Distance spectral radius of graphs with $r$ pendant vertices

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Let $G_r^n$ be the class of all connected graphs of order $n$ with $r$ pendant vertices. In this paper, we determine the unique graph with minimal distance spectral radius in $G_r^n$. In addition, we determine the unique graph with maximal distance spectral radius in $G_r^n$ for each $r \in \{2, 3, n-3, n-2, n-1\}$.

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1. Introduction

Let $G = (V, E)$ be a connected simple graph on $n$ vertices. The distance between two vertices $u, v \in V$ is denoted by $d_{uv}$ and is defined as the length of the shortest path between $u$ and $v$ in $G$. The distance matrix $D = (d_{uv})_{u,v \in V}$ is a symmetric real matrix, with real eigenvalues [7]. The distance spectral radius $\rho(G) = \rho_G$ of $G$ is the largest eigenvalue of the distance matrix $D$ of the graph $G$.

Distance energy $DE(G)$ is a newly introduced molecular graph-based analog of the total $\pi$-electron energy, and it is defined as the sum of the absolute eigenvalues of the molecular distance matrix. The distance spectra of trees and unicyclic graphs have exactly one positive eigenvalue, and therefore the distance energy for trees and unicyclic graphs is equal to the double of distance spectral radius [5,12].

The distance spectral radius is a useful molecular descriptor in QSRR modeling, as demonstrated by Consonni and Todeschini [6,18]. For more details on distance matrices and distance energy one may refer to [10,13,14,16].

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Balaban et al. [1] proposed the use of $\rho(G)$ as a molecular descriptor, while in [8] it was successfully used to infer the extent of branching and model boiling points of alkanes. Recently in [20] and [19], Zhou and Trinajstić provided upper and lower bounds for $\rho(G)$ in terms of the number of vertices, Wiener index and Zagreb index. Balasubramanian [2, 3] pointed out that the spectra of the distance matrices of many graphs such as the polyacenes, honeycomb and square lattice have exactly one positive eigenvalue, and he computed the spectrum of fullerenes $C_{60}$ and $C_{70}$.

Bapat et al. [5] showed various connections between the distance matrix $D(G)$ and the Laplacian matrix $L(G)$ of a graph. Bapat [4, 5] calculated the determinant and inverses of the distance matrices of weighted trees and unicyclic graphs. Merris [12] obtained an interlacing inequality involving the distance eigenvalues of trees.

2. Preliminaries

Let $e = uv$ be an edge of the connected graph $G$ such that $G' = G - e$ is also connected, and let $D'$ be the distance matrix of $G - e$. The removal of $e$ does not create shorter paths than the ones in $G$, and therefore, $d_{ij} \leq d'_{ij}$ for all $i, j \in V$. Moreover, $1 = d_{uv} < d'_{uv}$ and by the Perron–Frobenius theorem, one can conclude that

$$\rho(G) < \rho(G - e).$$

(1.1)

In particular, for any spanning tree $T$ of $G$, we have that

$$\rho(G) \leq \rho(T).$$

(1.2)

Similarly, adding a new edge $f = st$ to $G$ does not increase distances, while it does decrease at least one distance; the distance between $s$ and $t$ is one in $G + f$ and at least two in $G$. Again by the Perron–Frobenius theorem,

$$\rho(G + f) < \rho(G).$$

(1.3)

Inequality (1.3) tells us immediately that the complete graph $K_n$ has the minimum distance spectral radius among the connected graphs on $n$ vertices, while the inequality (1.2) shows that the maximum distance spectral radius will be attained for a particular tree.

Indulal [10] has found sharp bounds on the distance spectral radius and the distance energy of graphs. In [9], Ilić characterized $n$-vertex trees with given matching number $m$ which minimize the distance spectral radius. Liu has 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, respectively, [11]. Subhi and Powers [17] proved that for $n \geq 3$ the path $P_n$ has the maximum distance spectral radius among trees on $n$ vertices. Stevanović and Ilić [15] generalized this result, and proved that among trees with fixed maximum degree $\Delta$, the broom graph has maximum distance spectral radius and proved that the star $S_n$ is the unique graph with minimal distance spectral radius among trees on $n$ vertices.

