Harary index of regular dendrimers

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The Harary index of a connected graph *G* is defined as the half-sum of the off-diagonal elements of the reciprocal distance matrix of *G*. In this paper computation of the Harary index in regular dendrimers are proposed.

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1. Introduction

The Harary index (or reciprocal distance sum index) of a molecular graph *G*, denoted by *H(G)*, has been introduced independently by Plavši´c et al. [1] and by Ivanciuc et al. [2] in 1993 for the characterization of molecular graphs. The Harary index is defined as the half-sum of the elements in the reciprocal distance matrix, also called the Harary matrix [3]. This definition parallels the Hosoya definition of the Wiener index as the half-sum of the elements in the distance matrix [4]. The motivation for introduction of the Harary index was pragmatic-the aim was to design a distance index differing from the Wiener index [5] in that the contributions to it from the distant atoms in a molecule should be much smaller than from near atoms, since in many instances the distant atoms influence each other much less than near atoms. [6]

Let G be an undirected connected graph without loops or multiple edges with vertex-set $V(G) = \{v_1, v_2, \ldots, v_n\}$. For vertices v_i and v_j in $V(G)$, we denote by $d_G(v_i, v_j)$ the topological distance i.e., the number of edges on the shortest path, joining the two vertices of *G*. The distance matrix *D* of *G* is an $n\times n$ matrix (Dij) such that Dij is just the distance between the vertices v_i and v_j in *G*. The reciprocal distance matrix *RD* of *G* is an $n \times n$ matrix ($RDij$) such that [3]

$$RD_{ij} = \begin{cases} \dfrac{1}{D_{ij}} & if \quad i \neq j, \\ 0 & if \quad i = j. \end{cases}$$

The Harary index *H(G)* is defined as [1,2]

$$H(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} RD_{ij} = \sum_{i<j} RD_{ij}. \quad (1)$$

Dendrimers are hyperbranched molecules, synthesized by repeatable steps, either by adding branching blocks around a central *core* (thus obtaining a new, larger orbit or generation-the “divergent growth” approach) or by building large branched blocks starting from the periphery and then attaching them to the core (the “convergent growth” approach [6]). These rigorously tailored structures are mainly organic compounds, but inorganic components were also used [7,8].

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, *k***,** minus one: $p = k-1$. If all the branching points have the same degree, the dendrimer is called regular. Otherwise it is irregular.

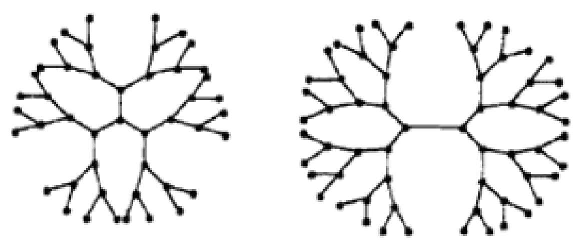

Fig. 1. Regular monocentric ($D_{2,4}$) and dicentric ($DD_{2,4}$) dendrimers.

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 [9]. It is well-known [10] 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* and generation *r* is herein denoted by $D_{p,r}$, whereas the corresponding dicentric dendrimer, by $DD_{p,r}$ [11]. In this paper the Harary index in regular monocentric and dicentric dendrimers are proposed.

Main results:

In this section at first we consider the graph of regular monocentric dendrimers as a rooted tree with *r+1* levels where central core of this graph is the rooted 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.

To compute the Harary index of $G=D_{p,r}$ the reciprocal distances between all of the vertices must be computed. For this purpose we compute the distances between each vertex of the graph and vertices in which are placed on lower levels of the graph. Let v be the rooted (central) vertex and E_i be the set of vertices where are placed on the *i*-th level of the graph. Thus $|E_i| = p(p-1)^{r-1}$ for $i = 2,3,...,r+1$ and

$$S(1) = \sum_{u\in V(G)} \frac{1}{d(v,u)} = \sum_{u\in E_i} \frac{|E_i|}{d(v,u)} = p\sum_{i=1}^{r} \frac{(p-1)^{i-1}}{i}. \quad (2)$$

Now suppose u is one of the $p(p-1)^{j-1}$ vertices where are placed on the *j*-th of the graph for $j = 2,3,...,r+1$. If V_j denotes the set of the children of u then by similar calculation

$$\sum_{x\in V_j} \frac{1}{d(u,x)} = \sum_{i=1}^{r-j} \frac{(p-1)^i}{i}.$$

Therefore the reciprocal distances between vertices on the *j*-th level and the their children for $j = 2,3,...,r+1$, calculated as

$$S(j) = p(p-1)^{j-1}\sum_{i=1}^{r-j} \frac{(p-1)^i}{i}. \quad (3)$$

If V^j denotes the set of the vertices where are placed on the *j*-th level or lower levels of the graph then

$$\sum_{x\in V^j - V_j} \frac{1}{d(u,x)} = \sum_{s=1}^{j-1}\sum_{i=s}^{r+s-j} \frac{(p-2)(p-1)^{i-1}}{i+s} + \sum_{i=j}^{r} \frac{(p-1)^i}{i+j}.$$

