Clique number and distance spectral radii of graphs *

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Abstract

The distance spectral radius of a connected graph G, denoted by $\rho(G)$, is the maximal eigenvalue of the distance matrix of G. In this paper we find a sharp lower bound as well as a sharp upper bound of $\rho(G)$ in terms of $\omega(G)$, the clique number of G. Furthermore, both extremal graphs are unique decided.

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1 Introduction

All graphs considered here are connected, simple and have at least one edge. The vertex set and edge set of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The set of vertices adjacent to a vertex v is denoted by $N_G(v)$ and the distance between a pair of vertices u, v is denoted by $d_G(u, v)$. A complete ω-partite graph with partition sets $V_1, V_2, \ldots, V_\omega$ is denoted by $K_{|V_1|,|V_2|,\ldots,|V_\omega|}$ and a complete graph of order k is denoted by K_k. The clique number $\omega(G)$ is the number of vertices in the largest clique

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in G. Let $D(G) = (d_{ij})$ be the distance matrix of G, where $d_{ij} = d_G(v_i, v_j)$. The maximal eigenvalue of $D(G)$ is called the distance spectral radius of G and is denoted by $\rho(G)$.

The distance matrix is very useful in different fields including the design of communication networks, graph embedding theory and molecular stability. In [1] Balaban et al. proposed the use of distance spectral radius as a molecular descriptor. While in [3] it was successfully used to infer the extent of branching and model boiling points of alkanes. Recently in [5] and [9] the authors provided some upper and lower bounds for $\rho(G)$. Stevanovíc and Ilić [7] showed that the broom graph has maximal distance spectral radius among all trees with fixed maximum degree. Ilić [4] determined the tree which attains minimal distance spectral radius among all trees with given matching number. Zhang and Godsil [8] characterized the extremal graphs with minimal distance spectral radii among all connected graphs with given number of cut vertices or cut edges.

This paper investigates the relationship between the distance spectral radius and the clique number of a graph. Let $T_{n,w}$ be the ω-partite Turán graph on n vertices and $K_\omega^{n-\omega}$ be the graph obtained from an ω-clique by attaching a path of length $n - w$ to a vertex of the clique. It is showed that $\rho(T_{n,w}) \leq \rho(G) \leq \rho(K_\omega^{n-\omega})$ for any graph G on n vertices with clique number ω. Furthermore, the left equality holds if and only if $G \cong T_{n,w}$ and the right equality holds if and only if $G \cong K_\omega^{n-\omega}$.

2 Lower bound on distance spectral radius

Since $D(G)$ is an irreducible nonnegative matrix for any connected graph G, by the Perron-Frobenius theorem, $\rho(G)$ is simple and there exists a positive unit eigenvector X associated with it, where X is called the Perron vector of $D(G)$. And by the Rayleigh-Ritz theorem,

$$\rho(G) = \max_{||Y||=1} Y^T D(G) Y = X^T D(G) X = \sum_{i,j} d_{ij} x_i x_j.$$

Let uv be an edge of a graph G such that $G - uv$ is still connected. Clearly, $d_{G-uv}(v_i, v_j) \geq d_G(v_i, v_j)$ for any pair of vertices v_i, v_j and $d_{G-uv}(u, v) > d_G(u, v)$. This implies that $\rho(G - uv) > \rho(G)$.

Let $G(|C_1|, |C_2|, \dots, |C_\omega|)$ denote the graph obtained from an ω-clique $C = \{v_1, v_2, \dots, v_\omega\}$ and an $(n - \omega)$-clique $C' = C_1 \cup C_2 \dots \cup C_\omega$ (see Figure 1) by joining v_k with each vertex of $C' \backslash C_k$ for $k = 1, 2, \dots, \omega$, where $|C_1| \leq |C_2| \leq \dots \leq |C_\omega|$, $\sum_{k=1}^{\omega} |C_k| = n - \omega$ and some C_k's may be empty. In fact, the complement of $G(|C_1|, |C_2|, \dots, |C_\omega|)$ is isomorphic to the disjoint union of $K_{1,|C_1|}, K_{1,|C_2|}, \dots, K_{1,|C_\omega|}$. And it is clear that $G(0, 0, \dots, 0, 1, 1, \dots, 1) \cong T_{n,\omega}$ when $\omega > \frac{n}{2}$.