Let $\mathcal{G}_n^r$ be the class of all connected graphs of order $n$ with $r$ pendant vertices. In this paper, we determine the unique graph with minimal distance spectral radius in $\mathcal{G}_n^r$. In addition, we determine the unique graph with maximal distance spectral radius in $\mathcal{G}_n^r$ for each $r \in \{2, 3, n - 3, n - 2, n - 1\}$. This paper is organized as follows. In Section 2, we give some preliminaries. In Section 3, we introduce some graph transformations which affect the distance spectral radius. In Section 4, we use the result obtained in Section 3, to determine the unique graph with minimal distance spectral radius in $\mathcal{G}_n^r$. Finally, in Section 5, we give the unique graph that maximizes the distance spectral radius in $\mathcal{G}_n^r$ for each $r \in \{2, 3, n - 3, n - 2, n - 1\}$.

2. Preliminaries

For a simple graph $G(V, E)$ and a subset $S$ of $V$, $G[S]$ denotes the induced subgraph on $S$ (i.e., the maximal subgraph of $G$ with vertex set $S$). Let $\deg(v)$ denote the degree of the vertex $v$ in $G$. If $\deg(v) = 1$, then $v$ is called a pendent vertex. The edge incident on a pendent vertex is known as a pendant edge. A quasi-pendent vertex of $G$ is a vertex adjacent to some pendant vertex. The star $S_n$ is a tree on $n$ vertices with one vertex of degree $n - 1$ and the remaining of degree 1. For positive integers $p, q$ denote by $S(p, q)$ a double star, namely a graph obtained from $K_2$ by attaching $p$ and $q$ pendant...
edges to end vertices. Note that \( S(p, q) \) is a graph of order \( p + q + 2 \). Also, according to this definition, the path \( P_4 \) is equal to \( S(1, 1) \).

Let \( x(G) = (x_1, x_2, \ldots, x_n)^t \) be an eigenvector of \( D(G) \) corresponding to \( \rho(G) \). Then

\[
\rho(G)x_i = \sum_{v_j \in V(G)} d_{ij}x_j. \tag{2.4}
\]

3. The transformations

Here we give some graph transformations in the form of lemmas which will be useful to derive our main results.

**Lemma 3.1.** Let \( G \) be a graph with a clique \( K_s \) of order \( s \) (\( s \geq 2 \)) and \( u, v \) be two vertices on the clique with \( p, q \) pendent vertices, respectively, where \( \text{deg}(v) = q + s - 1 \) in \( G \). If \( G' = G - vw + uw \), where \( w \) is a pendent vertex adjacent to \( v \) in \( G \), then for \( p \geq q \geq 1 \), \( \rho(G) > \rho(G') \).

**Proof.** Let the vertices of \( G \) and \( G' \) be labeled as in Fig. 1. We partition \( V(G) = V(G') \) into \( A_1 \cup A_2 \cup \{u\} \cup \{v\} \cup A \cup B \cup \{b_q\} \), where

\[
A_1 = \{w \mid d(w, u) < d(w, v)\}, \quad A_2 = \{w \mid d(w, u) = d(w, v)\}, \quad A = \{a_1, a_2, \ldots, a_p\},
\]
\[
B = \{b_1, b_2, \ldots, b_{q-1}\}.
\]

As we pass from \( G \) to \( G' \), the distances within \( A \cup A_1 \cup A_2 \cup \{u\} \cup \{v\} \cup B \) are unchanged; the distance of \( b_q \) with \( A_2 \) is also unchanged; the distance of \( b_q \) from a point in \( A \cup A_1 \cup \{u\} \) is decreased by 1, whereas the distance of \( b_q \) from a point in \( B \cup \{v\} \) is increased by 1. If the distance matrices are partitioned according to \( A_1, A_2, \{u\}, \{v\}, A, B \) and \( \{b_q\} \), then their difference is

\[
D(G) - D(G') = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & e_{A_1}^t \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & e_A \\
0 & 0 & 0 & 0 & 0 & -e_B \\
0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix},
\]

where \( e_i = (1, \ldots, 1)^t \) and \( i = A_1, A, B \). We denote \( \rho(G) \) by \( \rho \) and \( \rho(G') \) by \( \rho_1 \). Let \( x \) be an eigenvector of \( D(G') \) corresponding to \( \rho_1 \). By symmetry the components of \( x \) have the same value, say \( a \) for the vertices in \( A \cup \{b_q\} \) and \( b \) for the vertices in \( B \) whereas we take the components of \( x \) as

