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Distance spectral radius of digraphs with given connectivity☆

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ABSTRACT

Let $D(\overrightarrow{G})$ denote the distance matrix of a strongly connected digraph $\overrightarrow{G}$. The largest eigenvalue of $D(\overrightarrow{G})$ is called the distance spectral radius of a digraph $\overrightarrow{G}$, denoted by $\varrho(\overrightarrow{G})$. Recently, many studies proposed the use of $\varrho(\overrightarrow{G})$ as a molecular structure description of alkanes. In this paper, we characterize the extremal digraphs with minimum distance spectral radius among all digraphs with given vertex connectivity and the extremal graphs with minimum distance spectral radius among all graphs with given edge connectivity. Moreover, we give the exact value of the distance spectral radius of those extremal digraphs and graphs. We also characterize the graphs with the maximum distance spectral radius among all graphs of fixed order with given vertex connectivity 1 and 2.

1. Introduction

Unless stated otherwise, we follow [3] for terminology and notations, and we consider finite connected (and strongly connected) simple graphs (digraphs). In particular, denote $V(\overrightarrow{G}) = \{v_1, \dots, v_n\}$ the vertex set of $\overrightarrow{G}$, $E(\overrightarrow{G})$ the arc set of $\overrightarrow{G}$. Clearly, if G is an undirected graph, and $\overrightarrow{G}$ is the digraph obtained from G by replacing each edge with the pair of oppositely arcs joining the same pair of vertices. For a digraph $\overrightarrow{G} = (V, E)$, two vertices are called *adjacent* if they are connected by an arc. If there is an arc from vertex u to vertex v, we indicate this by writing uv, call v and u the head and the tail of uv, respectively. The digraph $\overrightarrow{G}$ is called *strongly connected* if for every pair of vertices $x, y \in V(\overrightarrow{G})$ there exists a directed path from x to y and a directed path from y to x. Recall that the *vertex connectivity* (edge connectivity) of a graph G, denoted by $\kappa(G)$ ($\eta(G)$), is the minimum number of vertices (edges) whose deletion yields the resulting graph disconnected. Similar to the definition of vertex connectivity of undirected graph, the vertex connectivity (arc connectivity) of a digraph, denoted by $\kappa(\overrightarrow{G})$ ($\eta(\overrightarrow{G})$), is the minimum number of vertices (arcs) whose deletion yields the resulting digraph non-strongly connected. The above two parameters are very important in characterizing digraph connectivity. The complete digraph of order n is the digraph $\overrightarrow{K_n}$ in which every pair of vertices is an arc. Let $D(\overrightarrow{G}) = (d_{ij})$ be the distance matrix of a digraph $\overrightarrow{G}$, where $d_{ij} = d_{\overrightarrow{G}}(v_i, v_j)$. $D_i = \sum_{j=1}^{n} d_{ij}$ $(i = 1, 2, \dots, n)$ is called the distance degree of vertex v_i. Clearly, we can assign the subscripts of vertices of $V(\overrightarrow{G})$ such that $D_1 \le D_2 \le \cdots \le D_n$, so we may let $\{v_1, v_2, \dots, v_n\}$ be such vertex ordering until stated otherwise. We call $\overrightarrow{G}$ *distance regular* if $D_1 = D_2 = \cdots = D_n$. The matrix $D(\overrightarrow{G})$ is nonnegative and

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irreducible when $\overrightarrow{G}$ is strongly connected. The largest eigenvalue of $D(\overrightarrow{G})$ is called the *distance spectral radius* of a digraph $\overrightarrow{G}$, denoted by $\varrho(D(\overrightarrow{G}))$. The positive unit eigenvector corresponding to $\varrho(D(\overrightarrow{G}))$ is called the *Perron vector* of $D(\overrightarrow{G})$.

Theorem 1.1 (*Perron–Frobenius [13]*). *Let A be a nonnegative irreducible square matrix with order n. Suppose $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of A. Then*

(i) *$\rho(A)$ is a simple eigenvalue of A and $|\lambda_i| \le \rho(A)$ for any eigenvalue λ_i $(1 \le i \le n)$;*
(ii) *there exists a positive unit eigenvector corresponding to $\rho(A)$, which is called the Perron vector of A;*
(iii) *if there are exactly h eigenvalues of A whose moduli are equal to $\varrho(A)$, say, $\lambda_1, \lambda_2, \ldots, \lambda_h$, then $\lambda_1, \lambda_2, \ldots, \lambda_h$ are the roots of $\lambda^h = \varrho(A)^h$.*

The distance matrix is very useful in different fields including the design of communication network, graph embedding theory as well as molecular stability. In [1] Balaban et al. proposed the use of distance spectral radius as a molecular descriptor. And in [5], it was successfully used to infer the extent of branching and model boiling points of alkanes. Recently in [18,19], Zhou and Trinajstić provided upper and lower bounds for $\varrho(G)$ in terms of the number of vertices, Wiener index and Zagreb index. Subhi and Powers in [16] proved that for $n \ge 3$ the path P_n has the maximum distance spectral radius among trees on n vertices. Stevanović and Ilić in [15] generalized this result, and proved that among trees with fixed maximum degree Δ, the broom has the maximal distance spectral radius. Furthermore, they proved that the star S_n is the unique graph with minimal distance spectral radius among trees on n vertices. In [6], Ilić characterized n-vertex trees with given matching number m which minimize the distance spectral radius. Recently, Bose et al. [4] determined the unique graph with minimal distance spectral radius with given pendent vertices. Yu et al. [17] proved that the graph S_n' (obtained from the star S_n on n $(n \ne 4, 5)$ vertices by adding an edge connecting two pendent vertices) has minimal distance spectral radius among unicyclic graphs on n vertices, and the graph P_n' (obtained from a triangle K_3 by attaching pendent path P_{n-3} to one of its vertices) has maximal distance spectral radius among unicyclic graphs. For other studies of distance spectral radius we suggest readers to refer to [2,7,8,10,11,14,20]. So far, there are fewer articles concern the distance spectral radius of digraphs.

