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## ON THE SPECTRA OF REDUCED DISTANCE MATRIX OF DENDRIMERS

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**ABSTRACT.** Let  $G$  be a simple connected graph and  $\{v_1, v_2, \dots, v_k\}$  be the set of pendent (vertices of degree one) vertices of  $G$ . The reduced distance matrix of  $G$  is a square matrix whose  $(i, j)$ -entry is the topological distance between  $v_i$  and  $v_j$  of  $G$ . In this paper, we obtain the spectrum of the reduced distance matrix of regular dendrimers.

### 1. Introduction

Let  $G$  be an undirected connected graph with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$ . The distance between the vertices  $v_i$  and  $v_j$  of  $G$ , is equal to the length (= number of edges) of a shortest path starting at  $v_i$  and ending at  $v_j$  (or vice versa) [1], and will be denoted by  $d_G(v_i, v_j)$ . The distance matrix of  $G$  is defined as the  $n \times n$  matrix  $D(G) = (d_{ij})$ , where  $d_{ij}$  is the distance between vertices  $v_i$  and  $v_j$  in  $G$ . This matrix has been much studied by mathematical chemists, for details see [2, 3]. In a number of recently published articles, the so-called reduced distance matrix [4] or terminal distance matrix [5, 6] of trees was considered. If an  $n$ -vertex graph  $G$  has  $k$  pendent vertices (= vertices of degree one), labeled by  $\{v_1, v_2, \dots, v_k\}$ , then its reduced distance matrix is the square matrix of order  $k$  whose  $(i, j)$ -entry is  $d_G(v_i, v_j)$  and will be denoted by  $RD(G)$ . Reduced distance matrices were used for modeling of amino acid sequences of proteins and of the genetic code [5, 6, 7], and were proposed to serve as a source of novel molecularstructure descriptors [5, 6].

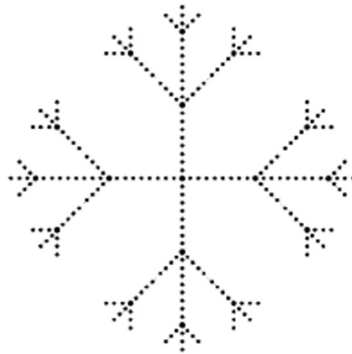
Dendrimers are hyperbranched molecules, synthesized by repeatable steps, either by adding branching blocks around a central core (thus obtaining a new, larger orbit or generation-the divergent growth approach) or by building large branched blocks starting from the periphery and then attaching them

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FIGURE 1. The graph of  $D_{3,3}$ .

to the core (the "convergent growth" approach [8]). The vertices of a dendrimer, except the extremal 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 branching points have the same degree, the dendrimer is called regular. Otherwise it is irregular. A regular monocentric dendrimer, of progressive degree  $p$  and generation  $r$  is herein denoted by  $D_{p,r}$  [9]-[11]. In this paper we will compute the spectrum of the reduced distance matrix of regular monocentric dendrimers.

## 2. Results and Discussion

As we mentioned the aim of this study is computing the spectra of reduced distance matrix of  $D_{p,r}$ . For this purpose, we represent the reduced distance matrix of  $D_{p,r}$  as a block matrix, and compute its eigenvalues. Suppose that  $I_n$  denotes the identity matrix of order  $n$  and  $J_n = (J_{ij})$  denotes an square matrix of order  $n$ , where

$$J_{ij} = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if } i \neq j. \end{cases}$$

Put  $B_n = I_n + J_n$ . So  $B_n$  is an square matrix whose each entry is equal to 1. To obtain the reduced distance matrix of  $D_{p,r}$  we first note that  $D_{p,1}$ , is the star of order  $p + 1$ . This is because that degree of the nonpendent vertices of  $D_{p,r}$  is  $p + 1$ . Thus the reduced distance matrix of  $D_{p,1}$  is given as follows:

$$RD(D_{p,1}) = 2J_p.$$

In what follows we will find the reduced distance matrix of  $D_{p,2}$ , which is obtained by making a new vertex adjacent to all central vertices of  $D_{p,1}$  (see Figure 2). For this purpose we shall use the tensor product of real matrices. Let  $A \otimes B$  denote the tensor product of two real matrices  $A$  and  $B$ .