![Fig. 1. The graphs G and G’ in Lemma 3.1.](image-url)
$y_1, y_2, \ldots, y_t$ for the vertices in $A_1, z_1, z_2, \ldots, z_t$ for the vertices in $A_2, x_1$ for $u$ and $x_2$ for $v$. Then $x$ can be written as,

$$x = \left( y_1, y_2, \ldots, y_t, z_1, z_2, \ldots, z_t, x_1, x_2, a, \ldots, a, b, \ldots, b, a \right)^t.$$  

We now have

$$\frac{1}{2} (\rho - \rho_1) \geq \frac{1}{2} x^t (D(G) - D(G')) x > a[x_1 - x_2 + pa - b(q - 1)].$$ \hfill (3.5)

From $D(G')x = \rho_1(G')x$, we have

$$\rho_1 x_2 - \rho_1 x_1 = x_1 + (p + 1)a - x_2 - (q - 1)b$$

$$\Rightarrow (\rho_1 + 1)(x_2 - x_1) = (p + 1)a - (q - 1)b$$ \hfill (3.6)

$$\rho_1 b - \rho_1 a = x_1 - x_2 - b - qb + pa + 3a$$

$$\Rightarrow (\rho_1 + 1)(b - a) = x_1 - x_2 - qb + pa + 2a$$ \hfill (3.7)

$$\rho_1 a - \rho_1 x_2 = z_1 + z_2 + \cdots + z_t + 2x_2 - 2a + 2(q - 1)b$$

$$\Rightarrow (\rho_1 + 2)(a - x_2) = z_1 + z_2 + \cdots + z_t + 2(q - 1)b.$$ \hfill (3.8)

From (3.8) we conclude that $a > x_2$. If we assume $a \geq b$, then the L.H.S. of (3.7) is nonpositive, whereas the R.H.S. of (3.7) is $x_1 + q(a - b) + (p - q)a + 2a - x_2$ which is positive as $a > x_2$, an absurdity, thus we must have $a < b$. Therefore by (3.7), we have

$$x_1 - x_2 - qb + pa + 2a > 0 \Rightarrow q(a - b) > x_2 - x_1 - (p - q)a - 2a.$$

Again by (3.6), we have

$$(\rho_1 + 1)(x_2 - x_1) = q(a - b) + (p - q)a + a + b > x_2 - x_1 + b - a, \text{ which gives } x_2 > x_1.$$

Since distance matrix is nonnegative and irreducible, its spectral radius is bounded by the minimum and maximum row sums and thus we have

$$s + 2q + p - 2 < \rho_1 < 2s + 2q + 3p - 2 \text{ i.e. } 2q + p < \rho_1 < 2s + 2q + 3p - 2.$$ \hfill (3.9)

If $p = q + t$ where $t \geq 0$ then,

$$pa - (q - 1)b = p(a - b) + (t + 1)b$$

$$= \frac{p}{\rho_1 + 1} [x_2 + (p - t)b - (p + 2)a - x_1] + (t + 1)b$$

$$= \frac{1}{\rho_1 + 1} [p(x_2 - x_1) + p^2(b - a) - ptb - 2pa + (t + 1)b(\rho_1 + 1)]$$

and

$$x_2 - x_1 = \frac{1}{\rho_1 + 1} [(p + 1)a - (p - t - 1)b]$$

$$= \frac{1}{\rho_1 + 1} [p(a - b) + a + (t + 1)b].$$

Therefore,

$$pa - (q - 1)b - (x_2 - x_1)$$

$$= \frac{1}{\rho_1 + 1} [p(x_2 - x_1) + (p^2 + p)(b - a) + (t + 1)b(\rho_1 - ptb - 2pa - a)].$$ \hfill (3.10)

From (3.9) we have, $\rho_1 > 2q + p = 3p - 2t$. 
Therefore,
\[
(t + 1)b\rho_1 > (t + 1)b(3p - 2t) \\
= ptb + 2bp + (2btp + bp - 2t^2b - 2tb) \\
> ptb + 2ap + b(2tp + p - 2t^2 - 2t).
\]
(3.11)

Since \( t \geq 0 \) and \( q \geq 1 \), so
\[
2tp + p - 2t^2 - 2t = 2(p - q)p + p - 2(p - q)^2 - 2(p - q) \\
= 2q(1 - q + p) - p \\
= 2q(1 + t) - p \\
= q + 2qt + q - p \\
= q + 2qt - t \geq 1.
\]

Therefore, (3.11) gives
\[
(t + 1)b\rho_1 > ptb + 2ap + b > ptb + 2ap + a \Rightarrow (t + 1)b\rho_1 - ptb - 2pa - a > 0.
\]
Using (3.10) and (3.12) in (3.5) we get, \( \rho > \rho_1 \).  \( \square \)

Applying the above lemma we have the following corollary for double star.

