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On the Characteristic Polynomial and the Spectrum of the Terminal Distance Matrix of Kragujevac Trees

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ABSTRACT

In this paper, the characteristic polynomial and the spectrum of the terminal distance matrix of some special types of Kragujevac trees is computed. As an application, we obtain an upper bound and a lower bound for the spectral radius of the terminal distance matrix of the Kragujevac trees.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2, v_3, \dots, v_n\}$. For vertices $v_1, v_2 \in V(G)$,we denote by $d(v_1, v_2)$ the topological distance (i.e., the number of edges on the shortest path) joining the two vertices of G. The square matrix of order n whose (i, j) entry is $d(v_i, v_j)$ is called the distance matrix of G.

A connected acyclic graph is called a tree. The number of vertices of a tree is its order. The terminal distance matrix or reduced distance matrix is defined for (molecular)

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trees [1]. Let T be a tree of order n with k pendent vertices (vertices of degree one), labeled by $v_1, v_2, \dots, v_k$, then $TD(T)$ the terminal distance matrix of T, is the square matrix of order k whose (i,j) entry is $d(v_i, v_j)$ for $1 \le i,j \le k$.

Terminal distance matrices were used in the mathematical modeling of proteins and genetic codes [2, 3, 5], and were proposed to serve as a source of a whole class of molecular-structure descriptors [3, 4].

A rooted tree is a tree in which one particular vertex is distinguished, this vertex is referred to as the root (of the rooted tree). In order to define the Kragujevac trees, we first explain the structure of its branches [6].

Definition 1.1. Let P_3 be the *3*-vertex tree, rooted at one of its terminal vertices. For $k = 2,3, \dots$ construct the rooted tree B_k by identifying the roots of k copies of P_3. The vertex obtained by identifying the roots of P_3-trees is the root of B_k.

Examples illustrating the structure of the rooted tree B_k are depicted in Figure 1.

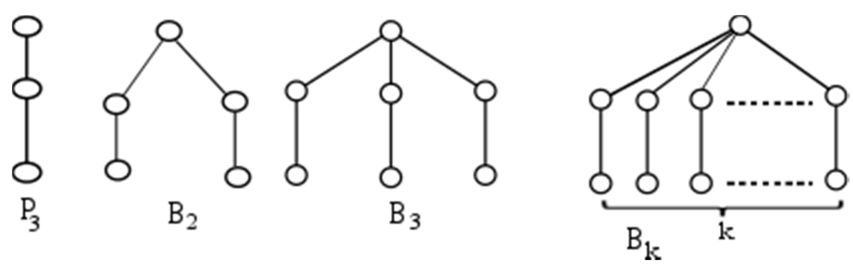

Figure 1. The rooted trees B_2, B_3, and B_k in the Definition 1.1.

Definition 1.2. Let $d \ge 2$ be an integer. Let $B_1, B_2, \dots, B_d$ be the rooted trees specified in Definition 1.1. A Kragujevac tree T is a tree possessing a vertex of degree d, adjacent to the roots of $B_1, B_2, \dots, B_d$. This vertex is said to be the central vertex of T, whereas d is the degree of T. The subgraphs $B_1, B_2, \dots, B_d$ are the branches of T (See Figure 2). Recall that some (or all) branches of T may be mutually isomorphic. If all branches of T are isomorphic, then T is called regular Kragujevac tree. We will denote by $T_{k,d}$ a regular Kragujevac tree with d branches isomorphic to B_k.

The class of Kragujevac trees emerged in several studies addressed to solve the problem of characterizing the tree with minimal atom-bond connectivity index [7,8].

