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A GROUP THEORETICAL METHOD FOR COMPUTING HARARY INDEX

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ABSTRACT. The Harary index of a molecular graph *G* is defined as the sum of the inverse of distances between the pair vertices of *G*. In this paper we report a group theoretical method for computing Harary index in some classes of dendrimers.

Keywords: *Graph automorphism, Harary index, Dendrimer.*

INTRODUCTION

A graph *G* is called a molecular graph if the set of vertices V(G) represent atoms and the set of edges E(G) collect the chemical bonds (*uv*) joining the atoms *u* and *v* in the molecule. The length of the shortest path between two vertices is called the topological distance and is denoted by *d*(*u*,*v*); the maximum distance between the vertex *u* and any vertex *v* in *G* is named the eccentricity of *u* and is denoted *e*(*u*).

Denote by *Aut*(*G*) the automorphism group of *G*. A topological index TI is a number that is invariant under the *Aut*(*G*). A variety of TIs have been proposed for characterization of chemical structures and used for structure-property correlations in QSPR models [1-3].

In particular, the Harary index of a graph, *H*(*G*), has been introduced in 1993, independently by Ivanciuc *et al*.[4] and by Plavšić *et al*. [5] Even earlier, the QSAR group in Timisoara, Romania, particularly Ciubotariu, [6] have used this index to express the decay of interactions between pair atoms in molecules as the distances between them increased. It has been named in the honor of Professor Frank Harary, on the occasion of his 70^{th} birthday. The Harary index is defined as follows:

$$H(G) = \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)}$$

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where the summation runs over all unordered pairs of vertices of the graph G and $d_G(u,v)$ denotes the topological distance between any two vertices u and v of G (i.e., the number of edges in a shortest path connecting u and v). Mathematical properties and some applications of H the reader can find in refs [7-14].

Dendrimers are hyper-branched synthetic polymers (i.e. macromolecules) with a well-defined molecular topology [4-6].

In this paper, we use a group theoretical method [15-19] for computing the Harary index.

According to this method, we compute the Harary index of the dendrimers $T[h,m]$ (Figure 1, 2). This dendrimer has a central vertex (denoted x_0) of degree $h + 1$ and every non-pendent vertex (i.e. branching vertex/atom) has degree $h + 1$, and m denote to the distance between the central vertex and each pendent vertices. The number of vertices of $T[h,m]$ is equal to $1+h\,((h-1)^m-1)/(h-2)$.

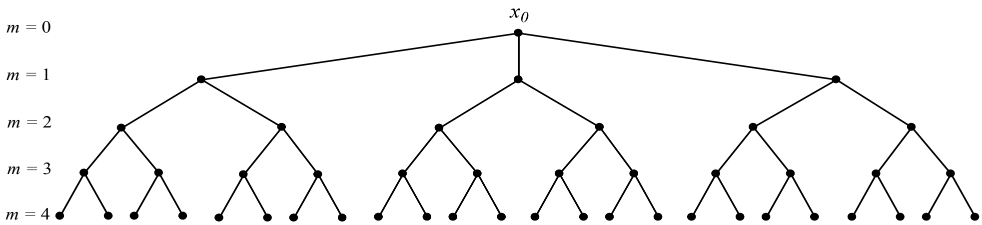

Figure 1. Dendrimer $T[2,4]$

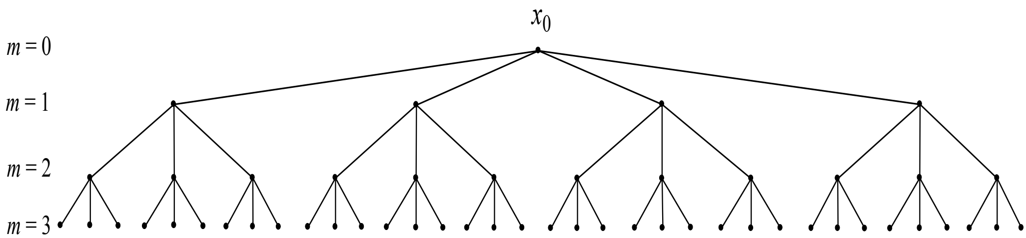

Figure 2. Dendrimer $T[3,3]$.