The rest of the paper is organized as follows: In Section 2, we give two useful lemmas. In Section 3, we characterize the extremal digraphs and graphs with the minimum distance spectral radius among all digraphs and graphs of fixed order with given vertex connectivity and edge connectivity. In addition, we compute the distance spectral radius of the extremal digraphs and graphs. In Section 4, we characterize the graphs with the maximum distance spectral radius among all graphs of fixed order with vertex connectivity 1 and 2.

2. Preliminaries

A reformulation of inequalities from the theory of nonnegative matrices [12, Chapter 2] yields the following lemma as follows.

Lemma 2.1. *If A is a nonnegative irreducible $n \times n$ matrix with the largest eigenvalue $\varrho(A)$ and row sums $s_1, s_2, \ldots, s_n$, then*

$$\min_{1 \le i \le n} s_i \le \varrho(A) \le \max_{1 \le i \le n} s_i.$$

Moreover, one of the equalities holds if and only if the row sums of A are all equal.

For a simple connected graph, we have the similar lemma.

Lemma 2.2. *Let G be a simple connected graph with n vertices. Then*

$$D_1 \le \varrho(D(G)) \le D_n.$$

Moreover, one of the equalities holds if and only if G is a distance regular graph.

The following lemma is an immediate consequence of the Perron–Frobenius Theorem.

Lemma 2.3. *Let $\overrightarrow{G}$ be a strongly connected digraph with $u, v \in V(\overrightarrow{G})$ and $uv \notin E(\overrightarrow{G})$. Then $\varrho(\overrightarrow{G}) > \varrho(\overrightarrow{G} + uv)$.*

3. Minimum distance spectral radius of digraphs and graphs with given connectivity

Let $\mathcal{D}_{n,k}$ be the set of strongly connected digraphs with order n and vertex connectivity $\kappa(\overrightarrow{G}) = k$. Let $\overrightarrow{G}_1 \triangledown \overrightarrow{G}_2$ denote the digraph obtained from two disjoint digraphs $\overrightarrow{G}_1$, $\overrightarrow{G}_2$ with vertex set $V(\overrightarrow{G}_1) \cup V(\overrightarrow{G}_2)$ and arc set $E = E(\overrightarrow{G}_1) \cup E(\overrightarrow{G}_2) \cup \{uv, vu | u \in V(\overrightarrow{G}_1), v \in V(\overrightarrow{G}_2)\}$. Let $\overrightarrow{\mathcal{K}}^{k,s}_{n-s}$ denote the set of digraphs $\overrightarrow{K_k} \triangledown (\overrightarrow{K_s} \cup \overrightarrow{K}_{n-s-k}) \cup E$ where E is an arc set and $E = \{uv | u \in V(\overrightarrow{K}_s), v \in V(\overrightarrow{K}_{n-s-k})\}$. A digraph $\overrightarrow{G}$ is a *minimizing digraph* of $\mathcal{D}_{n,k}$ if $\overrightarrow{G} \in \mathcal{D}_{n,k}$ and $\varrho(\overrightarrow{G}) = \min\{\varrho(\overrightarrow{G}) | \overrightarrow{G} \in \mathcal{D}_{n,k}\}$.

Let $J_{a\times b}$ be the $a \times b$ matrix whose entries are all equal to 1, I_n be the $n \times n$ unit matrix, $0_{a\times b}$ $(2_{a\times b})$ be the $a \times b$ matrix of entries are all equal to 0 (2).

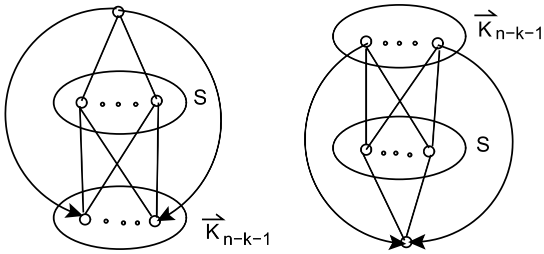

Fig. 1. The digraphs $\overrightarrow{\mathcal{K}}^{k,1}_{n-1}$ and $\overrightarrow{\mathcal{K}}^{k,n-k-1}_{k+1}$.

The following result can be found in [3], we cite it as our lemma.

