Balaban index of regular dendrimers

ABBAS HEYDARI
Department of Mathematics, Arak branch, Islamic Azad University, Arak, Iran

The Balaban index of a simple connected graph G is defined as $J(G)=\frac{m}{1+\mu}\sum_{uv\in E(G)}(d(u)d(v))^{\frac{-1}{2}}$ where m is the number of edges, μ is the cyclomatic number of G, $d(u)$ is sum of the distances between vertex u and all of the vertices of G, and the summation goes over all edges from the edge set $E(G)$. In this paper, computation of the Balaban index of regular dendrimers is purposed.

(Received August 1, 2011; accepted November 23, 2011)

Keywords: Topological Index, Balaban Index, Dendrimers

1. Introduction

A topological index is a numeric quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. It has been found that many properties of a chemical compound are closely related to some topological indices of its molecular graph [1, 2]. There are several topological indices have been defined and many of them have found applications as means for modeling chemical, pharmaceutical and other properties of molecules.

Let G be simple connected graph and the sets of vertices and edges of G be denoted by $V(G)$ and $E(G)$, respectively. For vertices u and v in $V(G)$, we denote by $d_G(u, v)$ the topological distance i.e., the number of edges on the shortest path, joining the two vertices u and v of G. Since G is connected, $d_G(u,v)$ exists for all vertices $u,v\in V(G)$. The distance sum of a vertex u of G is defined as $d(u)=\sum_{v\in V(G)}d_G(v,u)$. Let $e = uv$ denote the edge of G with end point u and v. The Balaban index of a molecular graph G was introduced by Balaban [3] in 1982 as one of less degenerated topological indices. It calculate the average distance sum connectivity index according to the following equation:

$$J(G)=\frac{m}{1+\mu}\sum_{uv\in E(G)}(d(u)d(v))^{\frac{-1}{2}} \qquad (1)$$

where m is number of edges of G and μ is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph (called cyclomatic number of G). If G is a connected graphs and n denote the number of vertices of G then $\mu=m-n+1$. The Balaban index appears to be a very useful molecular descriptor with attractive properties [1, 4]. It has also been extended to weighted graphs and used successfully in QSAR/QSPR modeling [2, 5].

Dendrimers are hyperbranched molecules, synthesized by repeatable steps, either by adding branching blocks around a central *core* or by building large branched blocks starting from the periphery and then attaching them to the core. The vertices of a dendrimer, except the external end points, are considered as branching points. The number of edges emerging from each branching point is called progressive degree, (i.e., the edges which enlarge the number of points of a newly added orbit). It equals the classical degree, minus one. If all the branching points have the same degree, the dendrimer is called regular. Otherwise it is irregular.

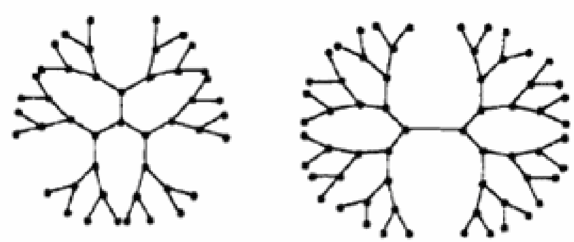

Fig. 1. Regular monocentric ($D_{3,4}$) and dicentric ($DD_{3,4}$) dendrimers.

A dendrimer is called *homogeneous* if all its radial chains (i.e., the chains starting from the core and ending in an external point) have the same length [6]. In graph theory, they correspond to the Bethe lattices [7]. It is well-known that any tree has either a monocenter or a dicenter (i.e., two points joined by an edge). Accordingly, the dendrimers are called *monocentric* and *dicentric,* respectively (Fig. 1). The numbering of orbits starts with zero for the core and ends with r, which equals the radius of the dendrimer (i.e., the number of edges from the core to the external nodes). A regular monocentric dendrimer, of progressive degree *p-1* and generation *r* is herein denoted by $D_{p,r}$, whereas the corresponding dicentric dendrimer, by $DD_{p,r}$ [8]. Recently topological indices of dendrimers have been studied in numerous research papers [8-10]. In this paper the Balaban index of regular monocentric and dicentric dendrimers are purposed.