Throughout this paper, our notation is standard and taken mainly from the standard books of graph theory as like as [20].

RESULTS AND DISCUSSION

Let v be a vertex of graph G. We write $N_i(v)$ for the set of vertices at distance i (of which maximum equals $e(v)$) from v. $N_1(v)$ is called the neighborhood of v. We call the partition of the vertex set $V(G) = N_0(v) \cup N_1(v) \cup \dots \cup N_{e(v)}(v)$ a representation of G with respect to v and denoted by $n_i(v)$, the cardinality of $N_i(v)$. Now set

$$Rd(v) = 1^{-1}n_1(v) + 2^{-1}n_1(v) + \dots + e(v)^{-1}n_{e(v)}(v)$$

and then rewrite the Harary index as

$$H(G) = \sum_{v\in V} Rd(v).$$

Lemma. If the action of automorphism group of G on $V(G)$ contains the orbits $V_1, V_2, \dots, V_k$, then $H(G) = \sum_{i=1}^{k} |V_i| Rd(v_i)$, where v_i is a vertex of the i–th orbit. In particular, if the action is transitive and v is a vertex of G then $H(G) = |V(G)|Rd(v)$.

Proof. Suppose v is a vertex of G. Consider the level representation of G with respect to v. For each vertex v_1 and v_2 in the same orbit, there exists an automorphism f such that $f(v_1) = v_2$. Thus they have the same level representation and $n_i(v_1) = n_i(v_2)$, so $Rd(v_1) = Rd(v_2)$ Since $V(G)$ is partitioned by orbits, then $H(G) = \sum_{i=1}^{k} \sum_{v_i \in V_i} Rd(v_i) = \sum_{i=1}^{k} |V_i| Rd(v_i)$. This completes the proof.

Example. Consider Q_n be the hypercube with 2^n vertices and $n2^{n-1}$ edges. The set vertex of Q_n is consist of the sequences $v = (v_1, v_2, \dots, v_n)$ where v_i is equals to 0 or 1 and two vertices u and v are adjacent if and only if they differ in an one place. This graph is vertex transitive and the automorphism group is isomorphic to group $Z_2 \sim S_n$. The distance of two vertices are i if and only if they differ in i places. Take 0 = (0, 0, …, 0) then $Rd(0) = F([1,1,1-n],[2,2],-1)_n$ where F is the generalized hyper geometric function. Then the Harary index of Q_n is as follow:

$$H(Q_n) = 2^n Rd(0).$$

In this section, we describe our computational method for computing Harary index of dendrimer $T_m = T[h,m]$. Choose the node x_0 of T_m, with minimum eccentricity, as the root and then consider the sets, $S[i]$ containing all vertices at the distance i from x_0 and $1 \le i \le m$. Therefore $V(T_m) = S[1] \cup S[2] \cup \dots \cup S[m]$. In order to characterize the symmetry of T_m, we notice that each dynamical symmetry operation of $S[1]$, considering the rotations of elements of T_1, in different generations of the whole T_m, is composed of m sequential physical operations. We first have a physical symmetry of the framework. Such operations form the group T_m of order $(h + 1)!$, which is isomorphic to S_{h+1} or $Sym(h + 1)$. We can see that, after accomplishing the first framework symmetry operation, there are two reflections isomorphic to S_h, for each $i \in T_m$. Therefore, we find a group isomorphic to

$$H = ((\ldots(S_h \sim S_h) \sim S_h) \sim \ldots) \sim S_h) \sim S_h$$

with n components. Thus, the automorphism graph of T_m is isomorphic to the wreath product $H \sim G$ of order $(h+1)!\times h^{(h+1)((h)^n-1)}$.

If $Aut(T_m)$ acts on $V(T_m)$ then the orbits of $Aut(T_m)$ are $S[i]$ for $0 \le i \le k$. Then, it is sufficient to obtained $R(v)$ for each vertices in $S[i]$.

