The distance spectral radius of graphs with given independence number*

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Abstract: Let $D(G)$ be the distance matrix of a connected graph G. The distance spectral radius of G is the largest eigenvalue of $D(G)$ and it has been proposed to be a molecular structure descriptor. In this paper, we study the distance spectral radius of graphs with given independence number. Special attention is paid to the graphs given independence number and maximal distance spectral radius.

1 Introduction

Let G be a connected simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. The *distance* between vertices u and v of G, denoted by $d_G(u, v)$, or $d(u, v)$ without confusion, is defined as the length of a shortest path from u to v. The *eccentricity* of a vertex v is the maximal distance from v to any other vertex. The *diameter*, denoted by d, of a graph G is the maximal eccentricity over all vertices in a graph. The *distance matrix* of G, denoted by $D(G)$, is an $n \times n$ matrix with its (u, v)-entry equal to $d_G(u, v)$. For a subset $S \subseteq V(G)$, $G[S]$ denotes the induced subgraph of G. We use $d_G(v)$ or $d(v)$ to denote the degree of v in G.

The *distance spectral radius* of G, denoted by $\varrho(G)$, is the largest eigenvalue of $D(G)$. Since $D(G)$ is a non-negative irreducible matrix, by Perron-Frobenius theorem [3], there is an eigenvector $\mathbf{x}$ corresponding to $\varrho(G)$ with positive coordinates, known as the Perron eigenvector of $D(G)$. Denote by x_i the coordinate of $\mathbf{x}$ corresponding to $v_i \in V(G)$.

For the Perron eigenvector $\mathbf{x}$ of G, we have

$$\varrho(G)x_i = \sum_{v_j \in V(G)} d_G(v_i, v_j)x_j.$$

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The *Wiener index* of a connected graph G is defined as the sum of all distances among vertices (see [4, 20, 27] for details)

$$W(G) = \sum_{i<j} d_G(v_i, v_j).$$

The distance spectral radius of graphs is well studied in the literature. Balaban et al. proposed the use of ϱ as a molecular descriptor, while in [8] it was successfully used to infer the extent of branching and model boiling points of alkanes. Apart from distance spectral radius, these exist many other topological molecular descriptors as well, including, for example, Wiener index [4], Wiener polarity index [22], Randić index [15], graph energy [12, 9], matching energy [13] and HOMO-LUMO index [14] and many others listed in [20, 27]. In [11, 32] the authors established various upper and lower bounds for distance spectral radius and distance energy of graphs. Liu [19] characterized graphs with minimal distance spectral radius in three classes of simple connected graphs with n vertices: with fixed (vertex) connectivity, matching number and chromatic number. Zhang and Godsil [31] studied the distance spectral radius of graphs with given number of cut vertices or cut edges. Bapat et al. in [1] showed various connections between distance matrix $D(G)$ and Laplacian matrix $L(G)$ of a graph G. Nath and Paul [24] recently obtained the maximal distance spectral radius of trees with given matching number, this resolved a conjecture posed in [10]. They also found the extremal tree of maximal distance spectral radius with given number of pendent vertices. Ilić [10] determined the minimal distance spectral radius of trees with given matching number. Du et al. [5] further studied the distance spectral radius of trees. Stevanović and Ilić in [25] proved that among trees with fixed maximum degree Δ, the broom graph is the unique graph with maximal distance spectral radius. Furthermore, the authors proved that the star $K_{1,n-1}$ is the unique graph with minimal distance spectral radius among tree on n vertices, i.e. for a tree G, it holds

$$\varrho(G) \geq \varrho(S_n) = n - 2 + \sqrt{(n-2)^2 + (n-1)}.$$

For more details on distance matrices and distance spectra, one may refer to [6, 7, 16, 18, 17, 21, 23] and the references therein.

Recall that the clique number $\omega(G)$ of a graph G is the largest number of pairwise adjacent vertices of G and the chromatic number $\chi(G)$ is the minimum number of colors to be assigned to the vertices of G such that no two adjacent vertices receive the same color. Obviously $\omega(G) \leq \chi(G)$. A subset S of $V(G)$ is called an *independent set* of G if no two vertices in S are adjacent in G. The *independence number* of G is the size of a maximum independent set of G, denoted by $\alpha(G)$.

