



# Ordering trees by their distance spectral radii<sup>☆</sup>



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## ABSTRACT

Let  $D(G)$  be the distance matrix of a connected graph  $G$ . The distance spectral radius of  $G$ , denoted by  $\partial_1(G)$ , is the largest eigenvalue of  $D(G)$ . In this paper we present a new transformation of a certain graph  $G$  that decreases  $\partial_1(G)$ . With the transformation, we partially confirm a conjecture proposed by Stevanović and Ilić [17] by showing that, if  $\Delta \geq \lceil \frac{n}{2} \rceil$ , the double star  $S_{\Delta, n-\Delta}$  uniquely minimizes the distance spectral radius among all trees on  $n$  vertices with maximum degree  $\Delta$ . Moreover, the trees on  $n \geq 10$  vertices with the fourth and fifth least distance spectral radii are characterized.

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## 1. Introduction

We consider only finite connected simple graphs. Let  $G$  be such a graph with vertex set  $V(G)$  and edge set  $E(G)$ . For  $u, v \in V(G)$ , the distance between  $u$  and  $v$ , denoted by  $d(u, v) = d_G(u, v)$ , is the length of a shortest path connecting  $u$  and  $v$ . The distance matrix of  $G$  is defined as  $D(G) = (d(u, v))_{u, v \in V(G)}$ . The eigenvalues of  $D(G)$  are called the distance eigenvalues of  $G$ . Since  $D(G)$  is non-negative and symmetric, the distance eigenvalues of  $G$  are real. The distance spectral radius of  $G$ , denoted by  $\partial_1(G)$ , is the largest distance eigenvalue of  $G$ . If  $|V(G)| \geq 2$ , since  $D(G)$  is irreducible, from the Perron–Frobenius theorem,  $\partial_1(G)$  is positive, simple, and there is a unique positive unit eigenvector  $x$  corresponding to  $\partial_1(G)$ , which is called the distance Perron vector of  $G$ .

The study of distance eigenvalues of graphs dates back to the classical work of Graham and Pollack [8], Graham and Lovász [7], and Edelberg et al. [6]. Balaban et al. [2] proposed the use of the distance spectral radius as a molecular descriptor. Hence the research of the distance spectral radii of graphs attracts the interests of a lot of mathematicians and chemists. Most of the known results can be found in the survey [1], for the developments after the survey paper was published see [11,13,14,16,23].

As usual,  $S_n$  and  $P_n$  will denote a star and a path on  $n$  vertices, respectively. A double star  $S_{a,b}$  ( $a, b \geq 2$ ) is the tree consisting of a star  $S_{a+1}$  with  $b-1$  pendent edges attached to an arbitrary pendent vertex of  $S_{a+1}$ . A spur  $A(n, m)$  ( $1 \leq m \leq \lfloor \frac{n}{2} \rfloor$ ) is the tree obtained from the star  $S_{n-m+1}$  by attaching a pendent edge to each of certain  $m-1$  pendent vertices of  $S_{n-m+1}$ . A broom  $B_{n,\Delta}$  is the tree consisting of a star  $S_{\Delta+1}$  with a path of length  $n-\Delta-1$  attached to an arbitrary pendent vertex of  $S_{\Delta+1}$ . A complete  $\Delta$ -ary tree is a tree on  $n$  vertices with maximum degree  $\Delta$  constructed as follows. Start with the root having  $\Delta$  children. Every vertex different from the root, which is not in the last two levels, has exactly  $\Delta-1$  children. While in the last level all vertices need not exist, those that do fill the level consecutively. Thus, at most one vertex on the level before the last has its degree different from  $\Delta$  and 1.

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Some extremal trees respective to the distance spectral radius among all trees on  $n$  vertices with specified invariants (including the maximum degree, diameter, number of pendent vertices, matching number, domination number) were characterized (see [5,9,15,17,19,20,22]). Stevanović and Ilić [17] proved that,  $B_{n,\Delta}$  uniquely maximizes the distance spectral radius among trees on  $n$  vertices with maximum degree  $\Delta$ , and proposed the following conjecture.

**Conjecture 1.1** ([17]). *The complete  $\Delta$ -ary tree has the minimum distance spectral radius among all trees on  $n$  vertices with maximum degree  $\Delta$ .*

In Section 2, we present a new transformation of a certain graph  $G$  that decreases  $\partial_1(G)$ . With this transformation Conjecture 1.1 is confirmed for  $\Delta \geq \lceil \frac{n}{2} \rceil$ . In Section 3, we consider to order the trees by their distance spectral radii, and characterize the trees on  $n \geq 10$  vertices with the fourth and fifth least distance spectral radii.

**2. A generalized transformation**

In order to investigate the perturbation of distance spectral radius of a graph, some transformations were presented (see [3–5,9,17,19–21,24]).