Lemma 3.1. *Let $\overrightarrow{G}$ be an arbitrary strongly connected digraph with vertex connectivity k. Suppose that S is a k-vertex cut of $\overrightarrow{G}$ and $\overrightarrow{G}_1, \ldots, \overrightarrow{G}_s$ are the strongly connected components of $\overrightarrow{G} - S$. Then there exists an ordering of $\overrightarrow{G}_1, \ldots, \overrightarrow{G}_s$ such that, for $1 \le i \le s$ and $v \in V(\overrightarrow{G}_i)$, every tail of v in $\overrightarrow{G}_1, \ldots, \overrightarrow{G}_i$.*

Remark 3.2. By Lemma 3.1, we know that there exists a strongly connected component of $\overrightarrow{G} - S$, say $\overrightarrow{G}_1$, such that no vertex of $V(\overrightarrow{G}_1)$ has in-neighbors in $\overrightarrow{G} - S - \overrightarrow{G}_1$. Let $\overrightarrow{G}'_1 = \overrightarrow{G} - S - \overrightarrow{G}_1$. Since $\overrightarrow{G}$ is strongly connected digraph with vertex connectivity $\kappa(\overrightarrow{G}) = k$, we add arcs to $\overrightarrow{G}[V(\overrightarrow{G}_1)]$, $\overrightarrow{G}[V(\overrightarrow{G}'_1)]$ and the arcs from $\overrightarrow{G}[V(\overrightarrow{G}_1)]$ to $\overrightarrow{G}[V(\overrightarrow{G}'_1)]$ unless no more arcs can be added to $\overrightarrow{G}$, the new digraph denoted by $\overrightarrow{G}'$. Clearly, $\overrightarrow{G}'$ is also k-connected and $\overrightarrow{G}' \in \overrightarrow{\mathcal{K}}^{k,s}_{n-s}$. Therefore, by Lemma 3.1, we have the digraphs which achieve the minimum distance spectral radius among all digraphs in $\mathcal{D}_{n,k}$ must be in $\overrightarrow{\mathcal{K}}^{k,s}_{n-s}$.

The following lemma shows that $\rho(\overrightarrow{\mathcal{K}}^{k,1}_{n-1}) = \rho(\overrightarrow{\mathcal{K}}^{k,n-k-1}_{k+1})$, where $\overrightarrow{\mathcal{K}}^{k,1}_{n-1}$ and $\overrightarrow{\mathcal{K}}^{k,n-k-1}_{k+1}$ are shown in Fig. 1.

Lemma 3.3. *Let D be the distance matrix of $\overrightarrow{\mathcal{K}}^{k,1}_{n-1}$ and D' be the distance matrix of $\overrightarrow{\mathcal{K}}^{k,n-k-1}_{k+1}$. Then $P_D(\lambda) = P_{D'}(\lambda)$.*

Proof. It is easy to see that $D' = D^t$. Therefore, we have $P_D(\lambda) = P_{D'}(\lambda)$. $\square$

Lemma 3.4. *Let $f(x) = -4x^2 + 4(n-k)x + 4n - 4$, $1 \le x \le n-k-1$. Then* $\min\{f(x) | 1 \le x \le n-k-1\} = f(1) = f(n-k-1) = 8n - 4k - 8$.

In the following, we will consider which digraphs minimize the spectral radius in $\overrightarrow{\mathcal{K}}^{k,s}_{n-s}$.

Theorem 3.5. *The digraphs $\overrightarrow{\mathcal{K}}^{k,1}_{n-1}$ and $\overrightarrow{\mathcal{K}}^{k,n-k-1}_{k+1}$ are the minimizing digraphs among all digraphs in $\overrightarrow{\mathcal{K}}^{k,s}_{n-s}$. Furthermore, if $\overrightarrow{G} \in \mathcal{D}_{n,k}$ then $\varrho(\overrightarrow{G}) \ge \frac{n-2+\sqrt{(n+2)^2-4k-8}}{2}$ with equality holding if and only if either $\overrightarrow{G} \cong \overrightarrow{\mathcal{K}}^{k,1}_{n-1}$ or $\overrightarrow{G} \cong \overrightarrow{\mathcal{K}}^{k,n-k+1}_{k+1}$.*

Proof. Let $\overrightarrow{G}$ be an arbitrary digraph in $\overrightarrow{\mathcal{K}}^{k,s}_{n-s}$ and S be a k-vertex cut of $\overrightarrow{G}$. Suppose that $\overrightarrow{G}_1$ and $\overrightarrow{G}_2$ (with $|V(\overrightarrow{G}_1)| = n_1$ and $|V(\overrightarrow{G}_2)| = n_2 = n - k - n_1$, respectively) are two strongly connected components of $\overrightarrow{G} - S$ and with arcs $E = \{u_1u_2 \in E | u_1 \in V(\overrightarrow{G}_1), u_2 \in V(\overrightarrow{G}_2)\}$. It is easy to see that $1 \le n_1 \le n-k-1$. Let D be the distance matrix of $\overrightarrow{G}$. Then

$$D = \begin{pmatrix} J_{n_1\times n_1} - I_{n_1\times n_1} & J_{n_1\times k} & J_{n_1\times n_2} \\ J_{k\times n_1} & J_{k\times k} - I_{k\times k} & J_{k\times n_2} \\ 2_{n_2\times n_1} & J_{n_2\times k} & J_{n_2\times n_2} - I_{n_2\times n_2} \end{pmatrix}$$