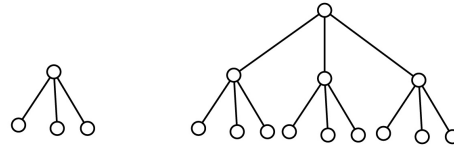


FIGURE 2. The graph of  $D_{3,1}$  and  $D_{3,2}$ .

The reduced distance matrix of  $D_{p,2}$  can be presented as

$$RD(D_{p,2}) = \begin{bmatrix} 2J_p & 4B_p & 4B_p & \dots & 4B_p \\ 4B_p & 2J_p & 4B_p & \dots & 4B_p \\ 4B_p & 4B_p & 2J_p & \dots & 4B_p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 4B_p & 4B_p & 4B_p & \dots & 2J_p \end{bmatrix} = 2J_P \otimes I_p + 4B_p \otimes J_p.$$

Thus the reduced distance matrix of  $D_{p,r}$  can be obtained recursively. In fact if we assume that  $D_1 = 2J_p$  and

$$(2.1) \quad D_n = D_{n-1} \otimes I_p + 2nB_{p^{n-1}} \otimes J_p$$

for  $n = 2, 3, \dots, r - 1$ , then the reduced distance matrix of  $D_{p,r}$  is given by

$$(2.2) \quad RD(D_{p,r}) = D_{r-1} \otimes I_{p+1} + 2rB_{p^{r-1}} \otimes J_{p+1}.$$

Therefore to compute the spectrum of  $DR(D_{p,r})$  we may find a method to calculating the eigenvalues of the block matrix where defined by the relation (1). First we recall a classical theorem of tensor product on two square matrices [12].

**Theorem A.** Let  $\{\lambda_i\}$  and  $\{x_i\}$  for  $1 \leq i \leq n$  be the eigenvalues and the corresponding eigenvectors for  $n$ -square matrix  $A$  respectively and  $\{\mu_j\}$  and  $\{y_j\}$  for  $1 \leq j \leq m$  be the eigenvalues and the corresponding eigenvectors for  $m$ -square matrix  $B$  respectively, then  $A \otimes B$  has eigenvalues  $\{\lambda_i \mu_j\}$  with corresponding eigenvectors  $\{x_i \otimes y_j\}$  for  $1 \leq i \leq n$  and  $1 \leq j \leq m$ .

Now let  $D_n$  be the block matrix given in equation (1). In the following Lemma we obtain an elementary result for  $D_n$  which is used to prove the main result of the paper. Recall that the spectrum of an  $n$ -square matrix that all its entries equal to 1 contains  $p$  and  $0$  with multiplicity  $n - 1$ .

**Lemma 1.** Let  $n \geq 1$  and  $B_{p^n}$  be a  $p^n$ -square matrix that all its entries are equal to 1. If  $x$  is an eigenvector of  $D_n$ , then  $B_{p^n}x = 0$  for all except  $x_0$ , one of the eigenvectors of  $D_n$  such that  $B_{p^n}x_0 = p^n x_0$ .

**Proof.** We prove the Lemma by induction on  $n$ . For  $n = 1$ , let  $\lambda$  be the eigenvalue of  $D_1 = 2J_p$  corresponding the eigenvector  $x$ , then

$$B_p x = (I_p + J_p)x = x + \frac{\lambda}{2}x.$$

Since  $\lambda = -2$  or  $\lambda = 2(p - 1)$ , so  $B_p x = 0$  or  $B_p x = px$ . Thus the result is true for  $n = 1$ .