Suppose that $G = \{G_1, G_{2,}, \dots, G_n\}$ is a sequence of simple graphs and H is a simple graph of order n. For $i = 1, 2, \dots, n$, choose a vertex x_i as the rooted vertex of G_i. The graph obtained by identifying x_i and i-th vertex of H is denoted by $H(G)$ and is called the rooted product of H by G [9]. If P_1 is the tree of order 1, S_{d+1} is the star graph of order $d+1$ and $G = \{P_1, B_{k_1}, B_{k_2}, \dots, B_{k_d}\}$, then the Kragujevac tree which is described in Definition 1.2, can be constructed by the rooted product of S_{d+1} by G as follows:

$$\mathrm{T} = S_{d+1}\left(P_1, B_{k_1}, B_{k_2}, \dots, B_{k_d}\right).$$

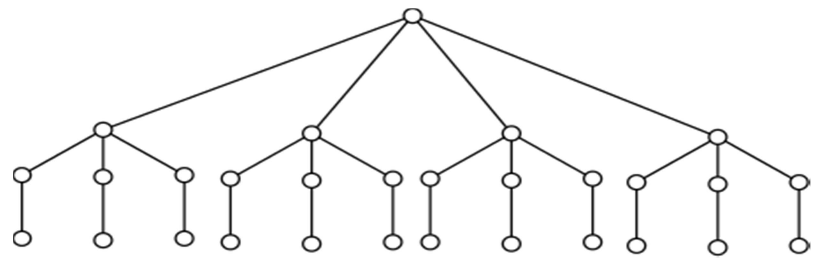

Figure 2. The graph of $T_{3,4}$, a regular Kragujevac tree of order 29 of degree 4.

Let A be a square matrix and $\bar{A}$ be the square matrix obtained from A, by deleting the first row and the first column. Suppose that $E_{m,n}$ denotes the $m \times n$ matrix whose (1,1) entry is 1 and others are 0. If $|A|$ denotes the determinant of square matrix A, then the following theorem obtain a method for computation of the characteristic polynomial of the rooted product of graphs [9].

Theorem 1.1. Let $A_{n_1}, A_{n_2}, \dots, A_{n_k}$ be symmetric matrices of order $n_1, n_2, \dots, n_k$ respectively. If

$$X = \begin{bmatrix} A_{n_1} & E_{n_1 n_2} & \cdots & E_{n_1 n_k} \\ E_{n_2 n_1} & A_{n_2} & \cdots & E_{n_2 n_k} \\ \vdots & \vdots & \ddots & \vdots \\ E_{n_k n_1} & E_{n_k n_2} & \cdots & A_{n_k} \end{bmatrix}, \text{ then } |X| = \begin{vmatrix} |A_{n_1}| & |\overline{A_{n_1}}| & \cdots & |\overline{A_{n_1}}| \\ |\overline{A_{n_2}}| & |A_{n_2}| & \cdots & |\overline{A_{n_2}}| \\ \vdots & \vdots & \ddots & \vdots \\ |\overline{A_{n_k}}| & |\overline{A_{n_k}}| & \cdots & |A_{n_k}| \end{vmatrix}.$$

In this paper, we compute the characteristic polynomial and the spectrum of the terminal distance matrix of $T_{k,d}$ in terms of positive integers d and k. As an application, we obtain an upper bound and a lower bound for the spectral radius of the terminal distance matrix of the Kragujevac trees.

2. CHARACTERISTIC POLYNOMIAL

In this section, the characteristic polynomial of the terminal distance matrix of some special types of Kragujevac trees is calculated by use of Theorem *1.1*. For this purpose the terminal distance matrix of these trees must be written in a suitable form of a block matrix.

