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On the Spectra of Reduced Distance Matrix of Thorn Graphs

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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 thorn graph of G, a graph which obtained by attaching some new vertices to pendent vertices of G. As an application we compute the spectrum of reduced distance matrix for some dendrimer graphs.

Keywords: Reduced distance matrix, spectrum, thorn graph, dendrimer graphs.

1. INTRODUCTION

Let G be a connected graph with vertex set $\{v_1, v_2, \ldots, v_n\}$. The distance between 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 vice versa) [1], 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, labelld 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 $RD(G)$.

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Reduced distance matrices were used for modeling of amino acid sequences of proteins and of the genetic code [5, 6, 8], and were proposed to serve as a source of novel molecular structure descriptors [5, 6].

Let G a connected n–vertex graph with vertex set $\{v_1, v_2, ..., v_n\}$, and let $P = (p_1, p_2, ..., p_n)$ be an n–tuple of non-negative integers. The thorn graph G_P is the graph obtained by attaching p_i pendent vertices to the vertex v_i of G for $i = 1, 2, ..., n$.

The p_i pendent vertices attached to the vertex v_i will be called the thorns of v_i. The concept of thorny graphs was introduced by Gutman [10], and eventually found a variety of chemical applications [11, 12]. In this paper, we obtain the spectrum of the reduced distance matrix of thorn graph of G where has been obtained by attaching p new vertices to pendent vertices of G.

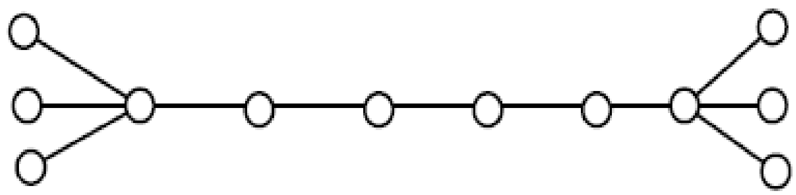

Figure 1. The Terminal Thorn Graph of Path of Order 6 for p = (3,0,0,0,0,3).

2. RESULTS AND DISCUSSION

Let G be a connected n-vertex graph and $P = (p_1, p_2, ..., p_n)$ be an n–tuple of non-negative integers such that for non-negative integer p, where $p_i = p$ if v_i is a pendent vertex of G and $p_i = 0$ if v_i is an non-pendent. So, G_P is obtained by attaching p new vertices to pendent vertices of G. This graph is called terminal p-thorn graph of G and is denoted by G_p. In this section we represent the reduced distance matrix of G_p as a block matrix, and compute the eigenvalues of it.

Suppose that I_n denotes the identity matrix of order n and $J_n = (J_{ij})$ denotes an square matrix of order n where

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

Put $B_n = I_n + J_n$. Thus B_n is an square matrix such that all of the its entries are equal to one. If for pendent vertices v_i and v_j of G, $d_{ij} = d_G(v_i, v_j) + 2$, then the reduced distance matrix of G_p can be represented as follows

$$RD(G_p) = \begin{bmatrix} 2J_p & d_{12}B_p & d_{13}B_p & \dots & d_{1k}B_p \\ d_{21}B_p & 2J_p & d_{23}B_p & \dots & d_{2k}B_p \\ d_{31}B_p & d_{32}B_p & 2J_p & \dots & d_{3k}B_p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ d_{k1}B_p & d_{k2}B_p & d_{k3}B_p & \dots & 2J_p \end{bmatrix}.$$

Now let $A \times B$ be the tensor product of two matrices A and B. If $D_k = (d_{ij})$ is k–square matrix such that $d_{ij} = d_G(v_i, v_j)+2$, where v_i and v_j are two pendent vertices of G, then

$$RD(G_p) = B_p \times D_k - 2I_{p^k}.$$

So to compute the eigenvalues of $RD(G_p)$ we can use the following theorem, which is a classical theorems of tensor product of two square complex matrices [9].

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 and $\{\mu_i\}$ and $\{y_i\}$ for $1 \le j \le m$ be the eigenvalues and the corresponding eigenvectors for m-square matrix B, then $A \times B$ has eigenvalues $\{\lambda_i \mu_j\}$ with corresponding eigenvectors $\{x_i \otimes y_j\}$ for $1 \le i \le n$ and for $1 \le i \le m$.

