Iranian J. Math. Chem. 8(3) September (2017) 291 − 298

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

On the Spectra of Reduced Distance Matrix of the Generalized Bethe Trees

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ARTICLE INFO

Article History:

Received: 8 June 2015
Accepted:8 June 2017
Published online14 July 2017
Academic Editor: Bijan Taeri

Keywords:

Reduced distance matrix
Generalized Bethe tree
Spectrum

ABSTRACT

Let G be a simple connected graph and $\{v_1, v_2, v_3, \dots, v_k\}$ be the set of pendant (vertices of degree one) vertices of G. The reduced distance matrix of G is a square matrix of order k whose (i, j)-entry is the topological distance between v_i and v_j of G. A rooted tree is called a generalized Bethe tree if its vertices at the same level have equal degree. In this paper, we compute the spectrum of the reduced distance matrix of the generalized Bethe trees.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2, v_3, \dots, v_n\}$. The distance between the vertices v_i and v_j of G, is equal to the length (= number of edges) of each shortest path starting at v_i and ending at v_j (or vice versa) [2], 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. While the problem of computing the characteristic polynomial of adjacency matrix and its spectrum appears to be solved for many large graphs, the related distance polynomials have received much less attention. The distance matrix is more complex than the ordinary adjacency matrix of a graph since the distance matrix is a complete matrix while in the adjacency matrix most of entries are zero. Thus the computation of the characteristic polynomial of the distance matrix is computationally a much more intense problem and, in general, there are no simple analytical solutions except for a few trees [6]. For this reason, distance polynomials of only trees have been studied extensively in the mathematical literature [6, 7]. The distance

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DOI: 10.22052/ijmc.2017.30051.1116

matrix of a graph and its spectrum has numerous applications to chemistry and other branches of science. The distance matrix, contains information on various walks and self-avoiding walks of chemical graphs, is immensely useful in the computation of topological indices such as the Wiener index, is useful in the computation of thermodynamic properties such as pressure and temperature coefficients and it contains more structural information compared to a simple adjacency matrix [1].

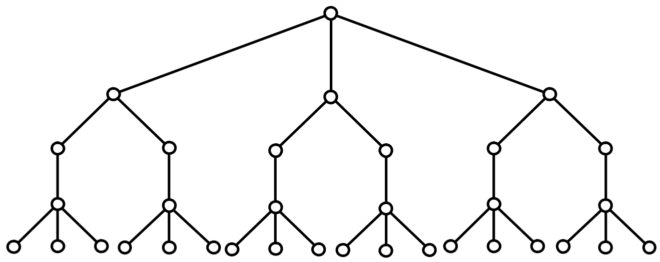

Figure 1: A Generalized Bethe Tree with 5 Levels.

In a number of recently published articles, the so-called reduced distance matrix [10] or terminal distance matrix [5, 8] of trees was considered. If an n-vertex graph G has n' pendant vertices (= vertices of degree one), labeled by $\{v_1, v_2, v_3, \dots, v_{n'}\}$, then its reduced distance matrix is the square matrix of order n' 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, and were proposed to serve as a source of novel molecular structure descriptors [5, 8].

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. Suppose T is an unweighted rooted tree such that its vertices at the same level have equal degrees. We agree that the root vertex is at level 1 and that T has k levels. In [9], Rojo and Robbiano, called such a tree with, generalized Bethe tree and denoted by β_k (see Figure 1). This class of trees has been much studied by mathematical chemists, for details see [3, 9].