In this paper, we study the distance spectral radius of graphs with given independence number. This paper is organized as follows. In Section 2, we consider the minimal distance spectral radius of graphs. In Section 3, we study the distance spectral radius of graphs with small independence number. In Section 4, graphs with large independence number and maximal distance spectral radius are considered.

2 The lower bound

Theorem 2.1. *Let G be a connected graph of order n with independence number r. Assume that $U = \{v_1, v_2, \ldots, v_r\}$ is an independent set, and $W = V(G) \setminus U = \{v_{r+1}, v_{r+2}, \ldots, v_n\}$. Let $\mathbf{x} = (x_1, \ldots, x_n)^T$ be the Perron vector of $D(G)$, where x_i corresponds to v_i for $i = 1, \ldots, n$. Let*

$$x_i = \min_{v_k \in U} x_k, \qquad x_j = \min_{v_k \in W} x_k.$$

Let A (resp. B) be the set of vertices adjacent to v_i (resp. v_j) in W (resp. in U) with $|A| = a \geq 1, |B| = b \geq 1$. Then we have $\varrho(G) \geq \frac{1}{2}(n + r - 3 + \sqrt{(n+r-3)^2 - 4((2r-2)(n-r-1) - (2n-2r-a)(2r-b))})$. (1)

Proof. For vertex v_i and its corresponding eigencomponent x_i, we have

$$\varrho x_i \geq a x_j + 2(r-1)x_i + 2(n-r-a)x_j, \tag{2}$$

and similarly, for x_j, we have

$$\varrho x_j \geq b x_i + 2(r-b)x_i + (n-r-1)x_j. \tag{3}$$

Thus it follows that

$$(\varrho - 2(r-1))\, x_i \geq (a + 2(n-r-a))\, x_j,$$
$$(\varrho - (n-r-1))\, x_j \geq (b + 2(r-b))\, x_i.$$

Simplifying the above two inequalities, one has

$$\varrho^2 - (n+r-3)\varrho + 2(r-1)(n-r-1) - (2n-2r-a)(2r-b) \geq 0.$$

Then the result follows immediately. □

Corollary 2.2. *Let G be a connected graph of order n with $\alpha(G) = r$. Then*

$$\varrho(G) \geq \tfrac{1}{2}\left(n + r - 3 + \sqrt{n^2 - 2(r-1)n + 5r^2 - 6r + 1}\right).$$

The equality holds if and only if $G \cong K_{n-r} \vee \overline{K_r}$, the join of the complete graph K_{n-r} and the empty graph $\overline{K_r}$.

Proof. Obviously, $a \le n-r$ and $b \le r$ in Theorem 2.1, therefore from (2) and (3) we can similarly have

$$\varrho x_i \ge a x_j + 2(r-1)x_i + 2(n-r-a)x_j \ge 2(r-1)x_i + (n-r)x_j, \tag{4}$$

$$\varrho x_j \ge b x_i + 2(r-b)x_i + (n-r-1)x_j \ge r x_i + (n-r-1)x_j. \tag{5}$$

Simplifying the above two inequalities, one has

$$\varrho^2 - (n+r-3)\varrho + 2(r-1)(n-r-1) - (n-r)r \ge 0.$$

Thus we get the desired result.

If the equality holds, then all the inequalities in the proof must be equalities, therefore $a = n-r$ and $b = r$. If equality of (4) holds, then all vertices in U (resp. W) have the same eigencomponents x_i (resp. x_j). Every vertex in U is adjacent to every vertex in W; every vertex in W is adjacent to every vertex in U. The equality of (5) implies that the degree of the vertices in W is $n-1$. Therefore we get the result. The converse is easy to check. □

3 The extremal graph with $\alpha = 2$ and $\lceil \frac{n}{2} \rceil - 1$

We denote by $L(p, q, n-p-q)$ the graph of order n obtained from the graphs K_p and K_q by joining $u \in K_p$, $v \in K_q$ with a path of order $n-p-q$ $(p \ge 2, q \ge 2)$. For simplicity, for $p \ge 2, q \ge 2, p+q = n$, let $L(p,q)$ denote the graphs K_p and K_q joined by a single edge uv with $u \in K_p$, $v \in K_q$.

