Augmented Eccentric Connectivity index of Dendrimers and Nanotubes

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Abstract.
In this paper, an algorithm is established for computing the augmented eccentric connectivity index of any simple connected graph. Also the augmented eccentricity connectivity index is calculated for dendrimers $T_{k,d}$, $VC_C[p,q]$ and $HC_C[p,q]$ nanotubes.

Keywords: Simple connected graph, Augmented eccentricity connectivity, Dendrimers, Nanotubes.

1. Introduction
An important aspect of application of graph theory 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, 10, 11, 22].

Let $G$ be a connected graph. The vertex-set and edge-set of $G$ are 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 $\xi(G) = \sum_{u \in V(G)} d(u)e(u)$, where $e(u)$ is the eccentricity of vertex $u$. The eccentric connectivity index was introduced by Madan et al. and used in a series of papers concerned with QSAR/QSPR studies [12, 23, 26]. The study of its mathematical properties was implemented recently [4-7, 13, 27]. The augmented eccentricity connectivity index $A_{\xi(G)} = \sum_{u \in V(G)} M(u)e(u)$ where $M(u)$ denotes the product of degrees of all neighbors of vertex $u$. It was introduced in another paper by the above mentioned group of authors [9]. Doslic and Saheli [8], reviewed basic mathematical properties of the augmented eccentric connectivity index and gave explicit formulae and presented
some open and closed unbranched polymers and nanostructures. Sedlar [25] established all extremal graphs with respect to augmented eccentric connectivity index among all simple connected graphs, among trees and among trees with perfect matching.

In this paper, an algorithm is presented for computing the augmented eccentric connectivity index of any simple connected graph. Furthermore the augmented eccentric connectivity index is computed for dendrimers \( T_{i,d} \), \( VC_5C_1[p,q] \) and \( HC_6C_1[p,q] \) 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 augmented eccentric connectivity index of any connected graph. Computation of augmented eccentric connectivity index of dendrimers has been discussed in section 3. In section 4, computation of the augmented eccentric connectivity index of \( VC_5C_1[p,q] \) nanotubes has been carried out. Computation of the augmented eccentric connectivity index of \( HC_6C_1[p,q] \) nanotubes has been explored in section 5. Concluding remarks has been given in the last section.

2. An algorithm for computing the augmented eccentric connectivity of any connected graph

In this section, we give an algorithm for computing the augmented eccentric connectivity index of any graph. The steps of the algorithm (AEC ALGORITHM) are as follows:

**AEC ALGORITHM**

<table>
<thead>
<tr>
<th>Notations:</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N(i) ) - Neighborhood of ith vertex</td>
</tr>
<tr>
<td>( d(i) ) - Degree of ith vertex</td>
</tr>
<tr>
<td>( D_{t,i} ) - The set of vertices that their distance to vertex ( i ) is equal to ( t ) ((t \geq 0))</td>
</tr>
<tr>
<td>( \varepsilon(u) = \text{Max}{t \in \varepsilon(u) \neq \emptyset} ) - Eccentricity of ith vertex</td>
</tr>
<tr>
<td>( M(u) = \prod_{j \in N(u)}</td>
</tr>
</tbody>
</table>

1. Assign every vertex with distinct numbers.
2. Find \( N(i) \) for every vertex \( i \).
3. Find \( D_{t,i} \) for every vertex \( i \) with \( t \geq 1 \), because the distance between vertex \( i \) and its adjacent vertices is equal to \( t \). For each vertex \( j \in D_{t,i} \), \((t \geq 1)\), the distance between each vertex of set \( N(j) \setminus \{D_{t,i} \cup D_{t+1-i} \} \) and the vertex \( i \) is equal to \( t + 1 \).)
4. Find \( \varepsilon(i) \) for every vertex \( i \)
5. Find \( M(i) \) for every vertex \( i \)
6. Calculate the augmented eccentricity connectivity index of the graph \( \Lambda_{A(i)} \)
Illustrated Example.
Consider the following simple graph with five vertices and edges to explain the above procedures to find the augmented eccentric connectivity index.

Fig 1. Sample Connected Graph with n=5

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

<table>
<thead>
<tr>
<th>Neighborhood of all the vertices</th>
<th>Eccentricity of all the vertices</th>
<th>M(i) - The product of degrees of all neighbors of vertex i</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_{1,0}={1}; D_{2,0}={2}; D_{3,0}={3}; D_{4,0}={4}; D_{5,0}={5}; )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( D_{1,1}={2,5}; D_{2,1}={1,3,4}; D_{3,1}={2}; D_{4,1}={2,5}; D_{5,1}={1,4}; )</td>
<td>Augmented eccentric connectivity index = 10.333</td>
<td></td>
</tr>
</tbody>
</table>

3. Computation of the Augmented eccentric connectivity index of dendrimers \( T_{k,d} \)

For computation of the augmented eccentric connectivity index 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, \( 1 \leq i \leq n \), and determine all of adjacent vertices set of the vertex (neighbourhood) \( N[i] \) by NEIGHBOURHOOD ALGORITHM. Next, we use AEC ALGORITHM to compute the augmented eccentric connectivity index of the \( T_{k,d} \) for arbitrary values of \( d \) and \( k \).