In the following corollary, we obtain the spectrum of $RD(G_p)$ in term of the eigenvalues of $RD(G)$ by using Theorem A. In continue we denote by $(\lambda)_m$ the eigenvalue λ of a square matrix with multiplicity m.

Corollary 1. Let G be a connected graph with k pendent vertices and D_k denote the reduced distance matrix of G. If $\{\lambda_i\}$ for $1 \le i \le n$ be the eigenvalues of D_k+2B_k, the spectrum of the reduced distance matrix of terminal p-thorn graph of G contains -2, with multiplicity $k(p-1)$ and $p\lambda_i - 2$ for $i = 1,2, \dots, k$.

Proof. By using (*1*), the reduced distance matrix of G_p is given by

$$B_p \times D_k - 2I_{p^k}.$$

Since the spectrum of square matrix B_p contains $(0)_{p-1}$ and $(p)_1$, by using Theorem A the spectrum of the reduced distance matrix of G_p contains $0 \times \lambda_i$ with multiplicity $k(p-1)$ and $p\lambda_i - 2$ for $i = 1,2, \dots, k$. Therefore proof is completed. ■

In what follows we compute the spectrum of reduced distance matrix of some dendrimer graphs by using Corollary *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” [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.

Example 1. As an application we consider a dendrimer series in which Corollary *1* is applicable (see Fig. *2*). This molecular structure can be seen in some of the dendrimer graphs such as tertiary phosphine dendrimers. Since G_2 is constructed by attaching two thorny vertices to pendent vertices of G_1, we have $p=2$ and $k=6$. If D_6 denotes the reduced distance matrix of G_1 then the spectrum of $D_6 + 2B_6$ contains -2, with multiplicity *3*, *–10* with multiplicity *32* and *38* with multiplicity *1* (or $(-2)_3$, $(-10)_{32}$ and $(38)_1$). Since

$$RD(D_2) = B_2 \times D_6 - 2I_6.$$

Corollary *1* implies that the reduced spectrum of G_2 contains $(-2)_6$, $(-6)_3$, $(-22)_2$ and $(74)_1$.

In the molecular graphs such as dendrimers and starlike trees usually the topological distances between pendent vertices are equal. In reduced distance matrix of this graph all of the entries are equal. So, we motivate to define the a special class of the connected graphs.

Definition 1. A connected graph is called *regular reduced distance graph* if distances between whose pendent vertices is equal.

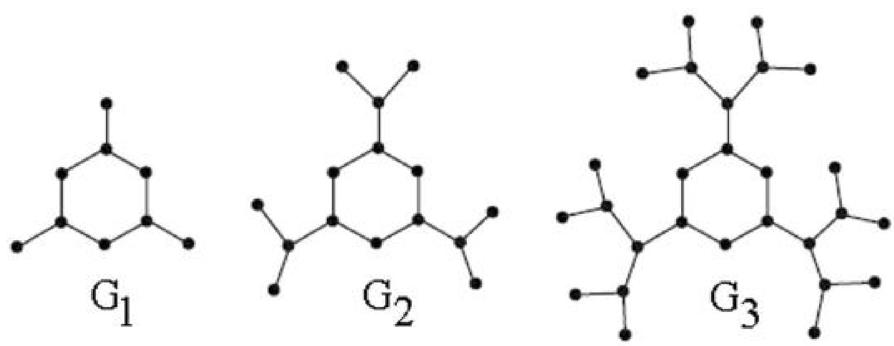

Figure 2. Dendrimer Series of Example 1.

If d be distance between pendent the vertices of regular distance graph G, then the reduced distance matrix of G_p can be computed as follows:

$$RD(G_p) = 2J_p \times I_k + dB_p \times J_k. \tag{2}$$

By using Theorem *A* the eigenvalues of G_p can be calculated in term of non–negative integers *p*, *d* and *k* where are introduced in previous paragraphs.

Theorem 1. Let *G* be a regular reduced distance graph with *k* pendent vertices. If *d* is the distance between the pendent vertices of *G* then the spectrum of the reduced distance matrix of terminal *p*–thorn graph of *G* contains -2, with multiplicity $k(p-1)$, $2(p-1)-pd$ with multiplicity $k-1$ and $2(p-1)+pd(k-1)$ with multiplicity one.

