ISSN: 0975-766X
CODEN: IJPTFI
Available Online through
Research Article
www.ijptonline.com

COMPUTING ECCENTRIC DISTANCE SUM OF DENDRIMERS AND NANOTUBES

***K.Balasubramanian, S.Balachandran, S.Raja Balachandar, S.G.Venkatesh**
Department of Mathematics, School of Humanities and Sciences, SASTRA University, Thanjavur-613401, India.
*Email: *k_bala27@yahoo.co.in*

Received on: 18-02-2017 *Accepted on: 29-03-2017*

Abstract.

In this paper, an algorithm is presented for computing the eccentric distance sum of any simple connected graph. Furthermore, the eccentric distance sum is computed for dendrimers $T_{k,d}$, $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes.

Keywords: Simple connected graph, Eccentric distance sum, Dendrimers, Nanotubes.

1.Introduction

An important graph theory application is the numerical characterization of chemical structures with graph invariants that can be polynomials, spectra, atomic or molecular topological indices [1, 2].

Topological indices of nanotubes are numerical descriptors that are derived from graphs of chemical compounds. Such indices based on the distances in graph are widely used for establishing relationships between the structure of nanotubes and their physicochemical properties. The main use of topological indices is that of numerical descriptors of the chemical structure in QSPR and QSAR models [3, 8, 9, 22].

Let G be a connected graph. The vertex-set and edge-set of G denoted by $V(G)$ and $E(G)$ respectively. The distance between the vertices u and v, $d(u,v)$, in a graph is the number of edges in a shortest path connecting them. Degree of a vertex u is denoted by $d(u)$.

The eccentric connectivity index $\xi(G)$ of a graph G is defined as $\xi(G)=\sum_{u\in V(G)} d(u)\varepsilon(u)$, where $\varepsilon(u)$ is the eccentricity of vertex u. The eccentric distance sum of G is defined as $\xi^d(G)=\sum_{v\in V(G)}\varepsilon(v)D_G(v)$, where $\varepsilon(v)$ is the eccentricity of the vertex v and $D_G(v)=\sum_{u\in V(G)} d(u,v)$ is the sum of all distances from vertex v. Eccentricity of a vertex u in a graph G is the path length from vertex u to vertex v that is farthest from u. The eccentric connectivity index was introduced by

Madan et al [10, 23, 25]. and used in a series of papers concerned with QSAR/QSPR studies. The study of its mathematical properties started only recently [4-7, 13, 27]. Recently, a novel graph invariant for predicting biological and physical properties – eccentric distance sum (EDS) was introduced by Gupta, Singh and Madan [11], defined as

$$\xi^d(G) = \sum_{v \in V(G)} \varepsilon(v) D_G(v).$$

This topological index has vast potential in structure activity/ property relationships; it also displays high discriminating power with respect to both biological activity and physical properties [11]. From [11], we also know that some structure activity and quantitative structure property studies using eccentric distance sum were better than the corresponding values obtained using the Wiener index.

It is also interesting to study the mathematical property of this topological index. Yu, Feng and Illic [26] identified the extremal unicyclic graphs of given girth having the minimal and second minimal EDS; they also characterized the trees with the minimal EDS among the n-vertex trees of a given diameter. Hua, Xu and Shu [12] obtained the sharp lower bound on EDS of n-vertex cacti.

In this paper, an algorithm is presented for computing the eccentric distance sum of any simple connected graph. Furthermore, the eccentric distance sum is computed for dendrimers $T_{k,d}$, $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes. Some topological indices are computed for certain nanotubes, which can be found in [14-21, 24].

In section 2..

We give an algorithm for computing the eccentric distance sum of any connected graph. Computation of the eccentric distance sum of dendrimers has been discussed in section 3. In section 4, computation of the eccentric distance sum of $VC_5C_7[p,q]$ nanotubes has been carried out. Computation of the eccentric distance sum of $HC_5C_7[p,q]$ nanotubes has been explored in section 5.

Concluding remarks are given in the final section.