**Corollary 3.2.** If \( p \geq q > 1 \), then \( \rho(S(p, q)) > \rho(S(p + 1, q - 1)) \).

**Lemma 3.3.** Let \( H_1 \) be a path \( P \equiv uvw \) with \( p, q (p \geq q) \) pendent vertices adjacent to \( u, w \), respectively, and one pendent vertex \( z \) adjacent to \( v \), \( H_2 \) is any connected graph. If \( G \) is a graph obtained by identifying the vertex \( v \) with any vertex of \( H_2 \) and \( G' = G - vz + wz \) then \( \rho(G') > \rho(G) \).

**Proof.** We partition \( V(G) = V(G') \) into \( A \cup \{u\} \cup \{v\} \cup \{w\} \cup B \cup C \cup \{z\} \), where \( A = \{a_1, a_2, \ldots, a_p\}, B = \{b_1, b_2, \ldots, b_q\}, C = V(G) \setminus (A \cup B \cup \{u\} \cup \{v\} \cup \{w\} \cup \{z\}) \).

As we pass from \( G \) to \( G' \), the distances within \( A \cup \{u\} \cup \{v\} \cup \{w\} \cup B \cup C \) are unchanged; the distance of \( z \) with \( A \cup \{u\} \cup \{v\} \cup \{w\} \cup C \) is increased by 1, whereas the distance of \( z \) with \( B \cup \{w\} \) is decreased by 1. If the distance matrices are partitioned according to \( A, \{u\}, \{v\}, \{w\}, B, C \) and \( \{z\} \), their difference is

\[
D(G') - D(G) = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & e_A \\
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & -e_B \\
0 & 0 & 0 & 0 & 0 & e_C \\
e_A^t & 1 & 1 & -1 & -e_B^t & e_C^t & 0
\end{bmatrix},
\]

where \( e_i = (1, \ldots, 1)^t \) and \( i = A, B, C \). We denote \( \rho(G) \) by \( \rho \) and \( \rho(G') \) by \( \rho_1 \). Let \( x \) be an eigenvector of \( D(G) \) corresponding to \( \rho \). Then by symmetry components of \( x \) have the same value, say \( a \) for the vertices in \( A, b \) for the vertices in \( B, c_1, c_2, \ldots, c_r \) for the vertices in \( C, x_1 \) for \( u, x_2 \) for \( v, x_3 \) for \( w \) and \( x_4 \) for \( z \), where \( r = n - (p + q + 4) \). Then \( x \) can be written as,
Fig. 2. The graphs $G$ and $G'$ in Lemma 3.3.

\[ x = \begin{pmatrix} a, \ldots, a, x_1, x_2, x_3, b, \ldots, b, c_1, c_2, \ldots, c_r, x_4 \end{pmatrix}^t. \]

We now have

\[ \frac{1}{2} (\rho_1 - \rho) \geq \frac{1}{2} x^t (D(G') - D(G)) x > x_4 [x_1 + x_2 - x_3 + pa - bq]. \]  

(3.12)

Now from $D(G)x = \rho x$, we have

\[ (\rho + 2)(b - a) = 2(pa - qb) + 2(x_1 - x_3) \]  

(3.13)

\[ (\rho + 2)(x_3 - x_1) = 2(pa - qb). \]  

(3.14)

Using (3.14) in (3.13) we get

\[ (\rho + 2)(b - a) = 2q(a - b) + 2(p - q)a + 2(x_1 - x_3) \]

\[ \Rightarrow (\rho + 2 + 2q)(b - a) = 2(p - q)a + \frac{4}{\rho + 2}(qb - pa) \]

\[ \Rightarrow (\rho + 2 + 2q)(\rho + 2)(b - a) = 2(p - q)(\rho + 2)a + 4qb - 4pa \]

\[ = 2(p - q)(\rho + 2)a + 4q(b - a) - 4a(p - q) \]

\[ \Rightarrow ((\rho + 2)^2 + 2\rho q)(b - a) = 2(p - q)\rho a \geq 0. \]

Thus $b \geq a$, so by (3.13) $pa - qb \geq x_3 - x_1$.