Lemma 3.1. *$\varrho(L(p,q)) \le \varrho(L(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor))$ with equality only if $L(p,q) \cong L(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor)$.*

Proof. Suppose that $V(L(p,q)) = \{v_1, \dots, v_n\}$. Let $\mathbf{x} = (x_1, \dots, x_n)^T$ be the Perron vector of $D(L(p,q))$ where x_i corresponds to v_i for $i = 1, \dots, n$. By symmetry, all the vertices in $V(K_p)\backslash\{u\}$ have the same coordinate, say x_0; all the vertices in $V(K_q)\backslash\{v\}$ have the same coordinate, say x_3; u corresponds to x_1 and v corresponds to x_2. Then

$$\begin{cases} \varrho(L(p,q))x_0 = (p-2)x_0 + x_1 + 2x_2 + 3(q-1)x_3, \\ \varrho(L(p,q))x_1 = (p-1)x_0 + x_2 + 2(q-1)x_3, \\ \varrho(L(p,q))x_2 = 2(p-1)x_0 + x_1 + (q-1)x_3, \\ \varrho(L(p,q))x_3 = 3(p-1)x_0 + 2x_1 + x_2 + (q-2)x_3. \end{cases}$$

Then ϱ is the Perron root of matrix M since $\varrho\mathbf{x}' = M\mathbf{x}'$, where $\mathbf{x}' = (x_0, x_1, x_2, x_3)'$ and

$$M = \begin{pmatrix} p-2 & 1 & 2 & 3q-3 \\ p-1 & 0 & 1 & 2q-2 \\ 2p-2 & 1 & 0 & q-1 \\ 3p-3 & 2 & 1 & q-2 \end{pmatrix}.$$

Then by a simple calculation, the characteristic polynomial of M is $\det(\lambda I-M) = \lambda^4-(n-4)\lambda^3+(2n+4-8pq)\lambda^2+(6n-14pq)\lambda+(2n-5pq) =: f(\lambda, p, q)$.

It can be checked that

$$f(\lambda, p, q) - f(\lambda, p-1, q+1) = (p-q-1)(8\lambda^2 + 14\lambda + 5).$$

Therefore, if $p \geq q-2$, then

$$f(\varrho, p-1, q+1) < f(\varrho, p, q) = 0.$$

This implies that the largest real root of $f(\lambda, p, q) = 0$ attains the maximum when $|p-q| \leq 1$. This completes the proof. □

Lemma 3.2. *Let G be a connected graph on $n \geq 4$ vertices with diameter 2. Then $\varrho(L(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor)) > \varrho(G)$.*

Proof. In [16], it is obtained that if the diameter of G is two, then $\varrho(G) \leq n-2+\sqrt{n^2-3n+3}$ with equality holding if and only if $G \cong K_{1,n-1}$.

By a simple calculation, we have

$$2W\left(L\left(\left\lceil \frac{n}{2} \right\rceil, \left\lfloor \frac{n}{2} \right\rfloor\right)\right) = \begin{cases} 2n^2-3n, & \text{if } n \text{ is even,} \\ 2n^2-3n-1, & \text{if } n \text{ is odd.} \end{cases}$$

Since $\varrho(L(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor)) \geq \frac{2W}{n}$ and $n \geq 4$, we have $\varrho(L(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor)) \geq 2n-3 > n-2+\sqrt{n^2-3n+3}$ if n is even; and $\varrho(L(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor))) \geq 2n-3-\frac{1}{n} > n-2+\sqrt{n^2-3n+3}$ if n is odd. Thus we complete the proof. □

In the following, we will consider the extremal graph with independence number 2 and maximal distance spectral radius.

Theorem 3.3. *Among all graphs with order n and independence number 2, the graph $L(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor)$ attains the maximum distance spectral radius.*

Proof. Let G be the extremal graph having maximum distance spectral radius among all graphs with independence number 2. The cases for $n \leq 3$ are easy to check, so we may assume that $n \geq 4$ in the sequel.

If the diameter of G is at least 4, then we can easily find three non-adjacent vertices, which contradicts to the fact that the independence number is 2.

If the diameter of G is 2, then by Lemma 3.2, $\varrho(G) < \varrho(L(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor))$.

If the diameter of G is 3, suppose that u and v are such candidates with $d(u, v) = 3$. Thus we can partition $V(G)$ into V_i and u, where $V_i = \{v_i | d(u, v_i) = i\}$ for $i = 1, 2, 3$. Since the independence number of G is two, thus $G[V_i]$ is a complete graph for $i = 1, 2, 3$ and $G[V_2 \cup V_3]$ is also a complete graph. Note that deleting edges of G would increase the distance spectral radius, then the number of edges between V_1 and V_2 is exactly one. Thus G is of the form $L(p, q)$. By Lemma 3.1, it follows that $G \cong L(\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor)$. This completes the proof. □

Recall that the unicyclic (resp. bicyclic) graph is a connected graph with the number of edges equal to the number of vertices (resp. plus one).

