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Wiener index of chemical trees from its subtree

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ABSTRACT

In chemical graph theory, Wiener index is a topological index of a molecule, defined as the sum of the lengths of the shortest paths between all pairs of vertices in the chemical graph representing the non-hydrogen atoms in the molecule. Calculation of Wiener index is usually done using distance matrix. For any matrix calculation smaller the matrix, better and fast are the computations. This paper aims to obtain the Wiener index of chemical trees by reducing the size of the distance matrix.

Key words: Wiener index, Distance matrix, Graph, Tree, Path.

INTRODUCTION

Mathematics is always used in graph theory in various ways. In [1] amino acid trees and Huffmann codes are used for arriving at a new genetic code. In [2] periodic table is used in drug encryption. Graph theory is one area of mathematics extensively used in chemistry.

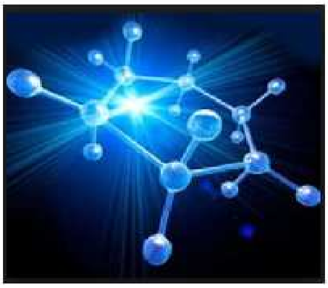
Wiener index has fast screening of ligands/molecules as it can be directly calculated from molecular structure, so its use in QSAR models is of immense utility compared to experimentally determined physicochemical parameters that are not always available for a particular molecular structure [3]. Calculation of Wiener index is usually done using distance matrix. This paper aims to reduce the size of the chemical graph. So the size of the distance matrix is smaller. This means the computational complexity of calculation of the Wiener index is reduced. The proposed method finally generates the Wiener index of the original chemical graph from this matrix.

Preliminary Note
In this section we provide the basic details of Wiener index and chemical graph that is required in the proposed calculation.

Wiener Index
In chemical graph theory, the Wiener index (also Wiener number) is a topological index of a molecule, defined as the sum of the lengths of the shortest paths between all pairs of vertices in the chemical graph representing the non-hydrogen atoms in the molecule [4].

Chemical Graph
In chemical graph theory and in mathematical chemistry, 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.[1] For particular purposes any of the labeling may be ignored [5].

In the Fig 1 the snapshot [6] on the left side is an example of a chemical graph and the graph on the right side is its respective graph structure.



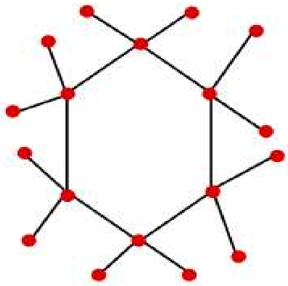


Fig. 1Wiener Index Calculation Using Distance Matrix

Snap shot 1 provides a method of Wiener index calculation using distance matrix [7].

The Wiener index can be defined for an arbitrary connected graph as follows. Without loss of generality, assume that G has vertices $1, 2, \ldots, n$. For each pair i, j of vertices, let d_{ij} denote the distance in G between i and j; i.e. the length of the shortest path between i and j. The distances d_{ij} form the so-called *distance matrix* $D(G) = [d_{ij}]$ of the graph G. The Wiener index of G is the number

$$W(G) = \sum_{i=1}^{n} \sum_{j=1}^{i} d_{ij} = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij} .$$

$UCJD_p$

	1	2	3	4	5	6	7	8	VS_i
1	0	1	1	1	1	1	1	1	7
2	7	0	3	3	3	3	7	3	29
3	5	5	0	5	5	5	5	7	37
4	3	3	3	0	6	6	3	3	27
5	2	2	2	2	0	7	2	2	19
6	1	1	1	1	1	0	1	1	7
7	1	1	1	1	1	1	0	1	7
8	1	1	1	1	1	1	1	0	7
CS_j	20	14	12	14	18	24	20	18	140

Wiener index $(W) = 70$

hyper-Cluj-distance index $(CJD_p) = 143$

D_UCJD_p

	1	2	3	4	5	6	7	8	VS_i
1	0	1	2	3	4	5	2	3	20
2	7	0	3	6	9	12	7	6	50
3	10	5	0	5	10	15	10	7	62
4	9	6	3	0	6	12	9	6	51
5	8	6	4	2	0	7	8	6	41
6	5	4	3	2	1	0	5	4	24
7	2	1	2	3	4	5	0	3	20
8	3	2	1	2	3	4	3	0	18
CS_j	44	25	18	23	37	60	44	35	286

$D^UCJD_p = 143$

$D^2CJD_p = 605$

Snapshot 1

The Wiener index of a path with n – vertices is $n\frac{(n^2-1)}{6}$ [8].