Now from (3.12),

\[ \frac{1}{2} (\rho_1 - \rho) > x_4 [x_1 + x_2 - x_3 + x_3 - x_1] = x_4 x_2, \]  

which is positive.

Thus $\rho(G') > \rho(G)$. □

For positive integers $p, q$, let $p + q + 3 = n$ and $D(n, p, q)$ consist of a path $P_3$ together with $p$ independent vertices adjacent to one pendent vertex of $P_3$ and $q$ independent vertices adjacent to the other pendent vertex.

Similar to the above lemma we have the following lemma.

**Lemma 3.4.** If $p \geq q > 1$, then $\rho(D(n, p, q)) > \rho(D(n, p + 1, q - 1))$.

4. Graphs with minimal distance spectral radii

In this section, we determine the unique graph with minimal distance spectral radius in $\sigma_n^r$. Let us denote the graph obtained by joining $k$ independent vertices to one vertex of $K_{n-k}$ by $K_n^k$. Further, we notice that $G_n^1 = \phi$. However, when $n \geq 4$ we have, $G_{n}^{\rho} \neq \phi$ if and only if $0 \leq r \leq n - 1$; furthermore, $G_{n}^{n-1}$ has only one graph, namely, $K_{1,n-1}$, and $G_{n}^{n-2}$ consists of precisely all double stars of order $n$. 


Theorem 4.1. For $n \geq 4$ and $0 \leq r \leq n - 1$, there is a unique graph in $G_n^r$ with minimal distance spectral radius, namely $K_n^r$ for $r \neq n - 2$ and the graph $S(n - 3, 1)$ for $r = n - 2$.

Proof. Suppose that $G^*$ is a graph with minimal distance spectral radius among all graphs in $G_n^r$. If $r = 0$, surely $G^* \cong K_n$ by (1.3). If $r = n - 1$, $G_n^r$ consists of only one graph, i.e. the star $K_{1,n-1} = K_{n-1}^n$, and the result follows in this case also. Assume that $1 \leq r \leq n - 3$. Let $P$ be the set of all the maximal distance vertex sets of $G^*$, and let $W$ be the set of all quasi-pendent vertices of $G^*$. We first claim that $G^*[V \setminus P]$ is a complete graph; otherwise by adding an edge between any two nonadjacent vertices of $V \setminus P$ the resulting graph still belongs to $G_n^r$ and by (1.3) it has a smaller distance spectral radius, which contradicts the minimality of $G^*$.

Thus, if $r = 1$, then clearly $G^* \cong K_n^1$. For $2 \leq r \leq n - 3$, we claim that $W$ contains exactly one point. Otherwise, let $w_1, w_2 \in W$ be two vertices such that there are $p$ and $q$ pendent vertices adjacent to $w_1$ and $w_2$, respectively, where, $p \geq q$, say. But then by Lemma 3.1, if we delete one of the pendent edges incident on $w_2$ and make the corresponding pendent vertex adjacent to $w_1$, the resulting graph still belongs to $G_n^r$ with a smaller distance spectral radius and that is a contradiction to the minimality of $G^*$. Therefore $G^* \cong K_n^r$, for $1 \leq r \leq n - 3$. Finally when $r = n - 2$, $G^*$ is a double star $S(p, q)$. And by repeated application of Corollary 3.2, we conclude that $G^* \cong S(n - 3, 1)$. □

5. Graphs with maximal distance spectral radii

In this section, we will characterize the graph in $G_n^r$ with maximal distance spectral radius for each $r \in \{2, 3, n - 3, n - 2, n - 1\}$. Clearly $G_n^{n-1} = \{K_{1,n-1}\}$ and hence for $r = n - 1$, the discussion is trivial.

Theorem 5.1. The path $P_n$ is the unique graph with maximal distance spectral radius in $G_n^2(n \geq 3)$.

Proof. It is obvious that $P_n \in G_n^2$. Let $G$ be any graph in $G_n^2$ and $G \neq P_n$. Then for any spanning tree $T$ of $G$, using (1.2) we have $\rho(G) \leq \rho(T)$. Again from [17], we know that among trees on $n$ vertices, the path $P_n$ has the maximal distance spectral radius where $n \geq 3$. So $\rho(G) < \rho(P_n)$ and the result follows. □

Theorem 5.2. $S(p, p)$ or $S(p, p + 1)$ uniquely maximizes the distance spectral radius in $G_n^{n-2}(n \geq 4)$, according as $n$ is even or odd.