If B_{k_i} for $1 \le i \le d$ is one of the branches of the Kragujevac tree $\mathrm{T} = S_{d+1}(P_1, B_{k_1}, B_{k_2}, \ldots, B_{k_d})$, then the terminal distance matrix of B_{k_i} is given as

$$TD(B_{k_i}) = \begin{bmatrix} 0 & 4 & \ldots & 4 \\ 4 & 0 & \ldots & 4 \\ \vdots & \vdots & \ddots & \vdots \\ 4 & 4 & \ldots & 0 \end{bmatrix}_{k_i \times k_i}.$$

If $C_{k_i \times k_j}$ is a $k_i \times k_j$ matrix whose all entries equal to 6, the terminal distance matrix of T is given as follows:

$$TD(T) = \begin{bmatrix} TD(B_{k_1}) & C_{k_1 \times k_2} & \ldots & C_{k_1 \times k_d} \\ C_{k_2 \times k_1} & TD(B_{k_2}) & \ldots & C_{k_2 \times k_d} \\ \vdots & \vdots & \ddots & \vdots \\ C_{k_d \times k_1} & C_{k_d \times k_2} & \ldots & TD(B_{k_d}) \end{bmatrix}_{d \times d}.$$

By subtracting the first row from the other rows, and then subtracting the first column of $C_{k_i \times k_j}$ from the other columns of this matrix, we can transform $C_{k_i \times k_j}$ to $6E_{k_i \times k_j}$ (whose $(1,1)$ entry is 6 and other entries are equal to 0). If D_i for $1 \le i \le d$, denotes the square matrix which is obtained by applying the used linear transformations to transform $C_{k_i \times k_j}$ to $6E_{k_i \times k_j}$ on $TD(B_{k_i})$, we have

$$TD(T) = \begin{bmatrix} D_1 & 6E_{k_1 \times k_2} & \ldots & 6E_{k_1 \times k_d} \\ 6E_{k_2 \times k_1} & D_2 & \ldots & 6E_{k_2 \times k_d} \\ \vdots & \vdots & \ddots & \vdots \\ 6E_{k_d \times k_1} & 6E_{k_d \times k_2} & \ldots & D_d \end{bmatrix}_{d \times d}.$$

Since $\det\left(\lambda I - TD(B_{k_i})\right) = \det(\lambda I - D_i)$, if $\Phi_{B_{k_i}}(\lambda)$ denotes the characteristic polynomial of $TD(B_{k_i})$ and $\overline{\Phi}_{B_{k_i}}(\lambda) = \det(\overline{D_i})$ for $1 \le i \le d$, then by using Theorem 1.1, the characteristic polynomial of the terminal distance matrix of T is given as

$$\Phi_T(\lambda) = \begin{vmatrix} \Phi_{B_{k_1}}(\lambda) & -6\overline{\Phi}_{B_{k_1}}(\lambda) & \ldots & -6\overline{\Phi}_{B_{k_1}}(\lambda) \\ -6\overline{\Phi}_{B_{k_2}}(\lambda) & \Phi_{B_{k_2}}(\lambda) & \ldots & -6\overline{\Phi}_{B_{k_2}}(\lambda) \\ \vdots & \vdots & \ddots & \vdots \\ -6\overline{\Phi}_{B_{k_d}}(\lambda) & -6\overline{\Phi}_{B_{k_d}}(\lambda) & \ldots & \Phi_{B_{k_d}}(\lambda) \end{vmatrix}_{d \times d}. \quad (1)$$

To compute Equation (1), we need to calculate the determinant of a special type of square matrices which is introduced in the following lemma.

Lemma 2.1. If the main diagonal of a square matrix contains $d_1$variable x and $d_2$variable y and the other entries are -6, then

$$\begin{vmatrix} x & -6 & \cdots & -6 & \cdots & -6 & \cdots & -6 \\ -6 & x & \cdots & -6 & \cdots & -6 & \cdots & -6 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & -6 \\ -6 & -6 & \cdots & x & -6 & -6 & \cdots & -6 \\ -6 & -6 & \cdots & -6 & y & -6 & \cdots & -6 \\ -6 & -6 & \cdots & -6 & -6 & y & \cdots & -6 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -6 & -6 & \cdots & -6 & -6 & -6 & \cdots & y \end{vmatrix}$$
$$= (x+6)^{d_1-1}(y+6)^{d_2-1}\big[x\big(y-\ 6(d_2-1)\big)-6(d_1-1)y-36(d_1+d_2-1)\big].$$