and

$$\begin{aligned} P_D(\lambda) &= |\lambda I - D| \\ &= \begin{vmatrix} (\lambda+1)I_{n_1\times n_1} - J_{n_1\times n_1} & -J_{n_1\times k} & -J_{n_1\times n_2} \\ -J_{k\times n_1} & (\lambda+1)I_{k\times k} - J_{k\times k} & -J_{k\times n_2} \\ -2_{n_2\times n_1} & -J_{n_2\times k} & (\lambda+1)I_{n_2\times n_2} - J_{n_2\times n_2} \end{vmatrix} \\ &= (\lambda+1)^{n-3} \begin{vmatrix} \lambda - n_1 + 1 & -k & -n_2 \\ -n_1 & \lambda - k + 1 & -n_2 \\ -2n_2 & -k & \lambda - n_2 + 1 \end{vmatrix} \\ &= (\lambda+1)^{n-2} \begin{vmatrix} \lambda - n_1 - k + 1 & -n_2 \\ -2n_1 - k & \lambda - n_2 + 1 \end{vmatrix} \\ &= (\lambda+1)^{n-2}[\lambda^2 - (n-2)\lambda - n_1n_2 - n + 1] = (\lambda+1)^{n-2}[\lambda^2 - (n-2)\lambda - n_1(n-k-n_1) - n + 1]. \end{aligned}$$

Thus we have $\varrho(\overrightarrow{G})$ as the largest root of the equation

$$x^2-(n-2)x-n_1(n-k-n_1)-n+1=0.$$

Then we have

$$\begin{aligned}\varrho(\overrightarrow{G}) &= \frac{n-2+\sqrt{(n-2)^2-4[n_1^2-(n-k)n_1-n+1]}}{2}\\ &\geq \frac{n-2+\sqrt{(n-2)^2+8n-4k-8}}{2} \quad \text{by Lemma 3.4}\\ &= \frac{n-2+\sqrt{(n+2)^2-4k-8}}{2}.\end{aligned}$$

If the above equality holds, then by Lemma 3.4, we have $n_1=1$ or $n_1=n-k-1$. If $n_1=1$, then $\overrightarrow{G}\cong\overrightarrow{\mathcal{K}}_{n-1}^{k,1}$, and if $n_1=n-k+1$, then $\overrightarrow{G}\cong\overrightarrow{\mathcal{K}}_{k}^{k,n-k+1}$.

For the converse, if $\overrightarrow{G}\cong\overrightarrow{\mathcal{K}}_{n-1}^{k,1}$ or $\overrightarrow{G}\cong\overrightarrow{\mathcal{K}}_{k}^{k,n-k+1}$, then it is routine to show that $\varrho(\overrightarrow{G})=\frac{n-2+\sqrt{(n+2)^2-4k-8}}{2}$, thus we complete the proof. □

Let $\overline{\mathcal{D}}_{n,k}$ be the set of strongly connected digraphs with order n and arc connectivity $\eta(\overrightarrow{G})=k$. In the following, we will consider the minimizing digraph when arc connectivity is equal to vertex connectivity, i.e. $\eta(\overrightarrow{G})=\kappa(\overrightarrow{G})=k$, we state it without proof.

Theorem 3.6. *For every $k\geq 1$, if $\eta(\overrightarrow{G})=\kappa(\overrightarrow{G})=k$, then the digraphs $\overrightarrow{\mathcal{K}}_{n-1}^{k,1}$ and $\overrightarrow{\mathcal{K}}_{k+1}^{k,n-k-1}$ are the minimizing digraphs in $\overline{\mathcal{D}}_{n,k}$.*

Let $\delta^0(\overrightarrow{G})=\min\{\delta^-(\overrightarrow{G}),\delta^+(\overrightarrow{G})\}$. The following result shows the minimizing digraphs when $\eta(\overrightarrow{G})=\delta^0(\overrightarrow{G})=k$.

Theorem 3.7. *For every $k\geq 1$, if $\eta(\overrightarrow{G})=\delta^0(\overrightarrow{G})=k$, then the digraphs $\overrightarrow{\mathcal{K}}_{n-1}^{k,1}$ and $\overrightarrow{\mathcal{K}}_{k+1}^{k,n-k-1}$ are the minimizing digraphs in $\overline{\mathcal{D}}_{n,k}$.*

Proof. If $\delta^0(\overrightarrow{G})=\delta^+(\overrightarrow{G})$, let u be a vertex of $V(\overrightarrow{G})$ with outdegree k. Then the arcs with the tail u form an arc cut, and $G-u$ is a complete digraph. By Lemma 2.3, we have the digraph $\overrightarrow{\mathcal{K}}_{n-1}^{k,1}$ as the minimum digraph in $\overline{\mathcal{D}}_{n,k}$. Similarly, we can show that if $\delta^0(\overrightarrow{G})=\delta^-(\overrightarrow{G})$, then the digraph $\overrightarrow{\mathcal{K}}_{k+1}^{k,n-k-1}$ is the minimizing digraph in $\overline{\mathcal{D}}_{n,k}$. Therefore, we complete the proof. □

However, the minimizing digraphs are not determined when $\delta^0(\overrightarrow{G})>\eta(\overrightarrow{G})>\kappa(\overrightarrow{G})$. According to the above results, we believe that the digraphs $\overrightarrow{\mathcal{K}}_{n-1}^{k,1}$ and $\overrightarrow{\mathcal{K}}_{k+1}^{k,n-k-1}$ are the minimizing digraphs in $\overline{\mathcal{D}}_{n,k}$. Thus we give the following conjecture.