The summation of reciprocal distances between vertices of the graph where are placed on same level calculated as follow

$$\sum_{s=1}^{j-1} \frac{p(p-2)(p-1)^{j+s-2}}{2s} + \frac{p(p-1)^{2j-1}}{2j}$$

Therefore the summation of reciprocal distances between vertices of the graph where are placed on *j*-th and other vertices where are belong to $V^j - V_j$ computed as

$$R(j) = p(p-1)^{j-1}\Big[\sum_{s=1}^{j-1}\sum_{i=s}^{r+s-j} \frac{(p-2)(p-1)^{i-1}}{i+s} + \sum_{i=j}^{r} \frac{(p-1)^i}{i+j} - \sum_{s=1}^{j-1} \frac{p(p-2)(p-1)^{j+s-2}}{2s} - \frac{p(p-1)^{2j-1}}{2j}\Big]. \quad (4)$$

So by considering *(1)-(4)* the Harary index of $D_{p,r}$ can be calculated as follow:

Theorem 1. The Harary index of mono centric regular dendrimers computed as

$$H(G) = p\sum_{i=1}^{r} \frac{(p-1)^{i-1}}{i} + \sum_{j=1}^{r} p(p-1)^{j-1}\Big[\sum_{s=1}^{j-1}\sum_{i=s}^{r+s-j} \frac{(p-2)(p-1)^{i-1}}{i+s} + \sum_{i=1}^{r-j} \frac{(p-1)^i}{i} + \sum_{i=j}^{r} \frac{(p-1)^i}{i+j} - \sum_{s=1}^{j-1} \frac{p(p-2)(p-1)^{j+s-2}}{2s} - \frac{p(p-1)^{2j-1}}{2j}\Big].$$

In continue we compute the Harary index of dicentric regular dendrimers. For this purpose we consider the graph of $DD_{p,r}$ as a monocentric dendrimer in which one of it's the subtrees induced by deleting central vertex has *r+1* level and others have *r* levels (see Fig. *2*). Let $\lambda(p,r)$ denote the summation of reciprocal distances of additional vertices on the *r+1*-th level and all of the vertices of the graph. Thus the Harary index of $DD_{p,r}$ can be computed by adding the Harary index of $D_{p,r}$ and $\lambda(p,r)$. The value of $\lambda(p,r)$ can be calculated by adding the reciprocal distances between vertices where are placed on the *i*-th for *i=1,2,…,r+1* and additional vertices where are placed on *r+1*-th of the graph. Thus

$$\lambda(p,r) = \sum_{i=0}^{r-1} \frac{(p-1)^r}{r-i} + \sum_{i=0}^{r} \frac{(p-1)^{r+i}}{r+i+1} + \sum_{i=1}^{r-1}\sum_{s=1}^{i} \frac{(p-2)(p-1)^{r+s-1}}{r-i+2s} + (p-2)(p-1)^r \sum_{i=1}^{r} \frac{(p-1)^{i-1}}{4i}.$$

Therefore the Harary index of $DD_{p,r}$ is computed by using Theorem *1* and the last equation as follow:

Theorem 2. The Harary index of dicentric regular dendrimers computed as

$$H(DD_{p,r}) = H(D_{p,r}) + (p-1)^r\Big[\sum_{i=0}^{r}\Big(\frac{(p-2)(p-1)^{i-1}}{4i} + \frac{1}{r-i} + \frac{(p-1)^i}{r+i+1}\Big) + \frac{1}{r+1} + (p-2)\sum_{i=1}^{r-1}\sum_{s=1}^{i} \frac{(p-1)^{s-1}}{r-i+2s}\Big].$$

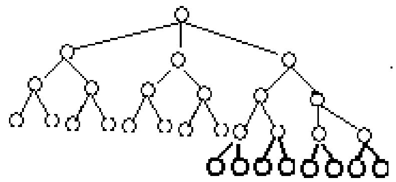

Fig. 2. The graph of $DD_{2,3}$ where is constructed by adding new vertices to the last level of $D_{2,3}$.

In Table 1 the numerical data for Harary index of monocentric and dicentric regular dendrimers of various dimensions are given.

Table 1.

p	r	$H(D_{p,r})$	$H(DD_{p,r})$
3	2	22	37.86
3	3	77.6	126.48
3	4	248.23	398.43
4	3	364.3	719.54
4	4	2332	4673.5
4	6	110480	229890
6	6	25292000	66141000

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