**Lemma 2.1** ([19]). *Let  $uv$  be a non-pendent cut edge of a graph  $G$ . Let  $G'$  be the graph obtained from  $G$  by contracting  $uv$  to a vertex  $u$  and attaching a pendent vertex  $v$  to  $u$ . Then  $\partial_1(G') < \partial_1(G)$ .*

**Lemma 2.2** ([17]). *Let  $v$  be a vertex in a nontrivial connected graph  $G$ . Denote by  $G_{k,l}$  the graph obtained from  $G$  by attaching a terminal vertex in each of  $P_k$  and  $P_l$  to  $v$ . If  $k \geq l \geq 1$ , then  $\partial_1(G_{k,l}) < \partial_1(G_{k+1,l-1})$ .*

**Lemma 2.3** ([3]). *Let  $G$  be a graph with a clique of order  $s \geq 2$ , and  $u$  and  $v$  two vertices on the clique with  $k, l$  pendent vertices, respectively, where the degree of  $v$  is  $l + s - 1$  in  $G$ . If  $G' = G - uv + uw$ , where  $w$  is a pendent vertex adjacent to  $v$  in  $G$ , then for  $k \geq l \geq 1$ ,  $\partial_1(G) > \partial_1(G')$ .*

If a vertex  $u$  is adjacent to  $v$  in  $G$ , then  $u$  is said to be a neighbor of  $v$ .  $N_G(v)$  will denote the set of neighbors of  $v$ . In particular, if  $u \in N_G(v)$  is a pendent vertex, then  $u$  is said to be a pendent neighbor of  $v$ .

**Lemma 2.4** ([19]). *Let  $G$  be a graph with  $u, v \in V(G)$ . Let  $u'$  and  $v'$  be the pendent neighbors of  $u$  and  $v$ , respectively. Let  $x_z$  be the entry of Perron vector  $x$  of  $G$  corresponding to vertex  $z \in V(G)$ . Then  $(\partial_1(G) + 2)(x'_u - x'_v) = \partial_1(G)(x_u - x_v)$ .*

With the following result we are to give a new transformation that generalizes Lemma 2.3.

**Theorem 2.5.** *Let  $u$  and  $v$  be two vertices in a connected graph  $G$  such that  $N_G(v) - \{u\} \subseteq N_G(u) - \{v\}$ . Denote by  $G_{k,l}^1$  the graph obtained from  $G$  by adding  $k$  pendent edges at vertex  $u$  and  $l$  pendent edges at vertex  $v$ . If  $k \geq l \geq 1$ , then  $\partial_1(G_{k,l}^1) > \partial_1(G_{k+1,l-1}^1)$ .*

**Proof.** Obviously,  $N_G(v) - \{u\} \subseteq N_G(u) - \{v\}$  implies  $d_G(w, v) \geq d_G(w, u)$  for each vertex  $w \in V(G) - \{u, v\}$ , and so  $d_G(u, v) = 1, 2$ . We distinguish the following two cases.

**Case 1.**  $d_G(u, v) = 2$ . Write  $H = G_{k,l}^1, H_1 = G_{k+1,l-1}^1, \rho = \partial_1(G_{k,l}^1)$ , and  $\rho_1 = \partial_1(G_{k+1,l-1}^1)$ . Denote by  $uu_1, uu_2, \dots, uu_k$  (resp.  $vv_1, vv_2, \dots, vv_l$ ) the  $k$  (resp.  $l$ ) pendent edges at vertex  $u$  (resp.  $v$ ) in  $H$ . Then  $H_1 = H - vv_l + uv_l$ . Let  $V(H) = V(H_1) = (V(G) - \{u, v\}) \cup \{u\} \cup \{v\} \cup A \cup B \cup \{v_i\}$ , where  $V(G) - \{u, v\} = \{w_1, w_2, \dots, w_s\}, A = \{u_1, u_2, \dots, u_k\}$ , and  $B = \{v_1, v_2, \dots, v_{l-1}\}$ . Let  $r_i = d_G(w_i, v) - d_G(w_i, u) \geq 0$  ( $i = 1, 2, \dots, s$ ),  $\alpha = (r_1, r_2, \dots, r_s)^T$ , and  $e_k$  a  $k$ -dimensional column vector with each entry equal to 1. It is easily seen that

$$D(H) - D(H_1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \alpha \\ 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 & 0 & 2e_k \\ 0 & 0 & 0 & 0 & 0 & -2e_{l-1} \\ \alpha^T & 2 & -2 & 2e_k^T & -2e_{l-1}^T & 0 \end{bmatrix}.$$

By symmetry, let  $x = (y_1, y_2, \dots, y_s, x_1, x_2, a, \dots, a, b, \dots, b, a)^T$  be the Perron vector of  $H_1$ , where  $y_i$  corresponds to  $w_i$  ( $i = 1, 2, \dots, s$ ),  $x_1$  to  $u, x_2$  to  $v, a$  to  $v_i$  and  $u_i$  ( $i = 1, 2, \dots, k$ ), and  $b$  to  $v_i$  ( $i = 1, 2, \dots, l - 1$ ). Let  $\sigma = \sum_{i=1}^s r_i y_i / 2 \geq 0$ . Then  $\frac{1}{4a}(\rho - \rho_1) \geq \frac{1}{4a}x^T(D(H) - D(H_1))x = \sigma + x_1 - x_2 + ka - (l - 1)b \geq \varepsilon$ .

From Lemma 2.4 and  $D(H_1)x = \rho_1 x$  we have

$$\begin{aligned} (\rho_1 + 2)(b - a) &= \rho_1(x_2 - x_1) = 2\sigma + 2(x_1 - x_2) + 2(k + 1)a - 2(l - 1)b \\ &\Rightarrow \begin{cases} \frac{1}{2}(\rho_1 + 2)(x_2 - x_1) = \sigma + (k + 1)a - (l - 1)b \\ \frac{1}{2}(\rho_1 + 2)(b - a) = \sigma + x_1 - x_2 + (k + 1)a - (l - 1)b. \end{cases} \end{aligned}$$

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