Proof. The lemma can be proved by induction on $n = d_1 + d_2$. □

Theorem 2.2. Let k, $d \geq 2$ be positive integers. The characteristic polynomial of the terminal distance matrix of the regular Kragujevac tree is computed as:

$$\Phi_{T_{k,d}}(\lambda) = (\lambda+4)^{d(k-1)}(\lambda+2k+4)^{d-1}(\lambda-k(6d-2)+4).$$

Proof. Let B_k be one of the branches of $T_{k,d}$. The characteristic polynomial of $TD(B_k)$ is given as follows:

$$\Phi_{B_k}(\lambda) = \begin{vmatrix} \lambda & -4 & \dots & -4 \\ -4 & \lambda & \dots & -4 \\ \vdots & \vdots & \ddots & \vdots \\ -4 & -4 & \dots & \lambda \end{vmatrix}_{k\times k} = (\lambda+4)^{k-1}\big(\lambda-4(k-1)\big). \qquad (2)$$

On the other hand, if M denotes the obtained determinant from $\Phi_{B_k}(\lambda)$ by subtracting the first row from the other rows and then subtracting the first column from the other columns of $\Phi_{B_k}(\lambda)$, then $\overline{\Phi}_{\beta_k}(\lambda) = \det(M)$. Hence

$$\overline{\Phi}_{B_k(\lambda)} = (\lambda+4)^{k-1} \begin{vmatrix} -2 & -1 & \dots & -1 \\ -1 & -2 & \dots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \dots & -2 \end{vmatrix}_{(k-1)\times(k-1)} = k(\lambda+4)^{k-1}. \qquad (3)$$

By Equation (1), the characteristic polynomial of the terminal distance matrix of $T_{k,d}$ is given as follows:

$$\Phi_{T_{k,d}}(\lambda) = \begin{vmatrix} \Phi_{B_k}(\lambda) & -6\overline{\Phi}_{B_k}(\lambda) & \dots & -6\overline{\Phi}_{B_k}(\lambda) \\ -6\overline{\Phi}_{B_k}(\lambda) & \Phi_{B_k}(\lambda) & \dots & -6\overline{\Phi}_{B_k}(\lambda) \\ \vdots & \vdots & \ddots & \vdots \\ -6\overline{\Phi}_{B_k}(\lambda) & -6\overline{\Phi}_{B_k}(\lambda) & \dots & \Phi_{B_k}(\lambda) \end{vmatrix}_{d\times d}.$$

Now by use of Lemma 2.1, we get

$$\Phi_{T_{k,d}}(\lambda) = \left(\overline{\Phi}_{B_k}(\lambda)\right)^d \left(\frac{\Phi_{B_k}(\lambda)}{\overline{\Phi}_{B_k}(\lambda)} + 6\right)^{d-1} \left(\frac{\Phi_{B_k}(\lambda)}{\overline{\Phi}_{B_k}(\lambda)} - 6(d-1)\right)$$
$$= \left(\Phi_{B_k}(\lambda) + 6\overline{\Phi}_{B_k}(\lambda)\right)^{d-1} \left(\Phi_{B_k}(\lambda) - 6(d-1)\overline{\Phi}_{B_k}(\lambda)\right)$$
$$= (\lambda+4)^{d(k-1)}(\lambda+2k+4)^{d-1}(\lambda - k(6d-2)+4).$$

Therefore, the proof is completed. □

Corollary 2.3. The spectrum of the terminal distance matrix of $T_{k,d}$ contains the integer numbers, -4 with multiplicity $d(k-1)$, $-2k-4$ with multiplicity $d-1$, and a positive integer equal to $k(6d-2)-4$.

In what follows, we compute the characteristic polynomial of the terminal distance matrix of two special types of Kragujevac trees which are used in the next section.