2. An algorithm for computing the eccentric distance sum of any connected graph

In this section, we give an algorithm for computing the eccentric distance sum of any graph. The steps of the algorithm (EDS ALGORITHM) are as follows:

EDS ALGORITHM

Notations:

$N(i)$- Neighborhood of ith vertex

$d(i)$- Degree of ith vertex

$D_{i,t}$- The set of vertices that their distance to vertex i is equal to t $(t \geq 0)$

$\varepsilon(u) = Max\{t \setminus D_{u,t} \neq \phi\}$- Eccentricity of ith vertex

d(i,j) – Shortest distance between the vertices i and j

1. Assign every vertex with distinct numbers.
2. Find $N(i)$ for every vertex i.
3. Find $D_{i,t}$ for every vertex i with t. ($D_{i,1} = N(i)$, because the distance between vertex i and its adjacent vertices is equal to 1, For each vertex $j \in D_{i,t}$, $(t \geq 1)$, the distance between each vertex of set $N(j) \setminus (D_{i,t} \cup D_{i,t-1})$ and the vertex i is equal to $t+1$.)
4. Find $\varepsilon(i)$ for every vertex i
5. Find $D_G(i)$ for every vertex i
6. Calculate the eccentric distance sum of the graph $\xi^d(G)$

Illustrated Example.

Consider the following simple graph with five vertices and edges to explain the above procedures to find the eccentric distance sum.

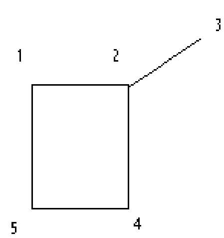

Fig 1. Sample Connected Graph with n=5.

By using the above algorithm in MATLAB, we have obtained the following values, namely N [I], $\varepsilon(i)$, $D_{i,t}, D_G(i)$, and the eccentric distance sum of Fig. 1 and they are displayed in the following table.

MATLAB output

Neighborhood of all the vertices	**Eccentricity of all the vertices**
N[1]=[2,5]; N[2]=[1,3,4]; N[3]=[2]; N[4]=[2,5]; N[5]=[1,4];	ε [1] =[2]; ε [2] =[2]; ε [3] =[3]; ε [4]=[2]; ε [5] =[3];
$D_{i,t}$ **- The set of vertices that their distance to vertex i is equal to t**	$D_G(i)$ **- the sum of all distances from vertex i**
$D_{1,0}$= [1]; $D_{2,0}$= [2]; $D_{3,0}$=[3]; $D_{4,0}$=[4]; $D_{5,0}$=[5];	$D_G(1)$=6; $D_G(2)$=5; $D_G(3)$=8; $D_G(4)$=6; $D_G(5)$=7.
$D_{1,1}$= [2,5]; $D_{2,1}$= [1,3,4]; $D_{3,1}$=[2]; D_{41}=[2,5]; $D_{5,1}$=[1,4];	
$D_{1,2}$= [3,4]; $D_{2,2}$= [5]; $D_{3,2}$=[1,4]; $D_{4,2}$=[1,3]; $D_{5,2}$=[2];	
$D_{1,3}$= []; D_{23}= []; $D_{3,3}$=[5]; $D_{4,3}$=[]; $D_{5,3}$=[3];	**Eccentric distance sum = 79**

3. Computation of the eccentric distance sum of dendrimers $T_{k,d}$

For computation of the eccentric distance sum of $T_{k,d}$, at first we assign to any vertex one number (See figure); according to this numbering, the set of vertices to each vertex, $1 \le i \le n$, and determine all of adjacent vertices set of the vertex (neighbourhood) , N[i] by NEIGHBOURHOOD ALGORITHM. Next we use EDS ALGORITHM for compute the eccentric distance sum of the $T_{k,d}$ for arbitrary values of d and k.

