ON THE SPECTRA OF REDUCED DISTANCE MATRIX OF DENDRIMERS

ABBAS HEYDARI

Communicated by Bijan Taeri

ABSTRACT. Let G be a simple connected graph and $\{v_1, v_2, \ldots, v_k\}$ 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 $V(G) = \{v_1 v_2, \ldots, v_n\}$. 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 $\{v_1, v_2, \ldots, v_k\}$, 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
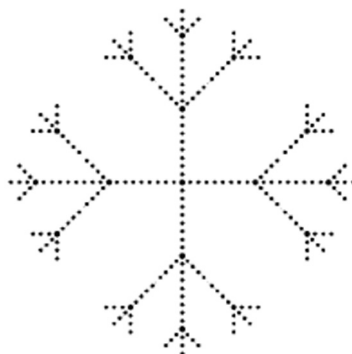
FIGURE 1. The graph of $D_{3,3}$.

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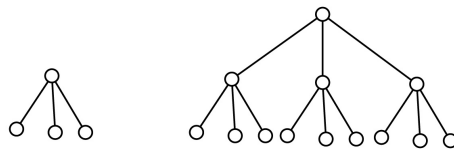
FIGURE 2. The graph of $D_{3,1}$ and $D_{3,2}$.

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

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

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

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

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

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 $1 \le i \le n$ be the eigenvalues and the corresponding eigenvectors for n-square matrix A respectively and $\{\mu_j\}$ and $\{y_j\}$ for $1 \le j \le m$ 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 $1 \le i \le n$ and $1 \le j \le m$.

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 $n \ge 1$ 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 λ 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 μ, 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. $\qquad\square$

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 λ_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 λ_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 λ and y be an eigenvector of J_p associated to the eigenvalue μ, then

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

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 λ_1 is an eigenvalue of D_{n-1} with multiplicity k and J_p is an square matrix of order p, so λ_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. $\qquad\square$

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 $m = 2, 3, \ldots, n$ 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 $m = 2, 3, \ldots, n-2$ 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 $m = 2, 3, \ldots, n-1$, $\sum_{i=1}^{n-1} 2i(p-1)p^{i-1} - 2np^{n-1}$ 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 $m = 2, 3, \ldots, n$ and $\sum_{i=1}^{n} 2i(p-1)p^{i-1}$ with multiplicity 1.

Therefore the proof is complete. $\qquad\qquad\square$

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 $m = 2, 3, \ldots, r$ 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. $\qquad\qquad\square$

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)

$$RD(D_{3,3}) = D_2 \otimes I_4 + 6B_9 \otimes J_4.$$
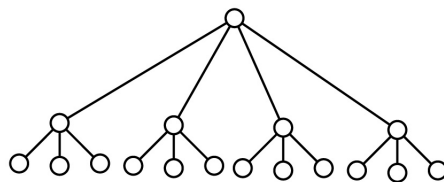
FIGURE 3. The graphs of $D_{3,1}$ and $D_{3,2}$.

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.

References

[1] F. Buckley and F. Harary,*Distance in Graphs*, Addison-Wesley Publishing Company, Advanced Book Program, Redwood City, 1990.

[2] D. H. Rouvray, *The role of the topological distance matrix in chemistry,* Mathematical and computational concepts in chemistry (Dubrovnik, 1985), Ellis Horwood Ser, Math. Appl., Horwood, Chichester, 1986 295–306.

[3] Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D. Plavsić and N. Trinajstić, The distance matrix in chemistry,*J. Math. Chem.*, **11** (1992) 223–258.

[4] E. A. Smolenskii, E. V. Shuvalova, L. K. Maslova, I. V. Chuvaeva and M. S. Molchanova, Reduced matrix of topological distances with a minimum number of independent parameters: distance vectors and molecular codes, *J. Math. Chem.*, **45** (2009) 1004-1020.

[5] B. Horvat, T. Pisanski and M. Randic, Terminal polynomials and star-like graphs, *MATCH Commun. Math. Comput. Chem.*, **60** (2008) 493-512.

[6] M. Randić, J. Zupan and D. Vikić-Topić, On representation of proteins by starlike graphs, *J. Mol. Graph. Modell.*, **26** (2007) 290-305.

[7] M. Randić and J. Zupan, Highly compact 2D graphical representation of DNA sequences, *SAR QSAR Environ. Res*, **15** (2004) 191-205.

[8] M. V. Diudea, Wiener Index of Dendrimers, *MATCH Commun. Math.Comput. Chem*, **32** (1995) 71-83.

[9] M. V. Diudea and B. Pârv, Molecular Topology. 25. Hyper-Wiener Index of Dendrimers, *J. Chem. Inf. Comput. Sci*, **35** (1995) 1015-1018.

[10] A. Heydari, Balaban index of regular dendrimers,*Optoelectron. Adv. Mater.-Rapid Commun.*, **5** no. 11 (2011) 1260-1262.

[11] A. Heydari, Harary index of regular dendrimers,*Optoelectron. Adv. Mater.-Rapid Commun.*, **4** no. 12 (2010) 2206-2208.

[12] F. Zhang, Matrix Theory, Basic Results and Techniques, Universitext, Springer-Verlag, New York, 1999.

Abbas Heydari

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

Email: a-heidari@iau-arak.ac.ir