2. Results and discussion

In this section at first we consider the lattice of regular monocentric dendrimers as a rooted tree with $r+1$ levels where its central core is considered as the root vertex of tree lying on the first level. Recall that a tree is a connected acyclic graph. In a tree, any vertex can be chosen as the root vertex. The level of a vertex on a tree is one more than its distance from the root vertex. The number of vertices of $D_{p,r}$ where are located on the *i*-th level of the graph can be computed as $n_i = p(p-1)^{i-2}$ for $i=2,\ldots,r+1$. Thus the number of all of the vertices of the graph is computed as

$$n = |V(D_{p,r})| = 1 + \sum_{i=0}^{r-1} p(p-1)^i.$$

Now suppose that *x* denotes the root vertex of $D_{p,r}$ and $e=xy$ denotes one of the *p* edges of $D_{p,r}$ where join *x* and one vertex on the *2*-th level of the graph. The sum distance of the *x* will be calculated as follow:

$$d(x) = p + 2p(p-1) + 3p(p-1)^2 + \ldots + rp(p-1)^{r-1} = p\frac{(p-1)^r(pr-2r-1)+1}{(p-2)^2}.$$

The sum distance of vertex *y* can be computed by using $d(x)$. Let $n_L(e)$ and $n_R(e)$ denote the number of vertices lying to the left and to the right of edge *e*. If $u \in n_L(e)$ and $v \in n_R(e)$, then $d(x,u) = d(x,v)+1$ and $d(y,v) = d(y,u)+1$. Hence

$$d(y) = \sum_{z\in V(D_{p,r})} d(y,z) = \sum_{u\in n_L(e)} d(y,u) + \sum_{v\in n_R(e)} d(y,v) = \sum_{u\in n_L(e)} (d(x,u)-1) + \sum_{y\in n_R(e)} (d(x,v)+1)$$
$$= d(x) + |n_R(e)| - |n_L(e)|.$$

Since $|n_L(e)| = \sum_{i=0}^{r-1}(p-1)^i$, so we have

$$|n_R(e)| = n - |n_L(e)| = 1 + \sum_{i=0}^{r-1} p(p-1)^i - \sum_{i=0}^{r-1}(p-1)^i.$$

Thus

$$d(y) = d(x) + n + 1 - 2\sum_{i=0}^{r-1}(p-1)^i.$$

Now suppose that E_j denotes the set of edges of the graph where join a vertex on *j*-th level and a vertex on *j+1*-th level of the graph. If $e = uv \in E_j$ and $\lambda(j) = |n_R(e)| - |n_L(e)|$ then

$$\lambda(j) = n + 1 - 2\sum_{i=0}^{r-j}(p-1)^i = \frac{(p-1)^r}{p-2}[p - 2(p-1)^{1-j}]. \qquad (2)$$

Also we have

$$d(u) = d(x) + \lambda(1) + \lambda(2) + \ldots + \lambda(j-1) \text{ and}$$
$$d(v) = d(x) + \lambda(1) + \lambda(2) + \ldots + \lambda(j). \qquad (3)$$

Now by using previous computation the Balaban index of regular monocentric dendrimer can be computed.

Theorem 1. The Balaban index of monocentric dendrimers is computed as

$$J(G) = p\frac{(p-1)^r - 1}{2(p-2)} \sum_{j=1}^{r} \frac{p(p-1)^{j-1}}{\sqrt{(d(j-1)d(j)}}.$$

Where

$$d(j) = p\frac{(p-1)^r(pr-2r-1)+1}{(p-2)^2} + \sum_{i=1}^{j}\frac{(p-1)^r}{p-2}[p-2(p-1)^{1-i}].$$

Proof: Let *m* denote the number of edges of $D_{p,r}$, then $m=n+1$, so $m = p\frac{(p-1)^r - 1}{2(p-2)}$ and $\mu = m - n + 1 = 2$.

Therefore by using *(1)* we have

$$J(D_{p,r}) = \frac{m}{\mu}\sum_{uv\in E(D_{p,r})}(d(u)d(v))^{\frac{-1}{2}} = \frac{m}{2}\sum_{j=1}^{r}\sum_{uv\in E_j}(d(u)d(v))^{\frac{-1}{2}} = \frac{p\sum_{i=0}^{r-1}(p-1)^i}{2}\sum_{j=1}^{r}\frac{p(p-1)^{j-1}}{\sqrt{d(u)d(v)}}.$$

If $e = uv \in E_j$, then by using of *(2)* and *(3)*, $d(u) = d(x) + \sum_{j=1}^{j-1}\lambda(j)$ and $d(v) = d(x) + \sum_{j=1}^{j}\lambda(j)$.

Put $d(j-1)=d(u)$ and $d(j)=d(v)$. We have

$$J(G) = p\frac{(p-1)^r - 1}{2(p-2)} \sum_{j=1}^{r} \frac{p(p-1)^{j-1}}{\sqrt{(d(j)d(j+1)}}.$$

Therefore proof is completed. □

As application in continue we compute the Balaban index of $D_{4,3}$. Since $p=4$ and $r=3$, we have

$$d(j) = 4\frac{3^3(4.3-2.3-1)+1}{2^2} + \sum_{i=1}^{j}\frac{3^3}{2}[4-2.3^{1-i}].$$

So *d(0)=136, d(1)=163, d(2)=208 and d(3)=259*. Therefore

$$J(D_{2,4})=4\frac{3^3-1}{4}\sum_{j=1}^{3}\frac{4.3^{j-1}}{\sqrt{d(j-1)d(j)}}=26(\frac{4}{\sqrt{136\times163}}+\frac{12}{\sqrt{163\times208}}+\frac{36}{\sqrt{163\times259}})=6.4257.$$