Now Suppose that the Lemma is true for all positive integers less than  $n$ . If  $y$  is the eigenvector of  $B_p$  associated to the eigenvalue  $\mu$ , then

$$B_{p^n}(x \otimes y) = (B_{p^{n-1}} \otimes B_p)(x \otimes y) = B_{p^{n-1}}x \otimes \mu y.$$

By induction hypothesis we have  $B_{p^{n-1}}x = 0$  or  $B_{p^{n-1}}x = p^{n-1}x$ . Since  $\mu = 0$  or  $\mu = p$  we have  $B_{p^n}x = p^n x$  or  $B_{p^n}x = 0$ . This completes the proof. □

Now by using Lemma 1 we can compute the eigenvalues of square matrix  $D_{n+1}$  defined in equation (1), by using the eigenvalues of  $D_n$  for  $n \geq 1$ .

**Lemma 2.** Let  $n \geq 2$  and  $x_0$  be the eigenvector of  $D_{n-1}$  associated to the eigenvalue  $\lambda_0$  where  $B_{p^{n-1}}x_0 = p^n x_0$ . If  $\lambda_1 \neq \lambda_0$  is an eigenvalue with multiplicity  $k$  of  $D_{n-1}$  then the spectrum of  $D_n$  contains  $\lambda_1$  with multiplicity  $pk$ ,  $\lambda_0 - 2np^{n-1}$  with multiplicity  $p - 1$  and  $\lambda_0 + 2np^{n-1}(p - 1)$  with multiplicity one.

**Proof.** Let  $x$  be an eigenvector of  $D_{n-1}$  associated to the eigenvalue  $\lambda$  and  $y$  be an eigenvector of  $J_p$  associated to the eigenvalue  $\mu$ , then

$$\begin{aligned} D_n(x \otimes y) &= (D_{n-1} \otimes I_p + 2nB_{p^{n-1}} \otimes J_p)(x \otimes y) \\ &= \lambda x \otimes y + 2nB_{p^{n-1}}x \otimes \mu y. \end{aligned}$$

If  $x \neq x_0$ , then by Lemma 1 we have  $B_{p^{n-1}}x = 0$ , thus

$$D_n(x \otimes y) = \lambda_1(x \otimes y).$$

Since  $\lambda_1$  is an eigenvalue of  $D_{n-1}$  with multiplicity  $k$  and  $J_p$  is an square matrix of order  $p$ , so  $\lambda_1$  is an eigenvalue of  $D_n$  with multiplicity  $pk$ .

Now suppose that  $x = x_0$ , then by Lemma 1 we have  $B_{p^{n-1}}x = p^{n-1}x$ . Note that  $\mu = -1$  with multiplicity  $p - 1$  or  $\mu = p - 1$  with multiplicity 1. If  $\mu = -1$  then

$$D_n(x \otimes y) = (\lambda_0 - 2np^{n-1})(x \otimes y).$$

Hence  $\lambda_0 - 2np^{n-1}$  is an eigenvalue of  $D_n$  with multiplicity  $p - 1$ .

If  $\mu = p - 1$  then

$$D_n(x \otimes y) = (\lambda_0 + 2np^{n-1}(p - 1))(x \otimes y).$$

Hence  $\lambda_0 + 2np^{n-1}(p - 1)$  is an eigenvalue of  $D_n$  with multiplicity 1.

Therefore the proof is complete. □

Now we can compute the spectrum of square block matrix  $D_n$  which is given in equation (1), using Lemma 2.

**Lemma 3.** Let  $n \geq 1$ . The spectrum of  $D_n$  contains  $-2$  with multiplicity  $(p - 1)p^{n-1}$ ,  $\sum_{i=1}^{m-1} 2i(p - 1)p^{i-1} - 2mp^{m-1}$  with multiplicity  $(p - 1)p^{n-m}$  for  $m = 2, 3, \dots, n$  and  $\sum_{i=1}^n 2i(p - 1)p^{i-1}$  with multiplicity 1.