In this paper we will compute the spectrum of the reduced distance matrix of the generalized Bethe trees by using methods of computation of eigenvalues of the tensor product of matrices. Recall that if A is a $m \times n$ matrix and B is a $p \times q$ matrix, then the tensor product $A \otimes B$ is the $mp \times nq$ block matrix as follows:

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \dots & a_{1n}B \\ a_{21}B & a_{22}B & \dots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \dots & a_{mn}B \end{bmatrix}.$$

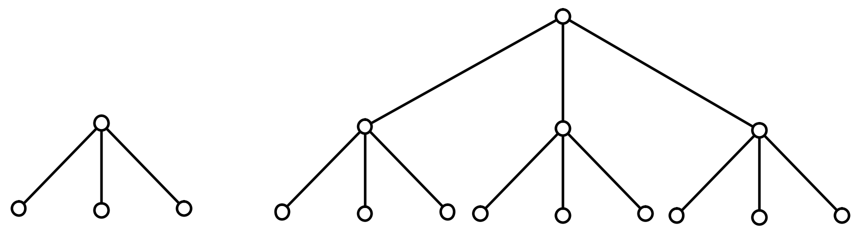

Figure 2: Simple Examples of β_2 and β_3.

Acyclic connected graphs or trees are wildly used in application of graph theory such as molecular graphs, telecommunication networks and the intellectual data analysis. Thus computation of numerical descriptors of trees has been studied in many recent papers [4−9]. The spectrum of the generalized Bethe trees can be used to obtain sharp bound for spectrum and some distance based topological indices of trees [9]. In this paper we will compute the spectrum of the reduced distance matrix of the generalized Bethe trees by exact formula in terms of its vertex degrees and the number of its levels.

2. RESULTS AND DISCUSSION

As we mentioned the computation of the characteristic polynomial and spectrum of the distance based matrices of a graph is computationally a much more intense problem and, in general, there are no simple analytical solutions except for graphs with simple structure. We will compute the spectrum of the reduced distance matrix of β_k by rewrite this matrix as a special type of block matrices, which can be described by the tensor product of some simple matrices. For this purpose, we assume that d_{k-j+1} denotes the degree of vertices on the j–th level of β_k , for $j = 1,2,\ldots,k$. Put

$$e_j = \begin{cases} d_j, & j = k,1 \\ d_j - 1, & 1 < j < k. \end{cases}$$

Thus e_j denotes the number of vertices on the (j+1)-th level which are adjacent with a vertex on the j-th level of β_k, for $j = 1,2,\ldots,k-1$. If n_k denotes the number of the pendant vertices of β_k, then $n_k = \prod_{j=1}^{k} e_j$. Suppose that I_n denotes the identity matrix of order n and $J = [J_{ij}]$ denotes a square matrix of order n, where

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

Put $B_n = I_n + J_n$. So B_n is asquare matrix of order n with all elements equal exactly 1. To obtain the reduced distance matrix of β_k we note that β_2, is a star of order $e_2 + 1$, see Figure 2. This is because that degree of the non-pendant vertices of β_2 must be e_2. Thus the reduced distance matrix of β_2 is given as $RD(\beta_2) = 2J_{e_2}$. In what follows, we will describe the reduced distance matrix of β_3, which is obtained by making a new vertex adjacent to all central vertices of e_3 copy of β_2, see Figure 2. For this purpose we shall use the tensor product of real matrices as follows:

$$RD(\beta_3) = \begin{bmatrix} 2J_{e_2} & 4B_{e_2} & 4B_{e_2} & \cdots & 4B_{e_2} \\ 4B_{e_2} & 2J_{e_2} & 4B_{e_2} & \cdots & 4B_{e_2} \\ 4B_{e_2} & 4B_{e_2} & 2J_{e_2} & \cdots & 4B_{e_2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 4B_{e_2} & 4B_{e_2} & 4B_{e_2} & \cdots & 2J_{e_2} \end{bmatrix}_{e_3 \times e_3} = I_{e_3} \otimes RD(\beta_2) + J_{e_3} \otimes 4B_{e_2}.$$