Now we will compute the Balaban index of dicentric dendrimers. If x denotes one of the two central vertices of $DD_{p,r}$ then

$$d(x)=\sum_{v\in V(DD_{p,r})}d(x,v)=\sum_{i=1}^{r}i(p-1)^i+\sum_{i=0}^{r}(i+1)(p-1)^i=\frac{(p-1)^{r+1}[2pr+p-4(r+1)]+p}{(p-2)^2}.$$

In this case the number of vertices of the graph is calculated as follow:

$$n=|V(DD_{p,r})|=2\sum_{i=0}^{r}(p-1)^r=\frac{2}{p-2}[(p-1)^{r+1}-1].$$

By using previous notations $\lambda(j)$ will be computed as follow

$$\lambda(j)=n-2\sum_{i=0}^{r-j}(p-1)^i=\frac{2(p-1)^{r+1}(1-(p-1)^{-j})}{p-2}$$

for $j=1,2,\ldots,r$. Now the Balaban index of $DD_{p,r}$ can be computed by recent calculations.

Theorem 2. The Balaban index of regular dicentric dendrimers is computed as

$$J(DD_{p,r})=[\frac{2}{p-2}((p-1)^{r+1}-1)-1]\sum_{j=1}^{r}\frac{(p-1)^j}{\sqrt{d(j-1)d(j)}}.$$

Where

$$d(j)=\frac{(p-1)^{r+1}[2pr+p-4(r+1)]+p}{(p-2)^2}+\sum_{i=1}^{j}\frac{2(p-1)^{r+1}(1-(p-1)^{-j})}{p-2}.$$

Proof: Let m denote the number of edges of the graph. Then $\mu=m-n+1=2$ and

$$m=n-1=\frac{2}{p-2}[(p-1)^{r+1}-1]-1.$$

Put $d(j)=d(x)+\sum_{j=1}^{j-1}\lambda(j)$. We have

$$d(j)=\frac{(p-1)^{r+1}[2pr+p-4(r+1)]+p}{(p-2)^2}+\sum_{i=1}^{j}\frac{2(p-1)^{r+1}(1-(p-1)^{-j})}{p-2}.$$

By using *(1)* the Balaban index of $DD_{p,r}$ will be computed as

$$J(DD_{p,r})=\frac{m}{2}\sum_{uv\in E(DD_{p,r})}[d(u)d(v)]^{\frac{-1}{2}}=2\frac{m}{2}\sum_{j=1}^{r}\sum_{uv\in E_j}[d(u)d(v)]^{\frac{-1}{2}}=$$

$$[\frac{2}{p-2}((p-1)^{r+1}-1)-1]\sum_{j=1}^{r}\frac{(p-1)^j}{\sqrt{d(j-1)d(j)}}.$$

Therefore proof is completed. □

For example we compute the Balaban index of $DD_{4,3}$. Since $p=4$ and $r=3$ thus

$$d(j)=\frac{3^4(2.4.3+4-4.4)+4}{2^2}+\sum_{i=1}^{j}2\frac{3^4(1-3^{-j})}{2}.$$

So *d(0)=244, d(1)=298, d(2)=370 and d(3)=448*. Therefore by using Theorem 2

$$J(DD_{2,4})=[\frac{2}{4-2}(3^4-1)-1]\sum_{j=1}^{3}\frac{3^j}{\sqrt{d(j-1)d(j)}}=79(\frac{3}{\sqrt{244\times298}}+\frac{9}{\sqrt{370\times298}}+\frac{27}{\sqrt{370\times448}})=8.259.$$

References

[1] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, (Wiley, Weinheim, 2000).
[2] N. Trinajstic, Chemical Graph Theory (CRC Press, Boca Raton, FL, 1983).
[3] A. T. Balaban, Chem. Phys. Lett. **89**, 399 (1982).
[4] M. V. Diudea, M. S. Florescu, P. V. Khadikar, Molecular Topology and Its Applications, EfiCon Press, Bucharest, 2006, p.57.
[5] J. Devillers, A. T. Balaban (Eds.), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon & Breach, Amsterdam, 1999.
[6] D. A. Tomalia, A. M. Naylor, W. A. Goddard, Angew. Chem., Int. Ed. Engl., **29**, 138 (1990).
[7] K. Balasubramanian, J. Math. Chem., **4**, 89 (1990).
[8] M. V. Diudea, B. Parv, J. Chem. Inf. Comput. Sci., **35**, 1015 (1995).
[9] A. Heydari, Optoelectron. Adv. Mater.-Rapid Commun, **4**(12), 2209 (2010).
[10] A. Heydari, Optoelectron. Adv. Mater.-Rapid Commun., **4**(12), 2206 (2010).

*Corresponding author: a-heidari@iau-arak.ac.ir