**NEIGHBOURHOOD ALGORITHM 1**

1. Read \( m, a, d \)
2. \( n = 14(d/(d-2))^{((d-1)\cdot k - 1)} \)
7. \( K2=[d+2..1+(d/(d-2))^{((d-1)\cdot(k-1) - 1)}] \)
8. for each \( i \) in \( K2 \)
7. \( N[i]=[(d-1)^{i+4}-d..(d-1)^{i+2}] \)
8. \( \text{Add}(N[i], \text{Int}((i+4)+d/(d-2))) \)
3. \( N := \emptyset \) (array)
4. \( K_1 := [2..d+1] \);
5. \( N[1] := K_1 \);
6. for each \( i \) in \( K_1 \)
   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
end for

9. \( K_3 := [2+(d/(d-2))((d-1)^{(k-1)} - 1)..'n] \)
10. for each \( i \) in \( K_3 \)
    if \( k = 1 \) then \( N[i] := [1] \)
    else
        \( N[i] := [\text{Int}(i/4+d)/(d-1)] \)
    end if
end for

Figure 2. Molecular graphs of dendrimers \( T_{k,d} \)

In table 1, the augmented eccentric connectivity index for various values of \( d, k \) and \( n \) have been given where \( n \) represents the number of vertices.

<table>
<thead>
<tr>
<th>( d )</th>
<th>( k )</th>
<th>( n )</th>
<th>Augmented Eccentricity Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1</td>
<td>4</td>
<td>11/2 = 5.5</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>10</td>
<td>21</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>22</td>
<td>777/20 = 38.85</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>5</td>
<td>9</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>17</td>
<td>436/3 = 145.33</td>
</tr>
</tbody>
</table>
Table 1. Augmented Eccentricity Index for $T_{k,d}$

<table>
<thead>
<tr>
<th>$k$</th>
<th>$d$</th>
<th>$v$</th>
<th>$\frac{v-\sum_{i=1}^{k} d_i}{k}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3</td>
<td>53</td>
<td>$\frac{5624}{15}=374.93$</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>161</td>
<td>$\frac{29938}{35}=855.37$</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>6</td>
<td>$\frac{27}{2}=13.5$</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>26</td>
<td>$\frac{9575}{6}=1595.83$</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>106</td>
<td>$\frac{60415}{12}=5,034.58$</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>426</td>
<td>$\frac{1224725}{84}=14,580.05$</td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>1706</td>
<td>$\frac{5572415}{126}=44,225.51$</td>
</tr>
</tbody>
</table>

4. Computation of the Augmented eccentricity connectivity index 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 augmented eccentricity connectivity index 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 occur alternatively and we denote the number of this repetitions 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 in this nanotube is equal to $16pq + 3p$.

We partition the vertices of the graph into 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 AEC ALGORITHM for compute the augmented eccentricity connectivity $VC_5C_7[p,q]$ nanotubes for arbitrary values of $p$ and $q$.
In table 2, the augmented eccentricity connectivity index for various values of $p, q$ and $n$ have been given where $n$ represents the number of vertices.

### Table 2. Augmented Eccentricity Index for VC$_5$C$_7$[p,q] nanotubes

<table>
<thead>
<tr>
<th>$p$</th>
<th>$q$</th>
<th>$n$</th>
<th>Augmented Eccentricity Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>4</td>
<td>201</td>
<td>$\frac{7865696}{284240}=27.67$</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>140</td>
<td>$\frac{6872}{35}=196.34$</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>268</td>
<td>$\frac{1889482143}{5720330}=330.30$</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>335</td>
<td>$\frac{99604107}{269192}=370.01$</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>792</td>
<td>$\frac{2163813468783}{3708514810}=583.47$</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>1630</td>
<td>$\frac{13394539577045978124651}{15645826737668687560}=856.10$</td>
</tr>
</tbody>
</table>

5. **Computation of the Augmented eccentricity connectivity index of $HC_5C_7[p,q]$ nanotubes**

In this section, we compute the augmented eccentricity connectivity index of $HC_5C_7[p,q]$ nanotubes similar to the previous section. $HC_5C_7[p,q]$ nanotubes consist 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 occur alternatively; we denote the number of this repetitions 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 in this nanotube is equal to $16pq+2p$.

Table 3 reveals the augmented eccentricity connectivity index for various value of $p, q$ and $n$ where $n$ denotes the number of vertices.
Figure 4. HC$_5$C$_7$[4,2] nanotube.

Table 3. Augmented Eccentricity Index for HC$_5$C$_7$[p,q]

<table>
<thead>
<tr>
<th>p</th>
<th>q</th>
<th>n</th>
<th>Augmented Eccentricity Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>4</td>
<td>198</td>
<td>$136259462392 / 557732175=244.30$</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>136</td>
<td>$20792 / 91=228.48$</td>
</tr>
<tr>
<td>4</td>
<td>264</td>
<td>264</td>
<td>$82950867215 / 267711444=309.85$</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>330</td>
<td>$79289169072 / 215656441=367.66$</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>784</td>
<td>$31583968485004887 / 54172924768820=583.02$</td>
</tr>
</tbody>
</table>

6. Conclusion

The computation of the Augmented eccentricity index of a graph is discussed and its algorithm is presented in this paper. We have implemented our algorithm to calculate the Augmented eccentricity index of dendermers $T_{d,k}$, $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes with MATLAB.

References