**Proof.** We prove the Lemma by induction on  $n$ . If  $n = 1$ , then  $D_1 = 2J_p$ , hence the spectrum of  $D_1$  contains  $-2$  with multiplicity  $p - 1$  and  $2(p - 1)$  with multiplicity 1. Thus the argument is true for  $n = 1$ .

Now Suppose that the Lemma is true for all positive integers less than  $n$ . Hence the spectrum of  $D_{n-1}$  contains  $-2$  with multiplicity  $(p - 1)p^{n-2}$ ,  $\sum_{i=1}^{m-1} 2i(p - 1)p^{i-1} - 2mp^{m-1}$  with multiplicity  $(p - 1)p^{n-m-1}$  for  $m = 2, 3, \dots, n - 2$  and  $\sum_{i=1}^{n-1} 2i(p - 1)p^{i-1}$  with multiplicity 1. By using Lemma 2 the spectrum of  $D_n$  contains  $-2$  with multiplicity  $p \times (p - 1)p^{n-2}$ ,  $\sum_{i=1}^{m-1} 2i(p - 1)p^{i-1} - 2mp^{m-1}$  with multiplicity  $p \times (p - 1)p^{n-m-1}$  for  $m = 2, 3, \dots, n - 1$ ,  $\sum_{i=1}^{n-1} 2i(p - 1)p^{i-1} - 2np^{n-1}$  with multiplicity  $p - 1$  and  $\sum_{i=1}^{n-1} 2i(p - 1)p^{i-1} + 2n(p - 1)p^{n-1}$  with multiplicity 1. Hence the spectrum of  $D_n$  contains  $-2$  with multiplicity  $(p - 1)p^{n-1}$ ,  $\sum_{i=1}^{m-1} 2i(p - 1)p^{i-1} - 2mp^{m-1}$  with multiplicity  $(p - 1)p^{n-m}$  for  $m = 2, 3, \dots, n$  and  $\sum_{i=1}^n 2i(p - 1)p^{i-1}$  with multiplicity 1.

Therefore the proof is complete. □

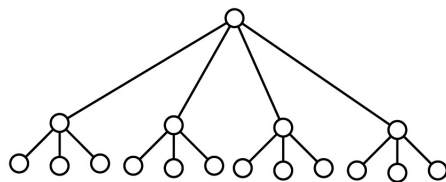
Now we can compute the spectrum of reduced distance matrix of regular monocentric dendrimers.

**Theorem 1.** The spectrum of reduced distance matrix of the regular monocentric dendrimer of progressive degree  $p$  and generation  $r$  contains  $-2$  with multiplicity  $(p^2 - 1)p^{r-2}$ ,  $\sum_{i=1}^{m-1} 2i(p - 1)p^{i-1} - 2mp^{m-1}$  with multiplicity  $(p^2 - 1)p^{r-m-1}$  for  $m = 2, 3, \dots, r$  and  $\sum_{i=1}^{r-1} 2i(p - 1)p^{i-1} + 2rp^r$  with multiplicity one.

**Proof.** The proof is straightforward by using Lemma 1 and 3. □

**Example 1.** As an application of Theorem 1 we compute the spectrum of the reduced distance matrix of  $D_{3,3}$  (see Figure 1). If  $D_2 = 2J_3 \otimes I_3 + 4B_3 \otimes J_3$ , then the reduced distance matrix of  $D_{3,3}$  is an square matrix of order 36 is given by equation (2)

$$RD(D_{3,3}) = D_2 \otimes I_4 + 6B_9 \otimes J_4.$$

FIGURE 3. The graphs of  $D_{3,1}$  and  $D_{3,2}$ .

By Theorem 1 the spectrum of  $RD(D_{3,3})$  contains  $-2$  with multiplicity 24,  $-8$  with multiplicity 8,  $-26$  with multiplicity 3 and 190 with multiplicity 1.

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