Conjecture 3.8. *For every $k\geq 1$, the digraphs $\overrightarrow{\mathcal{K}}_{n-1}^{k,1}$ and $\overrightarrow{\mathcal{K}}_{k+1}^{k,n-k-1}$ are the minimizing digraphs in $\overline{\mathcal{D}}_{n,k}$.*

Denote by $\mathcal{G}_n^k$ (respectively, $\bar{\mathcal{G}}_n^k$) the set of all graphs of order n with vertex connectivity k (respectively, edge connectivity k). A graph G is a *minimizing graph* of $\mathcal{G}_n^k$(or $\bar{\mathcal{G}}_n^k$) if $G\in\mathcal{G}_n^k$(or $\bar{\mathcal{G}}_n^k$) and $\varrho(G)=\min\{\varrho(G)|G\in\mathcal{G}_n^k(\text{or } \bar{\mathcal{G}}_n^k)\}$. Let $G_1\bigtriangledown G_2$ denote the graph obtained from two disjoint graphs G_1, G_2 by joining each vertex of G_1 to each vertex of G_2. Denote by $K_{n-s}^{k,s}$ the graph of $K_k\bigtriangledown(K_s\cup K_{n-s-k})$. In [9], Liu characterized that $K_{n-1}^{k,1}$ is the unique minimizing graph in the class $\mathcal{G}_n^k$, $k\geq 1$.

Theorem 3.9 (*[9]*)**.** *The graph $K_{n-1}^{k,1}$ is the unique minimizing graph in the class $\mathcal{G}_n^k$, $k\geq 1$.*

The following remark compute the smallest distance spectral radius among $\mathcal{G}_n^k$.

Remark 3.10. It is easy to see that

$$D(K_{n-1}^{k,1})=\begin{pmatrix}0 & J_{1\times k} & 2_{1\times(n-k+1)}\\ J_{k\times 1} & J_{k\times k}-I_{k\times k} & J_{k\times(n-k-1)}\\ 2_{(n-k-1)\times 1} & J_{(n-k-1)\times k} & J_{(n-k-1)\times(n-k-1)}-I_{(n-k-1)\times(n-k-1)}\end{pmatrix}.$$

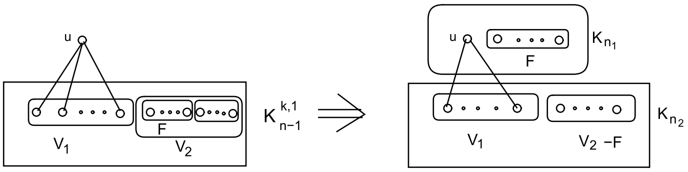

Fig. 2. A transformation from $K_{n-1}^{k,1}$ to G.

Therefore, we have

$$\begin{aligned} P_D(\lambda) &= \begin{vmatrix} \lambda & -J_{1\times k} & -2_{1\times(n-k+1)} \\ -J_{k\times 1} & (\lambda+1)I_{k\times k}-J_{k\times k} & -J_{k\times(n-k-1)} \\ -2_{(n-k-1)\times 1} & -J_{(n-k-1)\times k} & (\lambda+1)I_{(n-k-1)\times(n-k-1)}-J_{(n-k-1)\times(n-k-1)} \end{vmatrix} \\ &= (\lambda+1)^{n-3}\begin{vmatrix} \lambda & -k & -2(n-k-1) \\ -1 & \lambda-k+1 & -(n-k-1) \\ -2 & -k & \lambda-(n-k-2) \end{vmatrix} \\ &= (\lambda+1)^{n-3}[\lambda^3-(n-3)\lambda^2-(5n-3k-6)\lambda+kn-k^2+2k-4n+4]. \end{aligned}$$

That is, $\varrho(K_{n-1}^{k,1})$ is the largest root of the equation $x^3-(n-3)x^2-(5n-3k-6)x+kn-k^2+2k-4n+4=0$.

In the following, we will consider which graph minimizes the distance spectral radius among all connected graphs in $\overline{\mathcal{G}}_n^k$. If $k=n-1$, then G is the complete graph of order n. Thus, we may suppose $1\le k\le n-2$.

Theorem 3.11. *For every $1\le k\le n-2$, the graph $K_{n-1}^{k,1}$ is the unique minimizing graph in the class $\bar{\mathcal{G}}_n^k$.*

Proof. Let $K_{n-1}^{k,1}$ with $|V_1|=k$ and $|V_2|=n-k-1$ be the graph as shown in Fig. 2, and let x be the Perron vector of $K_{n-1}^{k,1}$. By symmetry, all the coordinates of V_1 are equal, say x_1, and all the coordinates of V_2 are equal, say x_2, and let $x_u = x_0$. Therefore, we have

$$\begin{cases} \varrho x_0 = kx_1+2(n-k-1)x_2, \\ \varrho x_1 = x_0+(k-1)x_1+(n-k-1)x_2, \\ \varrho x_2 = 2x_0+kx_1+(n-k-2)x_2, \end{cases}$$

and then $x_0>x_2>x_1$. Since $\varrho>n-1$, we have

$$\begin{cases} x_0 = x_1+\dfrac{n-k-1}{\varrho+1}x_2 < x_1+x_2, \\ x_1 = -x_0/(\varrho+1)+x_2, \end{cases} \tag{1}$$

and thus, we have

$$x_1 = \frac{(\varrho+1)^2-(n-k-1)}{(\varrho+1)(\varrho+2)}x_2. \tag{2}$$

Since $\varrho>n-1$, (2) implies $2x_1>x_2$.