Theorem 2.4. Let $k, d \geq 2$ be positive integers. The characteristic polynomial of the terminal distance matrix of $T = S_{d+1}(P_1, B_k, B_2, \dots, B_2)$, the Kragujevac tree which one of its branches is B_k and other branches are B_2, is given as follows:

$$\Phi_T(\lambda) = (\lambda+4)^{d+k-2}(\lambda+8)^{d-2}(\lambda^2 - (4k+12d-24)\lambda - 8k(3d+1) - 16(3d-5)).$$

Proof. By Equation (1), we have

$$\Phi_{\mathrm{T}}(\lambda) = \begin{vmatrix} \Phi_{B_k}(\lambda) & -6\overline{\Phi}_{B_k}(\lambda) & \cdots & -6\overline{\Phi}_{B_k}(\lambda) \\ -6\overline{\Phi}_{B_2}(\lambda) & \Phi_{B_2}(\lambda) & \cdots & -6\overline{\Phi}_{B_2}(\lambda) \\ \vdots & \vdots & \ddots & \vdots \\ -6\overline{\Phi}_{B_2}(\lambda) & -6\overline{\Phi}_{B_2}(\lambda) & \cdots & \Phi_{B_2}(\lambda) \end{vmatrix}$$
$$= \overline{\Phi}_{B_k}(\lambda)\left(\overline{\Phi}_{B_2}(\lambda)\right)^{d-1} \begin{vmatrix} \frac{\Phi_{B_k}(\lambda)}{\overline{\Phi}_{B_k}(\lambda)} & -6 & \cdots & -6 \\ -6 & \frac{\Phi_{B_2}(\lambda)}{\overline{\Phi}_{B_2}(\lambda)} & \cdots & -6 \\ \vdots & \vdots & \ddots & \vdots \\ -6 & -6 & \cdots & \frac{\Phi_{B_2}(\lambda)}{\overline{\Phi}_{B_2}(\lambda)} \end{vmatrix}.$$

Now, by applying Lemma 2.1, we get

$$\Phi_{\mathrm{T}}(\lambda) = \overline{\Phi}_{B_k}(\lambda)\left(\overline{\Phi}_{B_2}(\lambda)\right)^{d-1} \left(\frac{\Phi_{B_2}(\lambda)}{\overline{\Phi}_{B_2}(\lambda)} + 6\right)^{d-2} \left(\frac{\Phi_{B_k}(\lambda)}{\overline{\Phi}_{B_k}(\lambda)}\left(\frac{\Phi_{B_2}(\lambda)}{\overline{\Phi}_{B_2}(\lambda)} - 6(d-2)\right) - 36(d-1)\right)$$
$$= \left(\Phi_{B_2}(\lambda) + 6\overline{\Phi}_{B_2}(\lambda)\right)^{d-2} \left(\Phi_{B_k}(\lambda)(\Phi_{B_2}(\lambda) - 6(d-2)\overline{\Phi}_{B_2}(\lambda)) - 36(d-1)\overline{\Phi}_{B_2}(\lambda)\overline{\Phi}_{B_k}(\lambda)\right).$$

The result now follows from replacing $\Phi_{B_k}(\lambda)$, $\overline{\Phi}_{B_k}(\lambda)$, $\Phi_{B_2}(\lambda)$ and $\overline{\Phi}_{B_2}(\lambda)$ from Equations (2) and (3). □

Theorem 2.5. Let $k, d \geq 2$ be positive integers. The characteristic polynomial of the terminal distance matrix of $T = S_{d+1}(P_1, B_{k+1}, \dots, B_{k+1}, B_k \dots, B_k)$, a Kragujevac tree of degree d with d_1 branches equal to B_{k+1} and $d - d_1$ branches equal to B_k is given as follows:

$$\Phi_T(\lambda) = (\lambda + 4)^{(k-1)d+d_1}(\lambda + 2k + 6)^{d_1-1}(\lambda + 2k + 4)^{d-d_1-1}$$
$$(\lambda^2 - (6dk - 4k + 6\,d_1 - 10)\lambda - (12d-4)k^2 - (36d - 20)k - 24(d_1 - 1)).$$