Thus for j ≥ 2, the reduced distance matrix of β_{j+1} can be obtained by a recursive formula in terms of the reduced distance matrix of β_j by using the inductive method. Let $n_1 = 1$ and $n_j = \sum_{i=1}^{j} e_i$ denote the number of the pendant vertices of β_j, for $j = 2,3, \dots, k-1$. Since β_{j+1}, is obtained by making a new vertex adjacent to all central vertices of e_{j+1} copy of β_j, put $D_2 = 2J_{e_2}$ (the reduced distance matrix of β_2) and

$$D_{j+1} = I_{e_{j+1}} \otimes D_j + J_{e_{j+1}} \otimes 2jB_{n_j},$$

for $j = 2,3, \dots, k-1$. Then the reduced distance matrix of the generalized Bethe trees with k levels is given by $RD(\beta_k) = D_k$. Therefore to compute the spectrum of $RD(\beta_k)$ we must introduce a method to calculate the eigenvalues of the block matrix which is defined in (1). First we recall a classical theorem related to the tensor product of two square matrices [11].

Theorem A. Let $\{\lambda_i\}$ and $\{x_i\}, 1 \le i \le n$, denote the eigenvalues and the corresponding eigenvectors for n-square matrix A, respectively and $\{\mu_j\}$ and $\{y_j\}, 1 \le j \le m$, denote the eigenvalues and the corresponding eigenvectors for m-square matrix B, respectively. Then the eigenvalues of $A \otimes B$ are $\{\lambda_i \otimes \mu_j\}$ with corresponding eigenvectors $\{x_i \otimes y_j\}$, where $1 \le i \le n$ and $1 \le j \le m$.

In what follows, we introduce a method for computation the spectrum of the block matrices, which are defined in (1). Recall that the spectrum of an n-square matrix with all entries equal 1, contains n and 0 with multiplicity $n-1$.

Lemma 1. Let B_{n_j} denote an n_j-square matrix with all entries equal 1. If x denotes an eigenvector of $D_j, j \ge 2$, then $B_{n_j}x = 0$ for all eigenvector of D_j except x_0, one of the eigenvectors of D_j such that $B_{n_j}x_0 = n_j x_0$.

Proof. We proceed by induction on j. For $j = 2$, let λ be an eigenvalue of $D_2 = 2J_{e_2}$ with corresponding eigenvector x, then

$$B_{n_2}\mathrm{x} = \left(I_{n_2} + J_{n_2}\right)\mathrm{x} = \mathrm{x} + \frac{\lambda}{2}x,$$

since $n_2 = e_2$. Obviously, $\lambda = -2$ or $\lambda = 2(e_2 - 1)$, so $B_{n_2}\mathrm{x} = 0$ or $B_{n_2}\mathrm{x} = n_2\mathrm{x}$. Thus the result is true for $j = 2$. Now suppose that the lemma is true for all positive integers less than j. Since $n_j = e_j n_{j-1}$, if μ is an eigenvalue of B_{e_j} with associated eigenvector y, then

$$B_{n_j}(x\otimes y) = \left(B_{n_{j-1}}\otimes B_{e_j}\right)(x\otimes y) = B_{n_{j-1}}x\otimes \mu y.$$

By induction hypothesis, we have $B_{n_{j-1}}x = 0$ or $B_{n_{j-1}}x = n_{j-1}x$. Since $\mu = 0$ or $\mu = e_j$, $B_{n_j}x = 0$ or $B_{n_j}x = n_j x$. This completes the proof. □

Now by using Lemma 1, the spectrum of square matrix D_{j+1}, which is defined in equation (1), can be computed in terms of the eigenvalues of D_j for $j \geq 2$.

Lemma 2. Let as above, x_0 be an eigenvector of D_j associated to the eigenvalue λ_0 which $B_{n_j}x_0 = n_j x_0$ for $j \geq 2$. If $\lambda_1 \neq \lambda_0$ is an eigenvalue of D_j with multiplicity k, then the spectrum of D_{j+1} contains λ_1 with multiplicity $e_{j+1}k$, $\lambda_0 - 2jn_j$ with multiplicity $e_{j+1} - 1$ and $\lambda_0 + 2jn_j(e_{j+1} - 1)$ with multiplicity 1.