Proof. Since the spectrum of square matrix J_p contains $(-1)_{p-1}$ and $(p-1)_1$, we assume that *x* denotes one of the $p-1$ corresponding eigenvector of -1. Hence

$$B_p x = (I_p + J_p)x = x + J_p x = x - x = 0.$$

Now let *y* be one of the *k* eigenvectors of J_k. By using Theorem *A* and (2) we have

$$\begin{aligned} RD(G_p)(x\otimes y) &= (2J_p \otimes I_k)(x\otimes y) + (dB_p \otimes J_k)(x\otimes y) \\ &= 2J_p x \otimes I_k y + dB_p x \otimes J_k y \\ &= -2x\otimes y + 0x\otimes J_k y \\ &= -2(x\otimes y). \end{aligned}$$

Thus -2 is an eigenvalue of the $RD(G_p)$ with multiplicity $k(p-1)$. Now suppose that *x* is the eigenvector of J_p corresponding $p-1$. In this case we have

$$B_p x = (I_p + J_p)x = x + (p-1)x = x.$$

If *y* is one of the $k-1$ eigenvectors correspond to the eigenvalue -1 of J_k we have

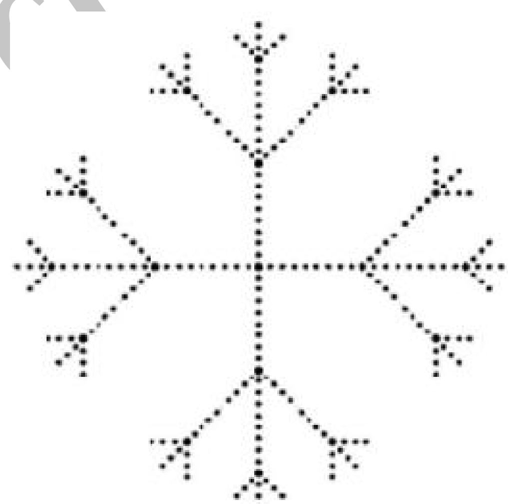

Figure 3. The Lattice of Regular Monocentric Dendrimer $D_{3,3}$.

$$\begin{aligned} RD(G_p)(x\otimes y) &= (2J_p\otimes I_k)(x\otimes y)+(dB_p\otimes J_k)(x\otimes y)\\ &= 2J_p x\otimes I_k y + dB_p x\otimes J_k y\\ &= 2(p-1)x\otimes y + pdx\otimes(-y)\\ &= (2(p-1)-dp)(x\otimes y). \end{aligned}$$

Hence $2(p-1)-pd$ is an eigenvalue of the $RD(G_p)$ with multiplicity $k-1$. At least assume that y is the corresponding eigenvector of the eigenvalue $k-1$ of J_k, then

$$\begin{aligned} RD(G_p)(x\otimes y) &= 2J_p x\otimes I_k y + dB_p x\otimes J_k y\\ &= 2(p-1)x\otimes y + pdx\otimes(k-1)y\\ &= (2(p-1)-dp(k-1))(x\otimes y). \end{aligned}$$

Hence $2(p-1) + pd(k-1)$ is an eigenvalue of the $RD(G_p)$ with multiplicity one. Therefore proof is completed. ∎

Example 2. Let $D_{p,2}$ be the regular monocentric dendrimer where its progressive degree is p (see Fig. 2). Since $D_{p,2}$ is constructed by attaching p horny vertices to the pendent vertices of S_{p+1}, the star graph of order $p+1$, we have $k = p + 1$ and $d = 4$. Hence Theorem 1 implies that the spectrum of reduced distance matrix of $D_{p,2}$ contains -2 with multiplicity p^2-1, $-2(p-1)$ with multiplicity p and $4p^2+2p-2$ with multiplicity one. For $r>2$, $D_{p,r}$ can be constructed by attaching p thorny vertex to pendent vertices of $D_{p,r-1}$. So the spectrum of reduced distance matrix of $D_{p,r}$ can be computed using Corollary 1.

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