Lemma 3.4 ([28]). *Among all unicyclic graphs, the graph $L(3, 2, n-5)$ attains the maximum distance spectral radius.*

Lemma 3.5 ([2]). *Among all bicyclic graphs with two edge disjoint cycles, the graph $L(3, 3, n-6)$ attains the maximum distance spectral radius.*

Lemma 3.6 ([29]). *Among all connected graphs with clique number $\omega(G)$, the graph $L(\omega, 2, n-\omega-2)$ attains the maximum distance spectral radius.*

Let G' be the graph of order n obtained from $K_4 - e$ by attaching a path of length $n-4$ at the vertex of degree 3 in $K_4 - e$.

Lemma 3.7 ([2]). *For G' described above, we have $\varrho(L(3, 3, n-6)) > \varrho(G')$.*

Theorem 3.8. *Among all connected graphs with independence number $r = \lceil \frac{n}{2} \rceil - 1$, the graph $L(3, 2, n-5)$ has the maximum distance spectral radius if n is odd; $L(3, 3, n-6)$ has the maximum distance spectral radius if n is even.*

Proof. Suppose that G has the maximum distance spectral radius among all graphs with independence number r.

If n is odd, then $r = \frac{n-1}{2}$. Thus G contains at lease one odd cycle (otherwise G is a bipartite graph, and thus $\alpha(G) > n/2$). Since deleting edges will increase the distance spectral radius and G has the maximum distance spectral radius among all graphs with independence number r. Thus we have G is a unicyclic graph with the length of the cycle odd. Then by Lemma 3.4, we have $G \cong L(3, 2, n-5)$.

If n is even, then $r = \frac{n-2}{2}$. Therefore G contains either at least two edge disjoint odd cycles or a K_4, if otherwise, we can delete a suitable vertex, say u, of G such that $G-u$ is bipartite, then $\alpha(G-u) = \lceil \frac{n-1}{2} \rceil = \frac{n}{2}$, a contradiction.

If G contain at least two edge disjoint odd cycles, then by Lemma 3.5, we have $G \cong L(3, 3, n-6)$.

If G contains K_4 as a subgraph, then by Lemmas 3.6 and 3.7, we have $\varrho(G) < \varrho(L(3, 3, n-6))$, which is a contradiction to the maximality of G. □

For graphs with independence number at most $\lceil \frac{n}{2} \rceil - 2$, we have the following general bound.

Lemma 3.9. *[32] Let G be a connected graph with n vertices, minimum degree δ_1 and second minimum degree δ_2. Let d be the diameter of G. Then*

$$\varrho(G) \le \sqrt{\left[dn - \frac{d(d-1)}{2} - 1 - \delta_1(d-1)\right]\left[dn - \frac{d(d-1)}{2} - 1 - \delta_2(d-1)\right]}$$

with equality if and only if G is a regular graph with $d \le 2$.

Theorem 3.10. *Let G be a connected graph of order n with independence number $r \le \lceil \frac{n}{2} \rceil - 2$. Then we have $\varrho(G) \le (n-r)(2r-1)$. The equality holds if and only if $G \cong K_n$.*

Proof. From Lemma 3.9, since $\delta_2 \ge \delta_1 \ge 1$, we have

$$\varrho(G) \le dn - \frac{d(d-1)}{2} - d =: f(d).$$

It is easy to check that $f(d)$ is strictly increasing with respect to d. Since $2 \le d+1 \le 2r$ for any graph, we find $d \le 2r-1$ and $f(d) \le f(2r-1)$ for $r \le \lceil \frac{n}{2} \rceil - 2$. This yields the result.

If the equality holds, then $d+1 = 2r$, and note that $d \le 2$ by Lemma 3.9, therefore $r = 1$ and this leads to the result. The converse is easy to check. □

To conclude this section, we pose the following conjecture regarding the extremal graph with maximal distance spectral radius and independent number at most $\lceil \frac{n}{2} \rceil - 1$.