Proof. Let x be an eigenvector of D_j associated to λ and y be an eigenvector of $J_{e_{j+1}}$ associated to μ, then by use of (1) we have

$$D_{j+1}(y\otimes x)=(I_{e_{j+1}}\otimes D_j + J_{e_{j+1}}\otimes 2jB_{n_j})(y\otimes x)= y\otimes \lambda x + \mu y\otimes 2jB_{n_j}x.$$

If $x \neq x_0$, then by Lemma 1 we get $B_{n_j}x = 0$, thus $D_{j+1}(y\otimes x) = y\otimes\lambda x$. Since λ_1 is an eigenvalue of D_j with multiplicity k and $J_{e_{j+1}}$ is a square matrix of order e_{j+1}, so λ_1 is an eigenvalue of D_{j+1} with multiplicity ke_{j+1}. Now suppose that $x \neq x_0$, by Lemma 1 we have $B_{n_j}x = n_j x$. Note that $\mu = -1$ with multiplicity $e_{j+1} - 1$ or $\mu = e_{j+1} - 1$ with multiplicity 1. If $\mu = -1$, then $D_{j+1}(y\otimes x) = \left(\lambda_0 - 2jn_j\right)(y\otimes x)$. Hence $\lambda_0 - 2jn_j$ is an eigenvalue of D_{j+1} with multiplicity $e_{j+1} - 1$. Otherwise if $\mu = e_{j+1} - 1$, then

$$D_{j+1}(y\otimes x) = \left(\lambda_0 + 2jn_j(e_{j+1} - 1)\right)(y\otimes x).$$

Hence $\lambda_0 + 2jn_j(e_{j+1} - 1)$ is an eigenvalue of D_{j+1} with multiplicity 1. Therefore the proof is complete. □

Now we can compute the spectrum of the square block matrix D_{j+1} which is given in equation (1), using Lemma 2 and determine the elements of the spectrum of β_k.

Theorem 1. The spectrum of the reduced distance matrix of β_k, the generalized Bethe tree of level k, contains -2 with multiplicity $(e_2-1)\prod_{i=3}^{k} e_i$, $\sum_{i=1}^{m-1} 2i(e_{i+1}-1)n_i - 2mn_m$ with multiplicity $(e_{m+1}-1)\prod_{j=m+2}^{k} e_j$ for $m = 2,3,\dots,k-1$ and $\sum_{i=1}^{k-1} 2i(e_{i+1}-1)n_i$ with multiplicity 1.

Proof. We proceed by induction on k. If $k = 2$, then the reduced distance matrix of β_2 is given by$D_2 = 2J_{e_2}$. Hence the spectrum of D_2 contains -2 with multiplicity e_2-1 and $2(e_2-1)$ with multiplicity 1. Thus the argument is true for $k = 2$. We now assume that the theorem is true for all positive integers less than k. By using the assumption of induction, the spectrum of $RD(\beta_{k-1})$ contains -2 with multiplicity $(e_2-1)\prod_{i=3}^{k-1} e_i$, $\sum_{i=1}^{m-1} 2i(e_{i+1}-1)n_i - 2mn_m$ with multiplicity$(e_{m+1}-1)\prod_{j=m+2}^{k-1} e_j$ for $m = 2,3,\dots,k-2$ and $\sum_{i=1}^{k-2} 2i(e_{i+1}-1)n_i$ with multiplicity 1. By using Lemma 2, the spectrum of $RD(\beta_k)$ contains -2 with multiplicity

$$e_k(e_2-1)\prod_{i=3}^{k-1} e_i = (e_2-1)\prod_{i=3}^{k} e_i.$$

On the other hand, the spectrum of $RD(\beta_k)$ should contain the elements $\sum_{i=1}^{m-1} 2i(e_{i+1}-1)n_i - 2mn_m$ of the spectrum of $RD(\beta_{k-1})$ for $m = 2,3,\dots,k-2$, with multiplicity