Proof. By Equation (1), $\Phi_T(\lambda)$ is given as follows:

$$\begin{vmatrix} \Phi_{B_{k+1}}(\lambda) & -6\overline{\Phi}_{B_{k+1}}(\lambda)\dots & -6\overline{\Phi}_{B_{k+1}}(\lambda) & \dots & -6\overline{\Phi}_{B_{k+1}}(\lambda)\dots & -6\overline{\Phi}_{B_{k+1}}(\lambda) \\ \vdots & \vdots & \vdots & \dots & -6\overline{\Phi}_{B_{k+1}}(\lambda)\dots & -6\overline{\Phi}_{B_{k+1}}(\lambda) \\ -6\overline{\Phi}_{B_{k+1}}(\lambda) & -6\overline{\Phi}_{B_{k+1}}(\lambda)\dots & \Phi_{B_{k+1}}(\lambda) & \dots & -6\overline{\Phi}_{B_{k+1}}(\lambda)\dots & -6\overline{\Phi}_{B_{k+1}}(\lambda) \\ -6\overline{\Phi}_{B_k}(\lambda) & -6\overline{\Phi}_{B_k}(\lambda)\dots & -6\overline{\Phi}_{B_k}(\lambda) & \dots & \Phi_{B_k}(\lambda)\dots & -6\overline{\Phi}_{B_k}(\lambda) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -6\overline{\Phi}_{B_k}(\lambda) & -6\overline{\Phi}_{B_k}(\lambda)\dots & -6\overline{\Phi}_{B_k}(\lambda) & \dots & -6\overline{\Phi}_{B_k}(\lambda) & \dots\ \Phi_{B_k}(\lambda) \end{vmatrix}$$

Now, by use of Lemma 2.1, we have

$$\Phi_T(\lambda) = \left(\overline{\Phi}_{B_{k+1}}(\lambda)\right)^{d_1}\left(\overline{\Phi}_{B_k}(\lambda)\right)^{d-d_1}\left(\frac{\Phi_{B_{k+1}}(\lambda)}{\overline{\Phi}_{B_{k+1}}(\lambda)} + 6\right)^{d_1-1} \times$$
$$\left(\frac{\Phi_{B_k}(\lambda)}{\overline{\Phi}_{B_k}(\lambda)} + 6\right)^{d-d_1-1}\left\langle\frac{\Phi_{k+1}(\lambda)}{\overline{\Phi}_{B_{k+1}}(\lambda)}\left(\frac{\Phi_k(\lambda)}{\overline{\Phi}_{B_k}(\lambda)} - 6(d - d_1 - 1)\right) - 6(d_1 - 1)\frac{\Phi_k(\lambda)}{\overline{\Phi}_{B_k}(\lambda)} - 36(d - 1)\right\rangle$$
$$= (\lambda + 4)^{(k-1)d+d_1}(\lambda + 2k + 6)^{d_1-1}(\lambda + 2k + 4)^{d-d_1-1} \times$$
$$(\lambda^2 - (6dk - 4k + 6\,d_1 - 10)\lambda - (12d-4)k^2 - (36d - 20)k - 24(d_1 - 1)).$$

This completes the proof. □

2. Spectral Radius

In this section, we obtain a lower bound and an upper bound for the spectral radius of Kragujevac trees of order n. Let $X = (x_1, x_2, \dots, x_n)$ be the Perron vector and ρ be the spectral radius of the terminal distance matrix of $T = S_{d+1}(P_1, B_{k_1}, B_{k_2}, \dots, B_{k_d})$. The components of X which are correspond to the pendant vertices of B_{k_i} are equal, so we will denote these components by x_{k_i} for $1 \leq i \leq d$.