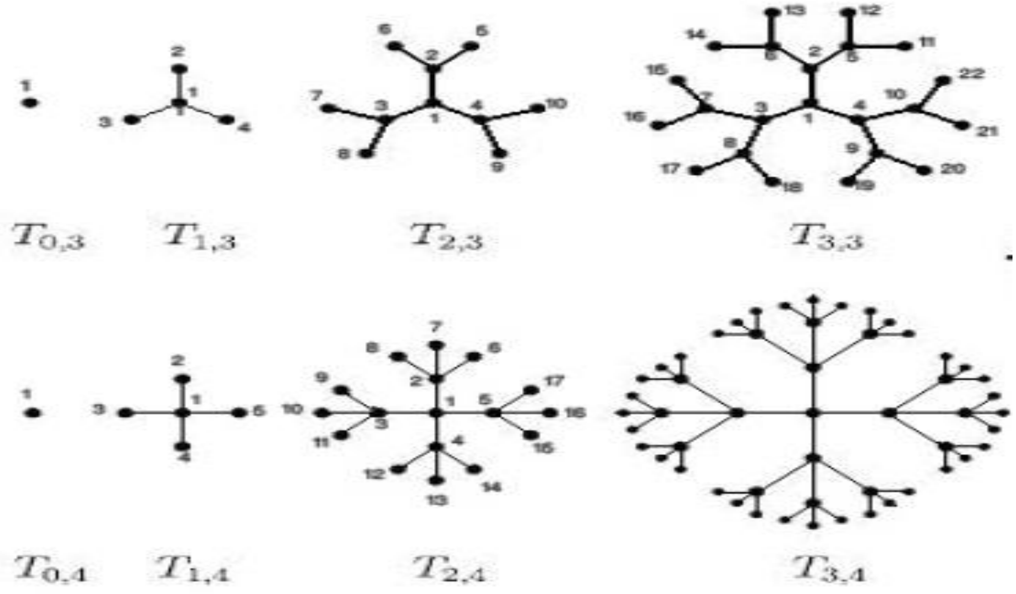

Figure 2. Molecular graphs of dendrimers $T_{k,d}$

Neighbourhood Algorithm 1.

1. Read m, a, d
2. n = 1+(d/(d-2))*((d-1)^k - 1)
3. N:=[] (array)
4. K1:=[2..d+1];
5 N[1]:=K1;
6 for each i in K1
if k=1 then N[i]:=[1]
else
N[i]:=[(d-1)*i+4-d..(d-1)*i+2]
Add(N[i],1)
End if
End for
	7. K2:=[d+2..1+(d/(d-2))*((d-1)^(k-1) - 1)]
	8 for each i in K2
	N[i]:=[(d-1)*i+4-d..(d-1)*i+2]
	Add(N[i],Int((i-4+d)/(d-1)))
	End for
	9. K3:=[2+(d/(d-2))*((d-1)^(k-1) - 1)..n]
	10 for each i in K3
	if k=1 then N[i]:=[1]
	else
	N[i]:=[Int((i-4+d)/(d-1))]
	End if
	End for

In table 1, the eccentric distance sum for various values of d,k and n have been given where n represents the number of vertices.

d	k	n	Eccentric Distance Sum
3	1	4	33
3	2	10	849
3	3	22	9951
4	1	5	60
4	2	17	2996
4	3	53	71440
4	4	161	1254768
5	1	6	95
5	2	26	7805
5	3	106	315855
5	4	426	9579345
5	5	1706	249111955

Table 1. Eccentric Distance Sum for $T_{k,d}$

4. Computation of the eccentric distance sum of $VC_5C_7[p,q]$ nanotubes

A C_5C_7 net is a trivalent decoration made by alternating C_5 and C_7. It can cover either a cylinder or a torus. In this section we compute the eccentric distance sum of $VC_5C_7[p,q]$ nanotubes.

We denote the number of pentagons in the first row by p, in this nanotubes the four first rows of vertices and edges are repeated alternately, we denote the number of this repetition by q.

In each period there are $16p$ vertices and $3p$ vertices which are joined to the end of the graph and hence the number of vertices n in this nanotube is equal to $16pq+3p$.

We partition the vertices of the graph to the following sets:

K_1 : The vertices of the first row whose number is $6p$.

K_2 : The vertices of the first row in each period except the first one whose number is

$6p(q-1)$.

K_3 : The vertices of the second row in each period whose number is $2pq$.

K_4 : The vertices of the third row in each period whose number is $6pq$.

K_5 : The vertices of the fourth row in each period whose number is $2pq$.

K_6 : The last vertices of the graph whose number is $3p$.

We write an algorithm to obtain the neighbourhood of vertices set to each vertex in the sets $K_i,\ i = 1...6$. Next we use EDS ALGORITHM for compute the eccentric distance sum $VC_5C_7[p,q]$ nanotubes for arbitrary values of p and q.

