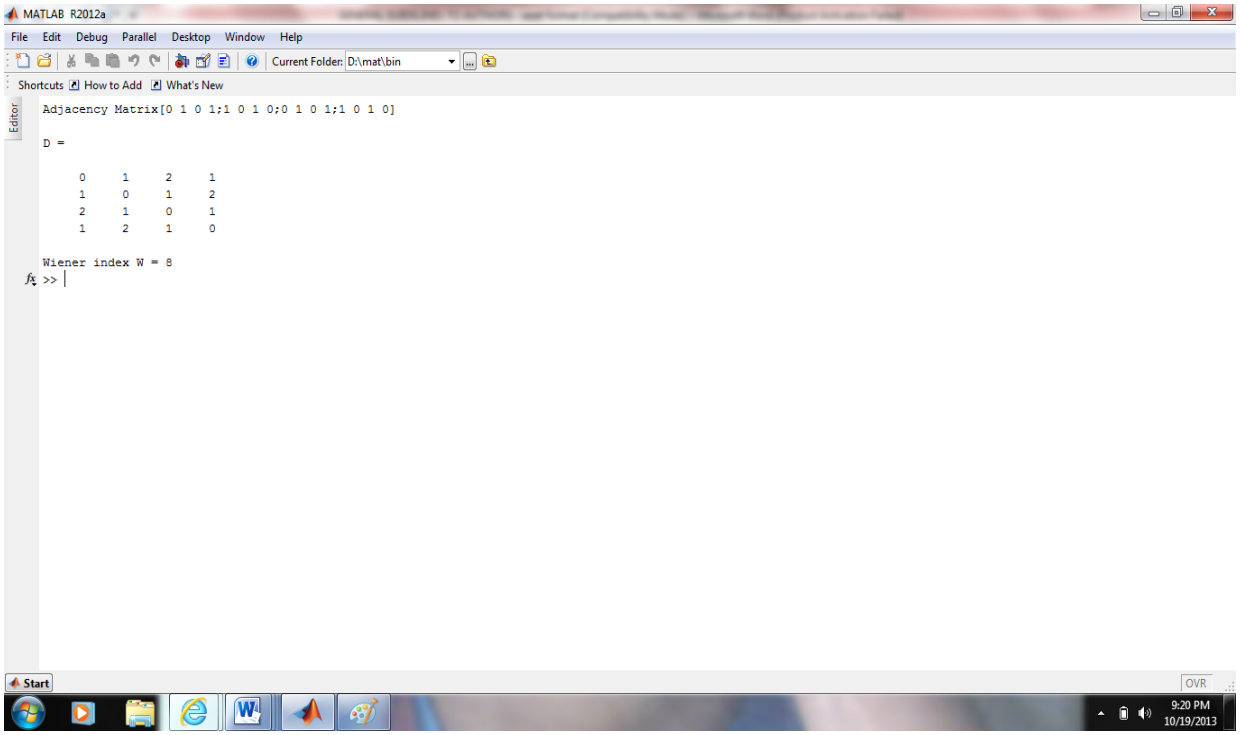

Figure 1

The graph generated by the program is shown below

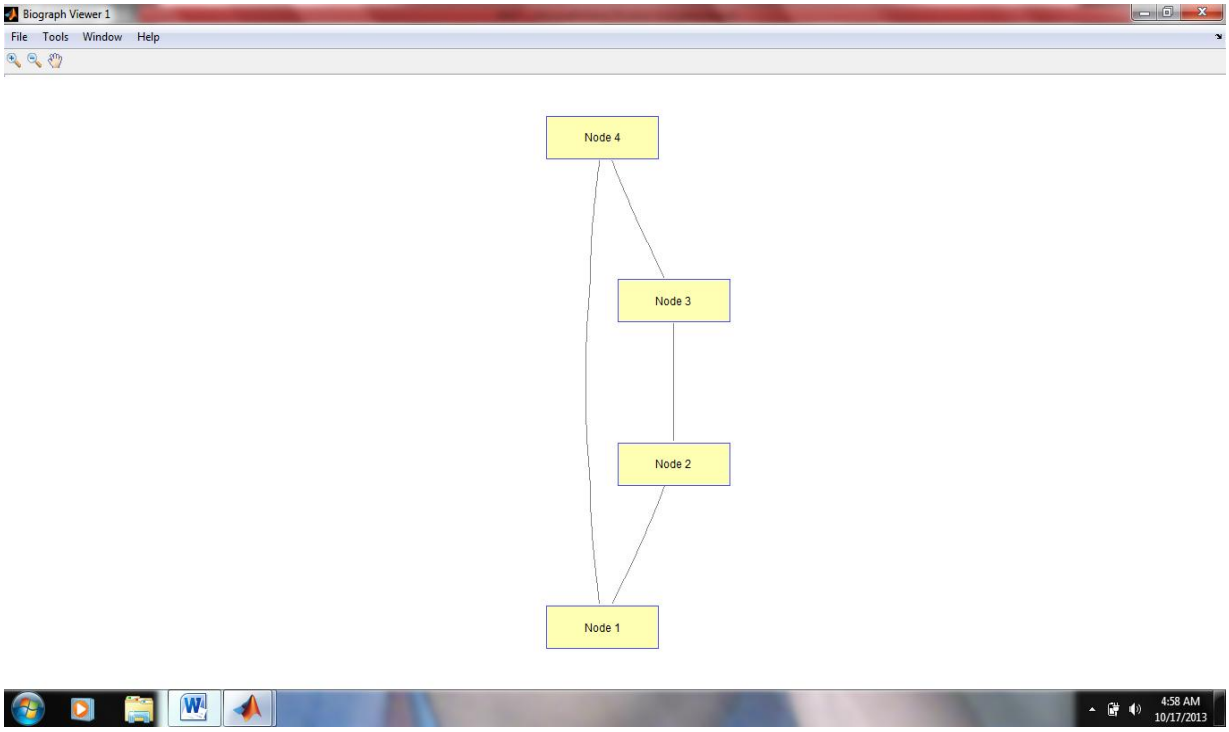

Figure 2

5. CONCLUSIONS

With the help of the MATLAB program, we can easily find out the Wiener index with the extension of shortest path between every pair of vertices of a graph. Other topological indices like Hyper Wiener index etc. can also be found with some slight modifications.

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