Conjecture 3.11. *Among all graphs with independence number $r \le \lceil \frac{n}{2} \rceil - 1$, the graph $L(\lceil \frac{n-2(r-2)}{2} \rceil, \lfloor \frac{n-2(r-2)}{2} \rfloor, 2(r-2))$ attains the maximum distance spectral.*

4 The extremal graph with $\alpha \ge \lceil \frac{n}{2} \rceil$

If the independence number equals to $\lceil \frac{n}{2} \rceil$, then the path P_n attains the maximum distance spectral radius.

For $s, p \ge 0$, the dumbbell graph $D(n; s, p)$ consists of a path P_{n-s-p}, s pendent edges attaching to a pendant vertex of P_{n-s-p}, and p pendent edges attaching to the other pendent vertex. Denote by $D(n,k; s,p) = D(n; s,p)$ with $s + p = k$.

Lemma 4.1 ([24]). *Among all connected graphs with k pendent vertices, the graph $D(n; \lceil \frac{k}{2} \rceil, \lfloor \frac{k}{2} \rfloor)$ attains the maximum distance spectral radius.*

Lemma 4.2 ([28]). *Suppose uv is a cut-edge of a connected graph G, but uv is not a pendent edge. If G_0 is the graph obtained from G by identifying u and v, and creating a new pendent vertex at the identified vertex, then $\varrho(G) > \varrho(G_0)$.*

By Lemma 4.2, we immediately get the following result.

Lemma 4.3. *For $k \geq 2$, we have $\varrho(D(n; \lceil \frac{k}{2} \rceil, \lfloor \frac{k}{2} \rfloor)) < \varrho(D(n; \lceil \frac{k-1}{2} \rceil, \lfloor \frac{k-1}{2} \rfloor))$.*

Let $\mathscr{T}_{n,r}$ denote the set of trees with n vertices and independence number $r \geq \lceil \frac{n}{2} \rceil + 1$. In the following, we shall find the minimum number of pendent vertices among $\mathscr{T}_{n,r}$.

Let $T \in \mathscr{T}_{n,r}$ and S be the maximum independent set in T. Obviously, there exists at least one pendent vertex u in S with its unique neighbor v. We will carry out the following two transformations:

(a). If $d(w) \geq 3$, then suppose that its neighbor set is $N(w) = \{w_1, \ldots, w_t\}$ and $d(w_i) = 1$, for $i = 1, \ldots, s$ where $s \leq t$. If $s < t$, then let $T' = T - \{ww_i | i = 1, \ldots, s\} + \{vw_i | i = 1, \ldots, s\}$. If $s = t$, then let $T' = T - \{ww_i | i = 1, \ldots t-1\} + \{vw_i | i = 1, \ldots, t-1\}$.

We carry out the transformation (a) recursively until the vertices other than v of the tree are adjacent to at most one pendent vertex.

(b). For $k, l \geq 2$, we denote by $T(w, k, l)$ the graph obtained from $T \cup P_k \cup P_l$ by adding edges between w and one of the end vertices in both P_k and P_l. Let $P_k = u_1 u_2 \ldots u_k w$ and $T' = T(w, 0, l + k - 1) \backslash \{u_1\} + \{vu_1\}$.

Clearly, when we run the above two transformations, the number of pendent vertices remains unchanged and the independence number does not decrease. Then we will have the following result.

Lemma 4.4. *Let $T \in \mathscr{T}_{n,r}$ ($r \geq \lceil \frac{n}{2} \rceil + 1$) be a tree with independence number r. If T has the minimum number of pendent vertices, say k, then $k = 2r - n + 1$.*

Proof. Let T_1 be the extremal tree with minimum number of pendent vertices after carrying out the above two transformations. Since the independence number does not decrease after carrying out the above two transformations, then $\alpha(T_1) = k + \lceil \frac{n-k-2}{2} \rceil = \lceil \frac{n+k-2}{2} \rceil = r$. If $n + k$ is even, then $n - k$ is even, at this moment we can subdivide the internal path one time and delete one pendent vertex, while the independence number also does not decrease but the number of pendent vertices decreases by one, this contradicts to the choice of T_1. Therefore $n + k$ is odd and $k = 2r - n + 1$. The result therefore follows. □

Then by Lemmas 4.1, 4.3 and 4.4, we have

Theorem 4.5. *Among all graphs in $\mathcal{T}_{n,r}$ ($r \geq \lceil \frac{n}{2} \rceil$), the graph $D(n; \lceil \frac{2r-n+1}{2} \rceil, \lfloor \frac{2r-n+1}{2} \rfloor)$ attains the maximum distance spectral radius.*