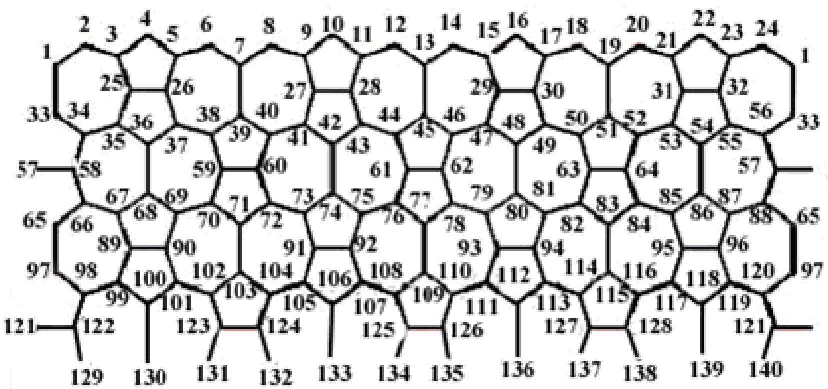

Figure 3. VC_5C_7[4,2] nanotube.

In table 2, the eccentric distance sum for various values of p,q and n have been given where n represents the number of vertices.

p	q	n	Eccentric Distance Sum
3	4	201	6821694
4	2	140	2335356
4	4	268	15102768

5	4	335	29103365
8	6	792	389754968
10	10	1630	3442876910

Table 2. Eccentric Distance Sum for $VC_5C_7[p,q]$

5. Computation of the eccentric distance sum of $HC_5C_7[p,q]$ nanotubes

In this section we compute the eccentric distance sum of $HC_5C_7[p,q]$ nanotubes similar to the previous section.

$HC_5C_7[p,q]$ nanotubes consists of heptagon and pentagon nets as seen below:

We denote the number of heptagons in the first row by p. In this nanotubes the four first rows of vertices and edges are repeated alternately; we denote the number of this repetition by q. In each period there are $16p$ vertices and $2p$ vertices which are joined to the end of the graph and hence the number of vertices n in this nanotube is equal to $16pq+2p$.

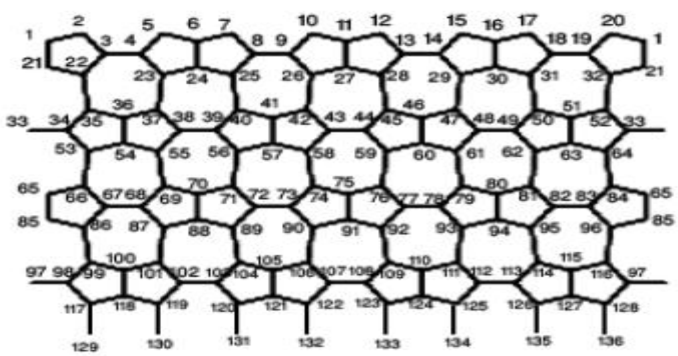

Figure 4. $HC_5C_7[4,2]$ nanotube.

Table 3 reveals the eccentric distance sum for various values of p,q and n where n denotes the number of vertices.

p	q	**n**	**Eccentric Distance Sum**
3	4	198	8603865
4	2	136	1904632
4	4	264	17193216
5	4	330	30218230
8	6	784	397621648

Table 3. Eccentric Distance Sum for $HC_5C_7[p,q]$

6. Conclusion

In this paper, we presented an algorithm to compute the eccentric distance sum of a graph with MATLAB coding. We also used our algorithm to calculate the eccentric distance sum of dendrimers $T_{k,d}$, $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes quickly.