MATERIALS AND METHODS

Wiener Index of a Tree from Sub tree

A Wiener index is the sum of the values of the distance between non hydrogen molecules. Wiener index is also calculated using distance matrix. Representation as a matrix enables easy calculation of the wiener index. In any calculation using matrices, as the size of the matrix decreases easy is the computation, either by manual calculation or calculation with aid of programs. Our main idea is to reduce the size of the distance matrix as far as possible still possible to calculate the Wiener index.

We shall discuss calculation of Wiener index for a tree, since in a tree there is exactly one path between every pair of vertices and easy for discussion.

Tree Reduction

In calculation of Wiener index, it is known that the Wiener index of any path of length n is $n\frac{(n^2-1)}{6}$. For example for path P_3, the value of the Weiner index is calculated as follows

Fig. 2

From vertex 1 the distance values are 1, 2, 3. From 2 the values are 1, 2 and from 3 it is 1 so the value is 12. We use any path as the basic subgraph that will be deleted from any graph. As an illustration consider the following graph in Fig. 3 .

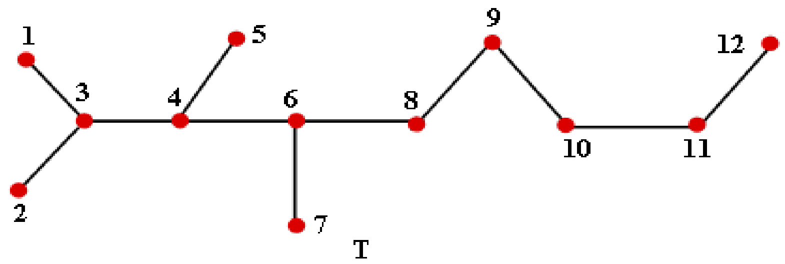


Fig. 3

We try to find a longest possible path that can be a subgraph of the graph and whose removal will not disconnect the graph. The possible path is from vertex 3 to 6 of length3. On removing this subgraph that is a path the graph in Fig . 3 gets reduced to the graph in Fig. 4 .

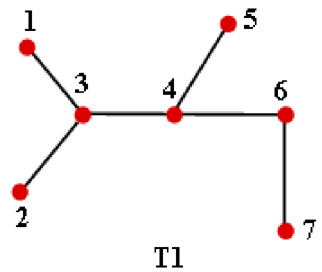


Fig. 4

This is the first part of the calculation, that is reducing the tree to a smaller tree. We basically track out a longest possible subgraph of the tree that is a path, whose removal will not disconnect the original tree.

Labelling of the Subtree

Let u be the vertex to which the longest path is attached. Let P_m be the path with m edges that has been removed. Now we redraw T1 so that it is rooted at u. For the tree T1 in Fig. 4. the rooted tree is as in Fig. 5.

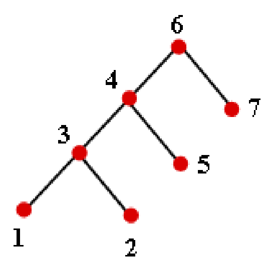


Fig. 5

For vertex u assign the value $\sum_{i=1}^{m} i$. This is because in the original tree T we need to calculate the distance from u to all the vertices in Pm. This value will be $\sum_{i=1}^{m} i$. For a next level vertex the distance value for the vertices in P_m is 2 + 3 + …. + (m+1). So for the next level vertices we assign a label $\sum_{i=1}^{m} i$ + m. For the next level vertices the distance values for the vertices in P_m is 3 + 4 + … + (m + 2). So for the next level vertices we assign a label $\sum_{i=1}^{m} i$ + 2m. In general for a tree rooted at u we assign labels as follows

Label of u = $\sum_{i=1}^{m} i$

For vertices at level k assign label $\sum_{i=1}^{m} i$ + km, k = 1, 2, ….., z where z is the height of the tree.

For the tree in Fig. 5 vertex 6 is the root. 4, 7 are level 1 vertices, 3, 5 are level 2 vertices, 1, 2 are level 3 vertices. Height of the tree is 3. The path removed is of length 5. So

Label of 6 = $\sum_{i=1}^{5} i = 1+2+3+4+5 = 15$.