Let G be a graph that attains the minimum distance spectral radius in $\bar{\mathcal{G}}_n^k$ and $G\ncong K_{n-1}^{k,1}$. Note that the assertion is easy to obtain when $n\le 5$. Then we assume $n\ge 6$ and $G\ncong K_n$ since $k\le n-2$. Note that each vertex of G has degree not less than k otherwise $G\in\bar{\mathcal{G}}_n^k$. If there exists a vertex u of G with degree k, then the edges incident to u form an edge cut, and $G-u$ is complete. The result follows in this case. So we may assume that all vertices of G have degrees greater than k. Let S be an edge cut of G containing k edges. Since G is k-edge connected, $G-S$ consists of exactly two components, G_1, G_2 of order n_1, n_2, respectively. Without loss of generality, we may assume that $n_2\ge n_1\ge 2$ since $\delta(G)\ge k+1$, and then $n_2\ge\frac{n}{2}\ge 3$.

Let u be a vertex of $V(G_1)$ which is incident to most of the edges in S. Assume that u joins t vertices of G_2. Surely $t\le\min\{k,n_2\}$. If $t=k$, there exists no edges joining G_1-u and G_2. Let F be a vertex set of V_2 with $|F|=n_1-1$. Then G can be obtained from $K_{n-1}^{k,1}$ by deleting the edges between F and $V(K_{n-1}^{k,1})-F-\{u\}$ and adding the edges between u and F as shown in Fig. 2. Therefore, we have

$$\begin{aligned} x^t[D(G)-D(K_{n-1}^{k,1})]x &= 2(n_1-1)x_2[kx_1+(n-n_1-k)x_2]-2(n_1-1)x_2x_0 \\ &= 2(n_1-1)x_2(kx_1+(n_2-k)x_2-x_0). \end{aligned} \tag{3}$$

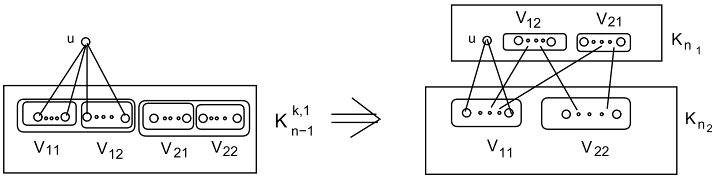

Fig. 3. A transformation from $K_{n-1}^{k,1}$ to G.

Now, we will consider the following two cases.

Case 1: $n_2 \geq k+1$.

Then we have $kx_1 + (n_2 - k)x_2 > x_1 + x_2 > x_0$, and

$$(3) > 2(n_1 - 1)x_2(x_1 + x_2 - x_0) > 0.$$

Therefore, we have $x^t D(G)x > x^t D(K_{n-1}^{k,1})x$, a contradiction.

Case 2: $n_2 = k$.

Then $k = n_2 \geq n/2 \geq 3$, and since $2x_1 > x_2$, thus we have

$$\begin{aligned}(3) &= 2(n_1 - 1)x_2(kx_1 - x_0) \geq 2(n_1 - 1)x_2(3x_1 - x_0) \\ &> 2(n_1 - 1)x_2(x_1 + x_2 - x_0) > 0,\end{aligned}$$

which implies $x^t D(G)x > x^t D(K_{n-1}^{k,1})x$, a contradiction.

So in the following, we may assume that $t < k$.

We partition $V(G)$ into $\{u\}, V_{ij}(G),\ i, j = 1, 2$ as shown in Fig. 3. Suppose $A_1(G) = [V_{12}(G), V_{11}(G)] \cap S, A_2(G) = [V_{12}(G), V_{22}(G)] \cap S, B_1(G) = [V_{21}(G), V_{11}(G)] \cap S$ and $B_2(G) = [V_{21}(G), V_{22}(G)] \cap S$. Suppose that $|A_i(G)| = a_i$ and $|B_i(G)| = b_i$, for $i = 1, 2$. Then $a_1 + a_2 + b_1 + b_2 = k - t$. Similarly, we may get G from $K_{n-1}^{k,1}$ by using the symmetry of G_1, G_2 and the structural properties of $K_{n-1}^{k,1}$. In fact, we can partition the vertex set $V(K_{n-1}^{k,1})$ into u, $V_{ij}(K_{n-1}^{k,1})$, $i, j = 1, 2$, as shown in Fig. 3, such that $|V_{ij}(G)| = |V_{ij}(K_{n-1}^{k,1})|$. Then we can easily construct a graph isomorphic to G from $K_{n-1}^{k,1}$ by deleting some of the edges between $V_{12}(K_{n-1}^{k,1}) \cup V_{21}(K_{n-1}^{k,1})$ and $V_{11}(K_{n-1}^{k,1}) \cup V_{22}(K_{n-1}^{k,1})$ such that the resulting graph satisfies $a_1 = |[V_{12}(K_{n-1}^{k,1}), V_{11}(K_{n-1}^{k,1})]|$, $a_2 = |[V_{12}(K_{n-1}^{k,1}), V_{22}(K_{n-1}^{k,1})]|$, $b_1 = |[V_{21}(K_{n-1}^{k,1}), V_{11}(K_{n-1}^{k,1})]|$, $b_2 = |[V_{21}(K_{n-1}^{k,1}), V_{22}(K_{n-1}^{k,1})]|$ and adding the edges between u and $V_{21}(K_{n-1}^{k,1})$; see Fig. 3.

