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

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ABSTRACT

Let $G$ be a simple connected graph and $\{v_1, v_2, v_3, \ldots, v_k\}$ 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.

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1. INTRODUCTION

Let $G$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, v_3, \ldots, v_n\}$. 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].

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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 \{$v_1, v_2, v_3, \ldots, v_{n'}$\}, 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 $\mathcal{B}_k$ (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:

$$A \otimes B = 
\begin{bmatrix}
    a_{11}B & a_{12}B & \ldots & a_{1n}B \\
    a_{21}B & a_{22}B & \ldots & a_{2n}B \\
    \vdots & \vdots & \ddots & \vdots \\
    a_{m1}B & a_{m2}B & \ldots & a_{mn}B
\end{bmatrix}.$$
Acyclic connected graphs or trees are widely 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 $\beta_k$ 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 $\beta_k$, for $j = 1, 2, ..., k$. 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 $\beta_k$, for $j = 1, 2, ..., k - 1$. If $n_k$ denotes the number of the pendant vertices of $\beta_k$, 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

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

Put $B_n = I_n + J_n$. So $B_n$ is square matrix of order $n$ with all elements equal exactly 1. To obtain the reduced distance matrix of $\beta_k$ we note that $\beta_2$, is a star of order $e_2 + 1$, see Figure 2. This is because that degree of the non-pendant vertices of $\beta_2$ must be $e_2$. Thus the reduced distance matrix of $\beta_2$ is given as $RD(\beta_2) = 2J_{e_2}$. In what follows, we

Figure 2: Simple Examples of $\beta_2$ and $\beta_3$. 
will describe the reduced distance matrix of $\beta_3$, which is obtained by making a new vertex adjacent to all central vertices of $e_3$ copy of $\beta_2$, see Figure 2. For this purpose we shall use the tensor product of real matrices as follows:

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

Thus for $j \geq 2$, the reduced distance matrix of $\beta_{j+1}$ can be obtained by a recursive formula in terms of the reduced distance matrix of $\beta_j$ 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 $\beta_j$, for $j = 2, 3, \ldots, k - 1$. Since $\beta_{j+1}$, is obtained by making a new vertex adjacent to all central vertices of $e_{j+1}$ copy of $\beta_j$, put $D_2 = 2J_{e_2}$ (the reduced distance matrix of $\beta_2$) and

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

for $j = 2, 3, \ldots, k - 1$. 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 $\{x_i\}, 1 \leq i \leq n$, denote the eigenvalues and the corresponding eigenvectors for $n$-square matrix $A$, respectively and $\{\mu_j\}$ and $\{y_j\}, 1 \leq j \leq m$, 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 $1 \leq i \leq n$ and $1 \leq j \leq m$.

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 $D_j, j \geq 2$, 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 $\lambda$ be an eigenvalue of $D_2 = 2J_{e_2}$ with corresponding eigenvector $x$, then
\[ B_{n_2}x = (I_{n_2} + J_{n_2})x = x + \frac{\lambda}{2}x, \]

since \( n_2 = e_2 \). Obviously, \( \lambda = -2 \) or \( \lambda = 2(e_2 - 1) \), so \( B_{n_2}x = 0 \) or \( B_{n_2}x = n_2x \). Thus the result is true for \( j = 2 \). Now suppose that the lemma is true for all positive integers less than \( j \). Since \( n_j = e_jn_{j-1} \), if \( \mu \) is an eigenvalue of \( B_{e_j} \) with associated eigenvector \( y \), then

\[ B_{n_j}(x \otimes y) = (B_{n_{j-1}} \otimes B_{e_j})(x \otimes y) = B_{n_{j-1}}x \otimes \mu y. \]

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 \( B_{n_j}x = n_jx \). This completes the proof. \( \square \)

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 \( \lambda_0 \) which \( B_{n_j}x_0 = n_jx_0 \) 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 \( \lambda_1 \) with multiplicity \( e_{j+1}k \), \( \lambda_0 - 2j\lambda_n \) 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 \( \lambda \) and \( y \) be an eigenvector of \( J_{e_{j+1}} \) associated to \( \mu \), 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 \( \lambda_1 \) is an eigenvalue of \( D_j \) with multiplicity \( k \) and \( J_{e_{j+1}} \) is a square matrix of order \( e_{j+1} \), so \( \lambda_1 \) is an eigenvalue of \( D_{j+1} \) with multiplicity \( ke_{j+1} \). Now suppose that \( x \neq x_0 \), by Lemma 1 we have \( B_{n_j}x = n_jx \). Note that \( \mu = -1 \) with multiplicity \( e_{j+1} - 1 \) or \( \mu = e_{j+1} - 1 \) with multiplicity 1. If \( \mu = -1 \), then \( D_{j+1}(y \otimes x) = (\lambda_0 - 2jn_j)(y \otimes x) \). 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

\[ D_{j+1}(y \otimes x) = (\lambda_0 + 2jn_j(e_{j+1} - 1))(y \otimes x). \]

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

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 \( \beta_k \).

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

**Proof.** We proceed by induction on $k$. If $k = 2$, then the reduced distance matrix of $\beta_2$ 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 $(e_2 - 1) \prod_{i=3}^{k-1} e_i$, $\Sigma_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m$ with multiplicity $(e_{m+1} - 1) \prod_{j=m+2}^{k-1} e_j$ for $m = 2, 3, \ldots, k - 2$ and $\Sigma_{i=1}^{k-2} 2i(e_{i+1} - 1)n_i$ 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 $\Sigma_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m$ of the spectrum of $RD(\beta_{k-1})$ for $m = 2, 3, \ldots, k - 2$, 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 $\Sigma_{i=1}^{k-2} 2i(e_{i+1} - 1)n_i$ of the spectrum of $RD(\beta_{k-1})$, by using Lemma 2, $\Sigma_{i=1}^{k-2} 2i(e_{i+1} - 1)n_i - 2(k - 1)n_{k-1}$ is an element of the spectrum of $RD(\beta_k)$. Hence the spectrum of $RD(\beta_k)$ contains $\Sigma_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m$ 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. \hfill \Box

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...
On the spectra of reduced distance matrix of the generalized Bethe trees

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 \(m = 4,\)
\(\sum_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m = 2(1) + 4(2)(2) + 6(2)(3)(2) - 8(18) = -54.\) 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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