Proof. Clearly $G_n^{n-2}$ contains only double stars $S(p, q)$ and by Corollary 3.2, we can conclude that the maximum distance spectral radius is attained at $S(p, q)$ only when $p - q$ is 0 or 1 depending on whether $n$ is even or odd, respectively. □

Let $G$ be a simple graph and $v$ be one of its vertices. A pendant path in $G$ is a path having one end vertex of degree at least 3, the other is of degree 1 and the intermediate points are of degree 2. For $k, l \geq 0$ we denote by $G(v, k, l)$ the graph obtained from $G \cup P_k \cup P_l$ by adding edges between $v$ and one of the end vertices in both $P_k$ and $P_l$. The broom $B_{n,3}$ is the tree consisting of a star $S_{3+1}$ along with a path $P_{n-s-1}$ attached to a pendent vertex of the star.

To prove our next results we need the following two lemmas.

Lemma 5.3 [15]. If $k \geq l \geq 1$, then $\rho(G(v, k, l)) < \rho(G(v, k + 1, l - 1))$.

Lemma 5.4 [15]. Let $T \neq B_{n,\Delta}$ be an arbitrary tree on $n$ vertices with the maximum vertex degree $\Delta$ where $3 \leq \Delta \leq n - 2$, then $\rho(B_{n,\Delta}) > \rho(T)$.

Theorem 5.5. $D(n, p, p)$ or $D(n, p, p + 1)$ uniquely maximizes the distance spectral radius in $G_n^{n-3}(n \geq 6)$, according as $n$ is odd or even.
Proof. Let $G_1 \in G_n^{n-3}$ be a graph with maximum distance spectral radius. Since $G_1$ has three non-pendent vertices, so they induce either a path or a triangle. If they induce a path then by Lemma 3.3, $G_1 \cong D(n, p, q)$ for some positive integer $p$ and $q$ and by Lemma 3.4, the result follows.

If they induce a triangle then there will be two cases.

Case 1. At least two vertices of the triangle are quasi-pendent vertices. If we remove an edge joining two quasi-pendent vertices then the resulting graph belongs to $G_n^{n-3}$ and has larger spectral radius than $G_1$, which is a contradiction.

Case 2. Exactly one vertex of the triangle is a quasi-pendent vertex. Then removing an edge of the triangle incident on the quasi-pendent vertex we get $S(n - 3, 1)$ and $\rho(S(n - 3, 1)) > \rho(G_1)$. Then by Lemma 5.3, we have $\rho(D(n, n - 4, 1)) > \rho(S(n - 3, 1))$ and $D(n, n - 4, 1)$ belongs to $G_n^{n-3}$, a contradiction. □

Theorem 5.6. The broom $B_{n,3}$ has the largest distance spectral radius in $G_n^3$ ($n \geq 4$).

Proof. Let $G_n^{(3)}$ be the class of all connected graphs on $n$ vertices, having at least three pendent vertices. Clearly $G_n^{(2)} \subset G_n^{(3)}$. Suppose $G \in G_n^{(3)}$ is a graph, having maximal distance spectral radius. We first observe that $G$ is a tree, as otherwise, the deletion of an edge from a cycle in $G$ results in a graph $G' \in G_n^{(3)}$ with $\rho(G) < \rho(G')$. We now claim that $G \in G_n^{(2)}$. If not, then $G$ has at least four pendent vertices. Then, we can find two pendent vertices $u$ and $v$ in $G$, which are the end points of two pendent paths $uu_1 \ldots uu_p$ and $vv_1 \ldots vv_q$, where $u_1, \ldots, u_p, v_1, \ldots, v_q$ are all distinct. Let $L_1 = uu_1 \ldots uu_p$ and $L_2 = vv_1 \ldots vv_q$. Then $G \cong H(w, p, q)$, where $H = G - (L_1 \cup L_2)$.

Applying Lemma 5.3, on $G \cong H(w, p, q)$ repeatedly we will end up in a graph $G''$ having at least three pendent vertices with $\rho(G) < \rho(G'')$. This contradicts the maximality of $G$ and so $G \in G_n^{(2)}$. But then $G$ is a tree with maximum degree 3. So by Lemma 5.4, $G \cong B_{n,3}$ and the result follows. □

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