Theorem 4.6. *Among all connected graphs with independence number $r \geq \lceil \frac{n}{2} \rceil$, the graph $D(n; \lceil \frac{2r-n+1}{2} \rceil, \lfloor \frac{2r-n+1}{2} \rfloor)$ attains the maximum distance spectral radius.*

Proof. Let G be a graph with independence number $r \geq \lceil \frac{n}{2} \rceil$. Suppose that $V_1 = \{v_1, v_2, \ldots, v_r\}$ is a maximum independent set of G and $V_2 = V \backslash V_1$. Assume that $G_i = G[V_i]$ are the subgraphs induced by V_i for $i = 1, 2$, and $C_1, \ldots, C_m$ are the components of G_2. Clearly, $1 \leq m \leq n - r$.

It is clear that either a pendent vertex or its neighbor must be contained in the maximum independent set. We may assume, without loss of generality, that $U = \{v_1, v_2, \ldots, v_t\}$ is the set of pendent vertices ($t \leq r$) in V_1 and set $V_1' = V_1 \setminus U$. Then all vertices in V_1' are of degree at least 2.

If $|V_1'| \leq m - 1$, then the number of pendent vertices of G is at least $r - m + 1 \geq 2r - n + 1$ as $m \leq n - r$. We delete edges of G until the graph is a tree, and denote the new graph by G'. Clearly, the pendent vertices of G' is at least $r - m + 1 \geq 2r - n + 1$. Then by Lemma 4.3 and Theorem 4.5, $\varrho(G) \leq \varrho(G') \leq \varrho(D(n; \lceil \frac{2r-n+1}{2} \rceil, \lfloor \frac{2r-n+1}{2} \rfloor))$. This completes the proof.

If $|V_1'| \geq m$, then we delete edges until G is a tree such that each component C_i ($i = 1, \cdots, m$) of G_2 is a tree. Denote the new graph by G''. Then each vertex of V_1 is adjacent to at most one vertex in C_i. Next we claim that at most $m-1$ vertices in V_1' are not pendent vertices. In fact, if otherwise, there exists a set $W \subseteq V_1'$ with m vertices of degree at least 2, then the induced subgraph $\tilde{G} = G[W \cup V_2]$ has $m + (n - r)$ vertices, note that the edges between W and V_2 is at least $2m$, one finds that the number of edges of $\tilde{G}$ is at least $2m + \sum_{i=1}^{m}(|C_i| - 1) = 2m + (n - r) - m = m + (n - r)$, which implies $\tilde{G}$ contains a cycle, and so does G, leading to a contradiction. Therefore the claim holds. Note that deleting an edge e of G (while keeping $G - e$ still connected) would increase the distance spectral radius, thus we have $\varrho(G'') \geq \varrho(G)$ with equality if and only if $G \cong G''$. Apparently G'' is a tree with the number of pendent vertices at least $r - m + 1 \geq 2r - n + 1$. Then by Lemma 4.3 and Theorem 4.5, $\varrho(G) \leq \varrho(G'') \leq \varrho(D(n; \lceil \frac{2r-n+1}{2} \rceil, \lfloor \frac{2r-n+1}{2} \rfloor))$. This completes the proof. □

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References

[1] R. B. Bapat, S. J. Kirkland, M. Neumann, *On distance matrices and Laplacians*, Linear Algebra Appl. 401 (2005) 193–209.

[2] S.S. Bose, M. Nath, S. Paul, *On the maximal distance spectral radius of graphs without a pendent vertex*, Linear Algebra Appl. 438 (2013) 4260–4278.

[3] D. Cvetković, M. Doob, H. Sachs, *Spectra of graphs – Theory and Application*, 3rd edition, Johann Ambrosius Barth Verlag, 1995.

[4] A. A. Dobrynin, R. Entringer, I. Gutman, *Wiener index of trees: theory and applications*, Acta Appl. Math. 66 (2001) 211–249.

[5] Z. Du, A. Ilić, L. Feng, *Further results on the distance spectral radius of graphs*, Linear Multilinear Algebra 61 (2013) 1287–1301.

[6] R. L. Graham, L. Lovász, *Distance matrix polynomials of trees*, Adv. in Math. 29 (1978) 60–88.