Label of vertices 4, 7 = $\sum_{i=1}^{5} i + m = 15+5 = 20$

Label of vertices 3, 5 = $\sum_{i=1}^{5} i + 2m = 15+10 = 25$

Label of vertices 1, 2 = $\sum_{i=1}^{5} i + 3m = 15+10 = 30$

$$\text{Wiener index of T1} = \begin{array}{c|ccccccc|c} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & \\ \hline 1 & 30 & 2 & 1 & 2 & 3 & 3 & 4 & 45 \\ 2 & - & 30 & 1 & 2 & 3 & 3 & 4 & 43 \\ 3 & - & - & 25 & 1 & 2 & 2 & 3 & 33 \\ 4 & - & - & - & 20 & 1 & 1 & 2 & 24 \\ 5 & - & - & - & - & 25 & 2 & 3 & 30 \\ 6 & - & - & - & - & - & 15 & 1 & 16 \\ 7 & - & - & - & - & - & - & 20 & 20 \end{array} = 211.$$

Wiener index of path P_4 = (1 + 2 + 3 + 4) + (1 + 2 + 3) + (1 + 2) + 1 = 20

So Wiener index of T = Wiener index of T1 + Wiener index of path P_4 = 211 + 20 = 231.

The above procedure can be summarized as follows.

Weiner Index Calculation of the Subtree
Construction of Distance Matrix D

We now calculate the Weiner index for the reduced tree T1. The off diagonal entry of the distance matrix remains the same as in any Weiner index calculation. In normal distance matrix all the diagonal entries are 0. But we assign nonzero values to the diagonal entries.

For the diagonal entry corresponding to vertex assign the value $\sum_{i=1}^{m} i$. For the remaining diagonal entries assign the value $\sum_{i=1}^{m} i$ + km, k = 1, 2, … , z. Now calculate the Weiner index as we normally calculate. The path of length m was removed from vertex u. Already vertex u is considered along with tree T1. So the Weiner index of the original tree T is the value of the Weiner index of the distance matrix D + Weiner index of the deleted path P_{m-1}, that is Weiner index of a tree with n – vertices = Wn = Weiner index of D + Weiner index of P_{m-1}.

Wiener index from reduced tree

Let T be the original tree with n – vertices

Step 1 Trace the longest possible path Pm in T so that T – { P_m } is connected.
Step 2 Let T1 = T – { u }, where u is the vertex common to T and T1.
Step 3 Redraw T1 as a rooted tree with u as the root.
Step 4 Assign labels to the vertices in T1 as follows

Label of u = $\sum_{i=1}^{m} i$

Label of level 1 vertices = $\sum_{i=1}^{m} i + m$

Label of level 2 vertices = $\sum_{i=1}^{m} i + 2m$ …..

Label of level k vertices = $\sum_{i=1}^{m} i + km$, where k is the level of the tree T1.

Step 5 Construct the distance matrix D as follows

$$a_{ij} = \begin{cases} \text{distance from i to j} & \text{if } i \neq j \\ \text{label of the corresponding vertex} & \text{if } i = j \end{cases}$$

Step 6 Calculate the Wiener index of D.

Step 7 Wiener index of T = Wiener index of T1 + Wiener index of path P_{m-1}.

RESULTS AND DISCUSSION

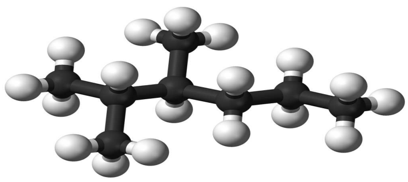
For the graph in Fig. 3 the distance matrix is

W =

	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	2	1	2	3	3	4	4	5	6	7	8	45
2	–	–	1	2	3	3	4	4	5	6	7	8	43
3	–	–	–	1	2	2	3	3	4	5	6	7	33
4	–	–	–	–	1	1	2	2	3	4	5	6	24
5	–	–	–	–	–	2	3	3	4	5	6	7	30
6	–	–	–	–	–	–	1	1	2	3	4	5	16
7	–	–	–	–	–	–	–	2	3	4	5	6	20
8	–	–	–	–	–	–	–	–	1	2	3	4	10
9	–	–	–	–	–	–	–	–	–	1	2	3	6
10	–	–	–	–	–	–	–	–	–	–	1	2	3
11	–	–	–	–	–	–	–	–	–	–	–	1	1
12	–	–	–	–	–	–	–	–	–	–	–	–	

So the Wiener index is 231 and it matches with the value calculated using the proposed procedure.