Let $\alpha_x(y, y+1+m) = x^y/(y+1+m)$. Then for vertex in $m = 0$ we have:

$$Rd(v_0) = (h+1)[\alpha_h(0,1) + \alpha_h(1,2) + \cdots + \alpha_h(k-1,k)];$$

and if $m \neq 0$ then for any vertex in row m:

$$\begin{aligned} Rd(v_m) &= h[\alpha_h(0,1) + \alpha_h(1,2) + \cdots + \alpha_h(k-m-1,k-m)] + h[\alpha_h(0,1+m) \\ &\quad + \alpha_h(1,2+m) + \cdots + \alpha_h(k-1,k+m)] + [1 + \frac{1}{2} + \cdots + \frac{1}{m}] \\ &\quad + 2^{h-2}\sum_{l=0}^{m-2}[\sum_{t=0}^{k-m+l}\alpha_h(t,t+l+2)]; \end{aligned}$$

so, the Harary index of T_m is equals to:

$$\begin{aligned} H(T[h,m]) &= Rd(v_0) + \sum_{m=1}^{k}((h+1)\times h^{(m-1)})Rd(v_m) \\ &= \frac{(h+1)}{2}\{\sum_{\alpha=0}^{k-1} v_h(\alpha,\alpha+1) + \sum_{m=1}^{k}[h^m[(\sum_{\alpha=0}^{k-m-1} v_h(\alpha,\alpha+1) \\ &\quad + \sum_{\alpha=0}^{k-1} v_h(\alpha,\alpha+m+1)) \\ &\quad + \frac{1}{h}(\sum_{p=1}^{m}\frac{1}{p} + 2^{(h-2)}\sum_{\alpha=0}^{k-m+l}[\sum_{l=0}^{m-2} v_h(\alpha,\alpha+l+2)])]]\}. \end{aligned}$$

For example, the Harary index of the two dendrimers $T[2,m]$ and $T[3,m]$ is equals to:

$$H(T[2,m]) = \frac{3}{2}\{\sum_{\alpha=0}^{k-1} v_2(\alpha,\alpha+1) + \sum_{m=1}^{k}[2^m[(\sum_{\alpha=0}^{k-m-1} v_2(\alpha,\alpha+1) + \sum_{\alpha=0}^{k-1} v_2(\alpha,\alpha+m+1))$$
$$+\frac{1}{2}(\sum_{p=1}^{m}\frac{1}{p} + \sum_{\alpha=0}^{k-m+l}[\sum_{l=0}^{m-2} v_2(\alpha,\alpha+l+2)])]]\};$$

$$H(T[3,m]) = 2\{\sum_{\alpha=0}^{k-1} v_3(\alpha,\alpha+1) + \sum_{m=1}^{k}[3^m[(\sum_{\alpha=0}^{k-m-1} v_3(\alpha,\alpha+1) + \sum_{\alpha=0}^{k-1} v_3(\alpha,\alpha+m+1))$$
$$+\frac{1}{3}(\sum_{p=1}^{m}\frac{1}{p} + 2\sum_{\alpha=0}^{k-m+l}[\sum_{l=0}^{m-2} v_3(\alpha,\alpha+l+2)])]]\}.$$

In Table 1, 2, the Harary index of *T*[2,*m*] and *T*[3,*m*] are computed, respectively.

Table 1. Computed Harary index

m	*H*(*T*[2,*m*])	*m*	*H*(*T*[2,*m*])
1	4.5	*11*	1064563.395
2	22	*12*	3802983.327
3	77.6	*13*	13753209.73
4	224.2285714	*14*	50236271.01
5	775.6190476	*15*	185005359.71
6	2442.472727	*16*	685960877.82
7	7855.125142	*17*	2557954484.97
8	25906.94426	*18*	9585125382.98
9	87570.42562	*19*	36068194256.98
10	302532.8129	*20*	136219894944.35

Table 2. Computed Harary index

m	*H*(*T*[3,*m*])	*m*	*H*(*T*[3,*m*])
1	7	*11*	3138719374.89
2	56.5	*12*	25643446199.96
3	291.4	*13*	211367664294.6
4	1527.128571	*14*	1754974615408.66
5	15634.53571	*15*	14661259143345.1
6	110475.5422	*16*	123126656175525
7	815803.798	*17*	1038739505017990
8	6228620.769	*18*	8798075520380730
9	48738232.29	*19*	74781213850513200
10	388404328.77	*20*	637606433725983000

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