Lemma 3.1. If $X = (x_1, x_2, \dots, x_n)$ is the Perron vector of the terminal distance matrix of $T = S_{d+1}(P_1, B_{k_1}, B_{k_2}, \dots, B_{k_d})$ and $k_i > k_j$ for some $1 \le i, j \le d$, then $x_{k_i} < x_{k_j}$.

Proof. If ρ denotes the spectral radius of T, then by use of the eigenvalue equation, we get $TD(T)X = \rho$X. Thus

$$\boldsymbol{\rho x_{k_i} = 4(k_i - 1)x_{k_i} + 6k_j x_{k_j} + \dots + 6k_d x_{k_d}}. \qquad \mathbf{(4)}$$

$$\rho x_{k_j} = 6k_i x_{k_i} + 4(k_j - 1)x_{k_j} + \dots + 6k_d x_{k_d}. \qquad (5)$$

By subtracting Equation (4) from Equation (5) we have

$$(\rho + 4 + 2k_i)x_{k_i} = (\rho + 4 + 2k_j)x_{k_j}.$$

Since $k_i > k_j$, hence $\mathrm{x}_{\mathrm{k_i}} < \mathrm{x}_{\mathrm{k_j}}$. □

Now let in $T = S_{d+1}(P_1, B_{k_1}, B_{k_2}, \dots, B_{k_d})$, k_i has maximum value and k_j has minimum value among branches of T. If $k_i - 1 > k_j$, then we denote by T^*, the Kragujevac three which is obtained from T by replacing B_{k_i} with $B_{k_i - 1}$ and replacing B_{k_j} with $B_{k_j + 1}$. The spectral radius of $TD(T)$ and $TD(T^*)$ will be compared in the following lemma.

Lemma 3.2. If ρ and ρ^* are the spectral radius of $TD(T)$ and $TD(T^*)$ respectively, then $\rho^* > \rho$.

Proof. Let D and D^* denote the terminal distance matrix of T and T^* respectively and X be the Perron vector of D. By use of the eigenvalue equation we get

$$\boldsymbol{X^t(D^* - D)X = 2(4k_j x_{k_i} x_{k_j} + 6(k_i - 1)x_{k_i}^2 - 4(k_i - 1)x_{k_i}^2 - 6k_j x_{k_i} x_{k_j})}$$

$$\boldsymbol{= 4x_{k_i}\Big((k_i - 1)x_{k_i} - k_j x_{k_j}\Big)}. \qquad \mathbf{(6)}$$

If $m = \sum_{i=1}^{d} k_i$, then by use of Equation (4) we get

$$\rho\, x_{k_i} > 4(k_i - 1)x_{k_i} + 6k_j x_{k_i} + 6(m - k_i - k_j)x_{k_i} \Rightarrow \rho + 4 > 6m - 2k_i. \qquad (7)$$

By subtracting Equations (4) and (5) we have

$$\rho\left(x_{k_j} - x_{k_i}\right) = (2k_i + 4)x_{k_i} - (2k_j + 4)x_{k_j} \Rightarrow (\rho + 4 + 2k_i)x_{k_i} = (\rho + 4 + 2k_j)x_{k_j}.$$

Hence,

$$(k_i - 1)x_i - k_j x_j = (k_i - 1)x_i - k_j \frac{\rho + 4 + 2k_i}{\rho + 4 + 2k_j} x_i = \frac{(\rho + 4)(k_i - 1 - k_j) - 2k_j}{\rho + 4 + 2k_j} x_i$$

Since $k_i - 1 - k_j > 1$, by use of Equation (7), we get

$$(k_i - 1)x_i - k_j x_j > \frac{6m - 2k_i - 2k_j}{\rho + 4 + 2k_j} x_i > 0. \quad (8)$$

Now by using Equations (6) and (8) we have $X^t(D^* - D)X > 0$ and from Riley equation, we get $\rho^* \geq \frac{X^t D^* X}{X^t X} > \frac{X^t D X}{X^t X} = \rho$. Therefore, the proof is completed. □

Let $k, d \geq 2$ be positive integers. In continue we suppose that

$$r = \left\lfloor \frac{n-d-1}{2d} \right\rfloor \text{ and } d_1 = \frac{n-(2r+1)d-1}{2}.$$

If T is a Kragujevac tree of order n with degree d, then d_1 is an positive integer.