References

1. A.T.Balaban, Chemical Applications of Graph Theory, Academic Press, London, 1976.
2. J.Devillers, A.T.Balaban(Eds), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon & Breach, Reading, 1999.
3. J.V.de Julian-Ortiz, C.de Gregorio Alapont, I.Rios-Santamarina, R.Garrcia-Domenech, J.Galvez, Prediction of properties of chiral compounds by molecular topology, J.Mol.Graphics Mod. 16(1998) 14-18.
4. T.Doslic, A.Graovac, O.Ori, Eccentric connectivity index of hexagonal belts and chains, MATCH Commun. Math. Comput. Chem., 65 (3) (2011) 745-752.
5. T.Doslic, A.Loghman, L.Badakshian, Computing topological indices by pulling a few strings, MATCH Commun. Math. Comput. Chem., 67 (1) (2012) 173-190.
6. T.Doslic, M.Saheli, Eccentric connectivity index of benzenoid graphs, in Noval Molecular Structure Descriptors-Theory and Applications II, I.Gutman and B.Furtula, Eds. Kragujevac:Univ. Kragujevac, 2010, 169-182.
7. T.Doslic, M.Saheli, D.Vukicevic, Eccentric connectivity index: extremal graphs and values, Iranian J. Math. Chem., 1, (2010) 45-56.
8. R.Garcia-Domenech, A.Villanueva, J.Galvez, R.Gozalbes, Application de la topologie moleculaire a la prediction de la viscosite liquid des composes organiques, J.Chim.Phys. 96, (1999) 1172-1185.
9. R.Garcia-Domenech, C.de Gregorio Alapont, J.V. de Ju lian-Ortiz, J.Galvez, L.Popa, Molecular connectivity to find betablockers with low toxicity, Bioorg. Med. Chem. Lett. 7, (1997) 567-572.
10. S.Gupta, M.K.Singh, A.K.Madan, Application of graph theory: relationship of eccentric connectivity index and wiener's index with anti-inflammatory activity, J. Math. Anal. Appl., 266(2), (2002) 259-268.
11. S.Gupta, M.K.Singh, A.K.Madan, Eccentric distance sum: A novel graph invariant for predicting biological and physical properties, J. Math. Anal. Appl. 275 (2002) 386-401.

12. H.B.Hua, K.X.Xu, W.N.Shu, A short and unified proof of Yu et al.'s two results on the eccentric distance sum, J.Math.Anal.Appl. 382 (2011) 364-366.

13. A.Ilic, Eccentric connectivity index, in Noval Molecular Structure Descriptors-Theory and Applications II, I.Gutman and B.Furtula, Eds. Kragujevac:Univ. Kragujevac, 2010, 139-168.

14. A.Iranmanesh, Y.Alizadeh, Computing Wiener and Schultz indices of $HAC_5C_7[p,q]$ nanotube by GAP program, Am. J. Appl. Sci. 5, (2008) 1754-1757.

15. A.Iranmanesh, Y.Alizadeh, Computing the Szeged and PI indices of $VC_5C_7[p,q]$ nanotubes, Int. J. Mol. Soc. 9, (2008) 131-144.

16. A.Iranmanesh, O.Khormali, PI index of $HAC_5C_7[p,q]$ nanotube, J. Comput. Theor. Nanosci. 5, (2008) 131-139.

17. A.Iranmanesh, Y.Alizadeh, Computing some topological indices by GAP program, MATCH Commun. Math. Comput. Chem. 60, (2008) 883-896.

18. A.Iranmanesh, Y.Pakravesh, Szeged index of $HAC_5C_6C_7[k,p]$ nanotubes, Ars Comb. 7, (2007) 3606-3617.

19. A.Iranmanesh, Y.Pakravesh, A.Mahmiani, PI index and edge-Szeged index of $HC_5C_7[k,p]$ nanotubes, Util. Math. 77, (2008) 65-78.

20. A.Iranmanesh, A.Mahmiani, Y.Pakravesh, Szeged index of $HC_5C_7[r,p]$ nanotubes, Ars Comb. 89, (2008) 309-319.

21. A.Iranmanesh, Y.Alizadeh, Eccentric connectivity index of $HAC_5C_7[p,q]$ and $HAC_5C_6C_7[p,q]$ nanotubes, MATCH Commun. Math. Comput. Chem. 69, (2013) 175-182.

22. L.B.Kier, L.H.Hall, Molecular Connectivity in Structure-Activity Analysis, Res. Studies Press, Letchworth, 1986.

23. S.Sardana, A.K.Madan, Application of graph theory: relationship of molecular connectivity index, Wiener's index and eccentric connectivity index with diuretic activity, MATCH Commun. Math. Comput. Chem., 43, (2001) 85-98.

24. M.Schonert, et al., GAP, Groups, Algorithms and Programming; Lehrstuhl D fuer Mathematik, RWTH: Achen, 1992.

25. V.Sharma, R.Goswami, A.K.Madan, Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies. J.Chem.Inf.Comput.Sci. 37, (1997) 273-282.

26. G.H.Yu, L.H.Feng, A.Ilic, On the eccentric distance sum of trees and unicyclic graphs, J.Math.Anal.Appl. 375 (2011) 99-107.

27. B.Zhou, Z.Du, On eccentric connectivity index, MATCH Commun. Math. Comput. Chem., 63(1), (2010) 181-198.