Consider 2, 3 dimethylhexane. The ball and stick structure of 2, 3 dimethylhexane is as seen in snapshot 2.



Snapshot 2

The tree representation of 2, 3 dimethylhexane is given in Fig. 6

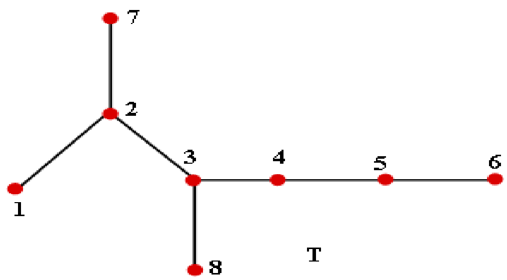
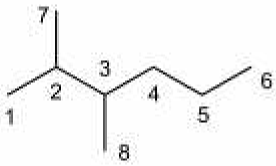


Fig. 6

The following snapshot [8] provides the Wiener index of 2, 3 dimethylhexane.

Example E7

Calculation of the expanded Wiener index and the Wiener index for 2,3-dimethylhexane.



D

	1	2	3	4	5	6	7	8	VS_i
1	0	1	2	3	4	5	2	3	20
2	1	0	1	2	3	4	1	2	14
3	2	1	0	1	2	3	2	1	12
4	3	2	1	0	1	2	3	2	14
5	4	3	2	1	0	1	4	3	18
6	5	4	3	2	1	0	5	4	24
7	2	1	2	3	4	5	0	3	20
8	3	2	1	2	3	4	3	0	18
CS_j	20	14	12	14	18	24	20	18	140

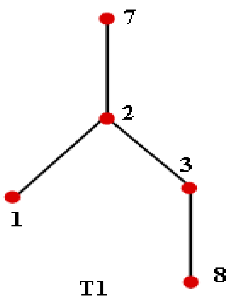
Wiener index $(W) = 70$

Snapshot 3

We now shall calculate the Wiener index of 2, 3 dimethylhexane using the proposed procedure.

We find a longest possible path that can be a subgraph of the graph and whose removal will not disconnect the graph. The path is from vertex 6 to 12 of length 5. On removing this

subgraph that is a path the graph in Fig. 6 gets reduced to the graph in Fig. 7 .



T1
Fig. 7

Redrawing this as a rooted tree we obtain the following graph in Fig. 8.

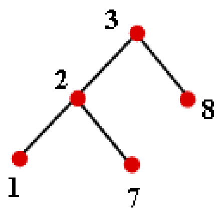


Fig. 8

For the tree in Fig. 8 vertex 3 is the root. 2, 8 are level 1 vertices, 1, 7 are level 2 vertices. Height of the tree is 2. The path removed is of length 3. So

Label of 3 = $\sum_{i=1}^{3} i = 1+2+3=6$.

Label of vertices 2 8 = $\sum_{i=1}^{3} i + m = 6 + 3 = 9$

Label of vertices 1 7 = $\sum_{i=1}^{3} i + 2m = 6 + 6 = 12$.

$$\text{Wiener index of T1} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 7 \\ 8 \end{array} \begin{array}{c} \begin{array}{ccccc} 1 & 2 & 3 & 7 & 8 \end{array} \\ \left[\begin{array}{ccccc} 12 & 1 & 2 & 2 & 3 \\ - & 9 & 1 & 1 & 2 \\ - & - & 6 & 2 & 1 \\ - & - & - & 12 & 3 \\ - & - & - & - & 9 \end{array}\right] \end{array} \begin{array}{c} \\ 20 \\ 13 \\ 9 \\ 15 \\ 9 \end{array} = 66$$

Wiener index of path P_2 = 1 + 2 + 1 = 4.

So Wiener index of T = Wiener index of T1 + Wiener index of path P_2 = 66 + 4 = 70.

This value matches with the Wiener index value as calculated in snapshot 3.

CONCLUSION

For a tree with ten vertices if a path with 3 vertices is removed, then calculation of the distance from all the remaining 6 vertices to these 3 vertices is reduced. For the diagonal entry values in the reduced distance matrix we only need to calculate the Wiener index of the path removed. All the diagonal entry values can be obtained by just addition of the path length to this value. This calculation is much easy than calculating the distance, specifically as the number of vertices increases. Also since the size of the matrix is reduced, computational complexity decreases. So this method can be adopted for much easy calculation of Wiener index.

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