[7] A. Güngör, S. Bozkurt, *On the distance spectral radius and the distance energy of graphs*, Linear Mutlinear Algebra 59 (2011) 365–370.

[8] I. Gutman, M. Medeleanu, *On the structure-dependence of the largest eigenvalue of the distance matrix of an alkane*, Indian J. Chem. A 37 (1998) 569–573.

[9] B.F. Huo, X.L. Li, Y.T. Shi, *Complete solution to a conjecture on the maximal energy of unicyclic graphs*, European J. Combin. 32(5) (2011) 662–673.

[10] A. Ilić, *Distance spectral radius of trees with given matching number*, Discrete Appl. Math. 158 (2010) 1799-1806.

[11] G. Indulal, *Sharp bounds on the distance spectral radius and the distance energy of graphs*, Linear Algebra Appl. 430 (2009) 106–113.

[12] J. Li, X.L. Li, Y.T. Shi, *On the maximal energy tree with two maximum degree vertices*, Linear Algebra Appl. 435 (2011) 2272–2284.

[13] S.J. Ji, X.L. Li, Y.T. Shi, *Extremal matching energy of bicyclic graphs*, MATCH Commun. Math. Comput. Chem. 70 (2013) 697–706.

[14] X.L. Li, Y.Y. Li, Y.T. Shi, I. Gutman, *Note on the HOMO-LUMO index of graphs*, MATCH Commun. Math. Comput. Chem. 70 (2013) 85–96.

[15] X.L. Li, Y.T. Shi, L.S. Wang, *On a relation between Randić index and algebraic connectivity*, MATCH Commun. Math. Comput. Chem. 68 (2012) 843–849.

[16] H. Lin, Y. Hong, J. Wang, J. Shu, *On the distance spectrum of graphs*, Linear Algebra Appl. 439 (2013) 1662–1669.

[17] H. Lin, J. Shu, *The distance spectral radius of digraphs*, Discrete Applied Mathematics, 161 (2013) 2537-2543.

[18] H. Lin, W. Yang, H. Zhang, J. Shu, *Distance spectral radius of digraphs with given connectivity*, Discrete Math. 312 (2012) 1849–1856.

[19] Z. Liu, *On spectral radius of the distance matrix*, Appl. Anal. Discrete Math. 4 (2010) 269–277.

[20] M. Liu, B. Liu, *A survey on recent results of variable Wiener index*, MATCH Commun. Math. Comput. Chem. 69 (2013), 491–520.

[21] R. Merris, *The distance spectrum of a tree*, J. Graph Theory 14 (1990) 365–369.

[22] J. Ma, Y.T. Shi, Y. Yue, *The Wiener polarity index of graph products*, Ars Combin. 116 (2014) 235–244.

[23] Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D. Plavšić, N. Trinajstić, *The distance matrix in chemistry*, J. Math. Chem. 11 (1992) 223–258.

[24] M. Nath, S. Paul, *On the distance spectral radius of trees*, Linear Multilinear Algebra 61 (2013) 847–855.

[25] D. Stevanović, A. Ilić, *Distance spectral radius of trees with fixed maximum degree*, Electron. J. Linear Algebra 20 (2010) 168–179.

[26] B. Wu, E. Xiao, Y. Hong, *The spectral radius of trees on k pendent vertices*, Linear Algebra Appl. 395 (2005) 343–349.

[27] K. Xu, M. Liu, Kinkar Ch. Das, I. Gutman, B. Furtula, *A survey on graphs extremal with respect to distance-based topological indices*, MATCH Commun. Math. Comput. Chem. 71 (2014) 461–508.

[28] G. Yu, Y. Wu, Y. Zhang, J. Shu, *Some graft transformations and its application on a distance spectrum*, Discrete Math. 311 (2011) 2117–2123.

[29] M. Zhai, G. Yu, J. Shu, *Clique number and distance spectral radii of graphs*, Ars Combin. 104 (2012) 385-392.

[30] Y.J. Zhang, *The distance spectrum of some kinds of graphs*, Master thesis, East China Normal University, 2011.

[31] X. Zhang, C.D. Godsil, *Connectivity and minimal distance spectral radius of graphs*, Linear Multilinear Algebra 59 (2011) 745–754.

[32] B. Zhou, A. Ilić, *On distance spectral radius and distance energy of graphs*, MATCH Commun. Math. Comput. Chem. 64 (2010) 261–280.