$$e_k(e_{m+1}-1)\prod_{j=m+2}^{k-1} e_j = (e_{m+1}-1)\prod_{j=m+2}^{k} e_j.$$

Also corresponding to the elements $\sum_{i=1}^{k-2} 2i(e_{i+1}-1)n_i$ of the spectrum of $RD(\beta_{k-1})$, by using Lemma 2, $\sum_{i=1}^{k-2} 2i(e_{i+1}-1)n_i - 2(k-1)n_{k-1}$ is an element of the spectrum of $RD(\beta_k)$. Hence the spectrum of $RD(\beta_k)$ contains $\sum_{i=1}^{m-1} 2i(e_{i+1}-1)n_i - 2mn_m$ with multiplicity $e_{m+1}-1$ for $m = k-1$. Finally, by using Lemma 2, the spectrum of $RD(\beta_k)$ should contain the following values with multiplicity 1:

$$\sum_{i=1}^{k-2} 2i(e_{i+1}-1)n_i + 2(k-1)n_{k-1}(e_k-1) = \sum_{i=1}^{k-1} 2i(e_{i+1}-1)n_i.$$

Therefore the proof is completed. □

By using Theorem 1, the spectrum of the reduced distance matrix of trees such that vertices on same level have equal degree can be computed. For example the reduced distance spectrum of the dendrimer trees, the caterpillar trees and the B-trees will be computed by using this method.

Example 1. As an application of Theorem 1, we compute the spectrum of the reduced distance matrix of T, a generalized Bethe tree of order 63 which is shown in Figure 3. Notice that T is a tree with 5 levels and $e_2 = 2$, $e_3 = 3$, $e_4 = 3$ and $e_5 = 2$. By using Theorem 1, the spectrum of $RD(T)$ contains -2 with multiplicity $(e_2-1)\prod_{i=3}^{5} e_i = 18$.

Also the reduced distance matrix of T contains the following integer numbers with multiplicity $(e_3 - 1)\prod_{i=4}^{m+1} e_i$ for $m = 2,3,4$,

$$\sum_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m.$$

If $m = 2$, then $\sum_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m = 2(1) - 2(2)(2) = -6$. If $m = 3$, then $\sum_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m = 2(1) + 4(2)(2) - 6(6) = -18$ and if $m = 4$, then $\sum_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m = 2(1) + 4(2)(2) + 6(2)(3)(2) - 8(18) = -54$. Hence, the spectrum of $RD(T)$ contains -6 with multiplicity 12, -18 with multiplicity 4 and 54 with multiplicity 1. Finally, the last element of the spectrum of $RD(T)$ with multiplicity 1 is computed as $\sum_{i=1}^{k-1} 2i(e_{i+1} - 1)n_i = 2(1)(1) + 4(2)(2) + 6(2)(6) + 8(1)(18) = 234$.

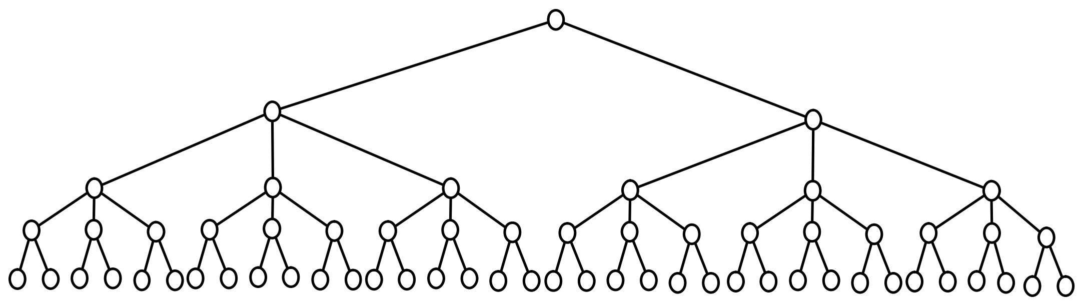

Figure 3: A Generalized Bethe Tree of Order 63.

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