Theorem 3.3. Among Kragujevac trees of order n and degree d, the terminal distance matrix of the Kragujevac tree with d_1 branches isomorphic to B_{r+1} and $d - d_1$ branches isomorphic to B_r, has maximum value of the spectral radius.

Proof. Let $T = S_{d+1}(P_1, B_{k_1}, B_{k_2}, \ldots, B_{k_d})$ be a Kragujevac tree of order n and degree d with maximum value of spectral radius. By use of Lemma 3.2, $|k_i - k_j| \leq 1$, for $1 \leq i, j \leq d$. Hence, $k_i = \left\lfloor \frac{n-d-1}{2d} \right\rfloor$ or $k_i = \left\lceil \frac{n-d-1}{2d} \right\rceil$, for $1 \leq i \leq d$. This completes the result. □

Corollary 3.4. If ρ is the spectral radius of the terminal distance matrix of a Kragujevac tree of order n and degree d, then

$$\rho \leq r(3\mathrm{d} - 2) + 3d_1 - 5 + \sqrt{9r^2d^2 + 18rdd_1 + 6r(d - 2d_1) + 3d_1(3d_1 - 2) + 1}.$$

Proof. By using Theorem 3.3, if $T = S_{d+1}(P_1, B_{r+1}, \ldots, B_{r+1}, B_r \ldots, B_r)$, then $TD(T)$ has maximum value of the spectral radius. Now by use of Theorem 2.5, ρ_T is the largest root of the equation $\lambda^2 - (6dr - 4r + 6\, d_1 - 10)\lambda - (12d - 4)r^2 - (36d - 20)r - 24(d_1 - 1) = 0$. Hence $\rho_T = r(3\mathrm{d} - 2) + 3d_1 - 5 + \sqrt{9r^2d^2 + 18rdd_1 + 6r(d - 2d_1) + 3d_1(3d_1 - 2) + 1}$. Thus the corollary is proved. □

Theorem 3.5. Among Kragujevac trees of order n and degree d, if $k = \frac{n-5d+3}{2}$ and $T = S_{d+1}(P_1, B_k, B_2, B_2 \ldots, B_2)$, then $TD(T)$ has minimum value of the spectral radius.

Proof. Let $T = S_{d+1}(P_1, B_{k_1}, B_{k_2}, \ldots, B_{k_d})$ be a Kragujevac tree of order n and degree d with minimum value of spectral radius. If $k_i = 2$, for $1 \leq i \leq d$, then the result of theorem is proved. Let for example $k_1 > 2$. If $k_i > 2$, for $2 \leq i \leq d$, then by using Lemma 3.2, we can obtain a Kragujevac tree of order n and degree d form T with larger spectral radius than ρ_T, which is a contradiction. Hence $k_i = 2$, $2 \leq i \leq d$, and the theorem is proved. □

Corollary 3.6. Let ρ be the spectral radius of the terminal distance matrix of a Kragujevac tree of order n and degree d. Then

$$\rho \geq 2k + 6d - 12 + 2\sqrt{(k+3d)^2 + 2k(3d-5) - 8(3d-2)}.$$

Proof. By use of Theorem 2.4, if $T = S_{d+1}(P_1, B_k, B_2, B_2 \ldots, B_2)$, then ρ_T is the greatest root of the following equation:

$$\lambda^2 - (4k + 12d - 24)\lambda - 8k(3d+1) - 16(3d-5) = 0,$$

Hence, $\rho_T = 2k + 6d - 12 + 2\sqrt{(k+3d)^2 + 2k(3d-5) - 8(3d-2)}$. We now apply Theorem 3.5 to deduce the result. □

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