Noting that $n_1 > k + 1 - t$ as the degree $d_G(u) > k$. Since $\varrho(G) > n - 1$, (2) implies

$$2x_1^2 > \left[\frac{2\varrho^2 + 2\varrho + 4}{(\varrho + 1)(\varrho + 2)}\right]^2 x_2^2 > x_2^2. \tag{4}$$

Since $x_2 > x_1$, we have $a_1x_1^2 + a_2x_1x_2 + b_1x_1x_2 + b_2x_2^2 < (k - t)x_2^2$. Therefore,

$$\begin{aligned}x^t[D(G) - D(K_{n-1}^{k,1})]x &= 2(k-t)x_1[tx_1 + (n - n_1 - (k-t))x_2] \\ &\quad + 2(n_1 - (k-t) - 1)x_2[tx_1 + (n - n_1 - (k-t))x_2] \\ &\quad - a_1x_1^2 - a_2x_1x_2 - b_1x_1x_2 - b_2x_2^2 - (n_1 - 1 - (k-t))x_1x_0 \\ &\geq (k-t)(2tx_1^2 - x_2^2) + 2(k-t)x_1(n - n_1 - t)x_2 \\ &\quad + 2(n_1 - 1 - (k-t))x_2[tx_1 + (n - n_1 - t)x_2 - x_0].\end{aligned} \tag{5}$$

Now, we consider the following two cases.

Case 1: $n_2 \geq t + 1$.

Then we have

$$(5) > (k-t)(2x_1^2 - x_2^2) + 2(n_1 - 1 - (k-t))x_2(x_1 + x_2 - x_0) > 0,$$

which implies $x^t D(K_{n-1}^{k,1})x < x^t D(G)x$, a contradiction.

Case 2: $n_2 = t$.

Then $n - n_1 - t = n_2 - t = 0$, and we have $n_2 = t \geq n/2 \geq 3$. Since $2x_1 > x_2$, we obtain

$$\begin{aligned}(5) &\geq (k-t)(2x_1^2 - x_2^2) + 2(n_1 - 1 - (k-t))x_2(3x_1 - x_0) \\ &> (k-t)(2x_1^2 - x_2^2) + 2(n_1 - 1 - (k-t))x_2(x_1 + x_2 - x_0) > 0.\end{aligned}$$

Hence we have $x^t D(K_{n-1}^{k,1})x < x^t D(G)x$, a contradiction. Therefore, we complete the proof. □

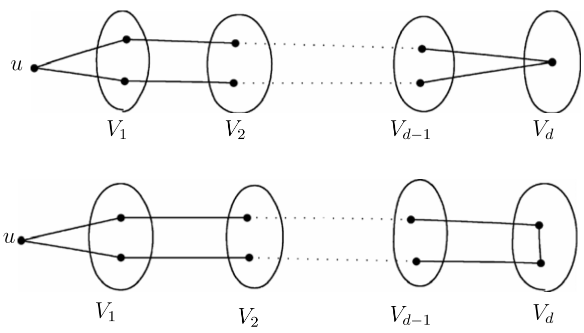

Fig. 4. The graph $G^{\star}$.

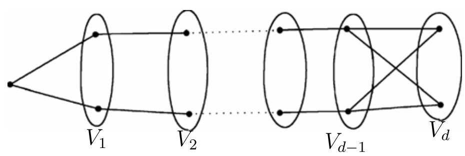

Fig. 5. The graph H.

4. Maximum distance spectral radius of graphs with given connectivity

A graph G is a *maximizing graph* of $\mathcal{G}_n^k$ if $G \in \mathcal{G}_n^k$ and $\varrho(G) = \max\{\varrho(G)|G \in \mathcal{G}_n^k\}$. Subhi and Powers in [16] proved that for $n \geq 3$ the path P_n has the maximum distance spectral radius among trees on n vertices. It is not difficult to see that P_n also has the maximum distance spectral radius among all connected graphs. Then we will have the following theorem. Noticing that the graph in section may do not satisfy the inequality $D_1 \leq D_2 \leq \cdots \leq D_n$.

Theorem 4.1. *The graph P_n is the unique maximizing graph in the class $\mathcal{G}_n^1$.*

Proof. Since $\kappa(P_n) = 1$ and by the result of Subhi and Powers', we have P_n as the maximizing graph in $\mathcal{G}_n^1$. □

Next we will consider the maximizing graphs in the class $\mathcal{G}_n^2$. Let $G \in \mathcal{G}_n^2$ be a graph with diameter d. Let x be a vertex such that $d(x, y) = d$ for some $y \in V(G)$. Note that G is 2-connected, then $V(G)$ has a partition $V(G) = \{x\} \cup V_1 \cup \cdots \cup V_d$, where V_i is the set of all vertices satisfying $d(x, z) = i, z \in V_i$, $|V_i| \geq 2$ for each $i = 1, 2, \ldots, d-1$. Let $G^{\star} = \{G|G$ be a 2-connected graph with diameter $d = \lfloor \frac{n}{2} \rfloor\}$. Thus, for any $G \in G^{\star}$, there is a partition $V(G) = \{x\} \cup V_1 \cup \cdots \cup V_d$ such that $|V_i| = 2$ for each $i = 1, 2, \ldots, d-1$ and $|V_d| = 1$ when n is even; $|V_d| = 2$ when n is odd; see Fig. 4. Let $G \in \mathcal{G}_n^2$, $x \in V(G)$, and $d(x, y) = d$ for some $y \in V(G)$ be the largest length of the distance from x. Thus, $V(G)$ can be decomposed into $V = \{x\} \cup V_1 \cup \cdots \cup V_d$, where V_i is the set of all vertices satisfying $d(x, z) = i, z \in V_i$. Note that $|V_i| \geq 2$, then it is not difficult to see that either

$$|V_1| + 2|V_2| + \cdots + d|V_d| \leq 2 \times 1 + 2 \times 2 + \cdots + 2 \times \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right) + \left\lfloor \frac{n}{2} \right\rfloor \tag{6}$$

if n is even, and equality holds if and only if $d = \lfloor \frac{n}{2} \rfloor$, or

$$|V_1| + 2|V_2| + \cdots + d|V_d| \leq 2 \times 1 + 2 \times 2 + \cdots + 2 \times \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right) + 2\left\lfloor \frac{n}{2} \right\rfloor \tag{7}$$

if n is odd, and equality holds if and only if $d = \lfloor \frac{n}{2} \rfloor$.

Lemma 4.2. *Let G be a graph of $\mathcal{G}_n^2$ and G' be a graph of $G^{\star}$. Then $D_n(G') \geq D_n(G)$, the equality holds if and only if $G \in G^{\star}$.*

Proof. Let $x \in V(G)$ and $d(x, y) = d$ for some $y \in V(G)$ be the largest length of the distance from x. Then $V(G)$ can be decomposed into $V = \{x\} \cup V_1 \cup \cdots \cup V_d$, where V_i is the set of all vertices satisfying $d(x, z) = i, z \in V_i$. Obviously, V_i is a cut-set of vertices of G for each $i = 1, 2, \ldots, d-1$ since G is 2-connected, thus we have $|V_i| \geq 2$ for each $i = 1, 2, \ldots, d-1$. Noticing that the diameter of G is at most $\lfloor \frac{n}{2} \rfloor$. Assume $f = \max\{\sum_{v \in V(G)} d(x, v)|x \in V(G), G \in \mathcal{G}_n^2\}$. It follows from inequalities (6) and (7) that $\sum_{v \in V(G)} d(x, v) = f$ if and only if $d = \lfloor \frac{n}{2} \rfloor$ i.e. $G \in G^{\star}$. We complete the proof. □

For $A, B \subset V(G)$, denote $[A, B]$ the set of edges (of G) whose one end is in A and the other end is in B. Let H be a graph with vertex connectivity 2 and $|V(H)| = n = 2d + 1$ such that $V(H)$ has a partition $V(H) = \{x\} \cup V_1 \cup \cdots \cup V_d$ for some $y \in V(H)$, $|V_i| = 2$ and V_i is an independent set of H for each $i = 1, 2, \ldots, d$, and $|[V_i, V_{i+1}]| = 2$ for $i = 1, 2, \ldots, d-2$ and $|[V_{d-1}, V_d]| = 4$; see Fig. 5.

Lemma 4.3. *Let H be a graph defined as above (see Fig. 5). Then $\varrho(C_n) > \varrho(H)$.*

Proof. It is easy to see that $D_n(H) > D_{n-1}(H)$ and $D_n(H) = D_n(C_n)$. Suppose that $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ is the Perron vector of $D(H)$, $x_s = \max_{1\le i\le n} x_i$ and $x_t = \max_{j\neq s} x_j$. Then

$$\rho(D(H))x_s \le D_s(H)x_t,\ \rho(D(H))x_t \le D_t(H)x_s.$$

Hence $\rho(D(H)) \le \sqrt{D_{n-1}(H)D_n(H)} < D_n(H) = D_n(C_n) = \varrho(C_n)$. $\square$

Using Lemmas 4.2 and 4.3, we immediately have the following result.

Theorem 4.4. *The graph C_n is the unique maximizing graph in the graph $\mathcal{G}_n^2$.*

Proof. Let G be a graph in $\mathcal{G}_n^2$ and $G' \in G^\star$. By Lemma 4.2, we have $D_n(G') \ge D_n(G)$, the equality holds if and only if $G \in G^\star$. It is well known that $\varrho(G+e) < \varrho(G)$, for any $e\bar{\in}E(G)$. We have $\varrho(G') \le \varrho(C_n)$ or $\varrho(G') \le \varrho(H) < \varrho(C_n)$ since G' can be obtained by adding some edges to C_n or H, and the equality holds if and only if $G' \cong C_n$. Thus we complete the proof. $\square$

Remark 4.5. It is easy to see that

$$\varrho(C_n) = D_i(C_n) = \begin{cases} \dfrac{n^2-1}{4} & n \text{ is odd;} \\ \dfrac{n^2}{4} & n \text{ is even.} \end{cases}$$

Thus, we have for any graph G with $|V(G)| = n$, if G is k-connected ($k \ge 2$), then

$$\varrho(D(G)) \le \begin{cases} \dfrac{n^2-1}{4} & n \text{ is odd;} \\ \dfrac{n^2}{4} & n \text{ is even} \end{cases}$$

the equality holds if and only if $k = 2$ and $G \cong C_n$.

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