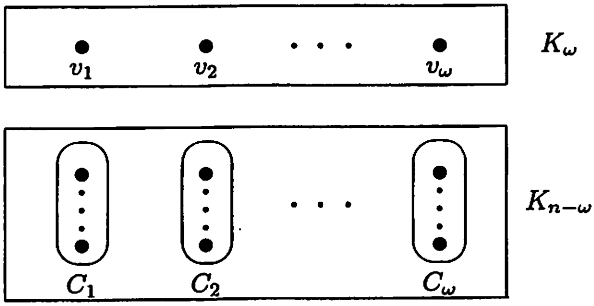

Figure 1 An ω-clique and an $(n-\omega)$-clique in $G(|C_1|, |C_2|, \dots, |C_\omega|)$.

Theorem 2.1 *Let G be a graph on n vertices with clique number ω. If $\omega > \frac{n}{2}$, then $\rho(G) \geq \rho(T_{n,\omega})$ and the equality holds if and only if $G \cong T_{n,\omega}$.*

Proof. Let $C = \{v_1, v_2, \dots, v_\omega\}$ be a clique of G and $C' = V(G) \backslash C$. Then any vertex of C' has at most $\omega - 1$ neighbors in C. This implies that under graph isomorphism G is a spanning subgraph of $G(|C_1|, |C_2|, \dots, |C_\omega|)$ for some partition $C_1, C_2, \dots, C_\omega$ of C'. Therefore, $\rho(G) \geq \rho(G(|C_1|, |C_2|, \dots, |C_\omega|))$. Let

$$\mathcal{G}_{n,\omega} = \{G(|C_1|, |C_2|, \dots, |C_\omega|) | \sum_{k=1}^{\omega} |C_k| = n - \omega, |C_1| \leq |C_2| \leq \dots \leq |C_\omega|\}.$$

and $G^* = G(|C_1|, |C_2|, \dots, |C_\omega|)$ be an extremal graph in $\mathcal{G}_{n,\omega}$ with minimal distance spectral radius. Although all graphs in $\mathcal{G}_{n,\omega}$ but $G(0, 0, \dots, 0, 1, 1, \dots, 1)$ have clique number greater than ω, it suffices to show that $G^* \cong G(0, 0, \dots, 0, 1, 1, \dots, 1)$.

Assume to the contrary that $G^* \ncong G(0, 0, \dots, 0, 1, 1, \dots, 1)$. Let i be the minimal index such that $|C_i| \geq 2$, j be the maximal index such that $C_j = \emptyset$ (Such j does exist, since $\sum_{k=1}^{\omega} |C_k| = n - \omega < \omega$) and $G' = G(|C'_1|, |C'_2|, \dots, |C'_\omega|)$, where $C'_i = C_i \setminus \{u\}$ for some vertex $u \in C_i$, $C'_j = \{u\}$ and $C'_k = C_k$ for else k (see Figure 2). Then $G' \in \mathcal{G}_{n,\omega}$. We now get a contradiction by proving that $\rho(G^*) > \rho(G')$.

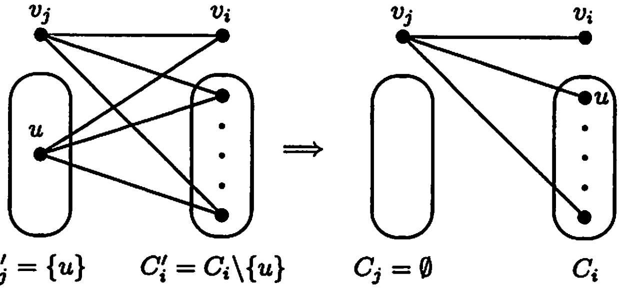

Figure 2 The local transformation from G' to G^*.

Let X be the Perron vector of $D(G')$ with component x_{v_k} corresponding to vertex v_k for $k = 1, 2, \ldots, \omega$. By symmetry, all the vertices of C_k' have the same Perron component and we may use x_k' to denote the Perron component of the vertices in C_k' for $k = 1, 2, \ldots, \omega$. Since $d_{G^*}(u, v_i) = d_{G'}(u, v_i) + 1 = 2$, $d_{G^*}(u, v_j) = d_{G'}(u, v_j) - 1 = 1$ and $d_{G^*}(s, t) = d_{G'}(s, t)$ for any else pair of vertices s and t, we have

$$\rho(G^*) - \rho(G') \geq X^T[D(G^*) - D(G')]X = 2x_j'(x_{v_i} - x_{v_j}).$$

Further,

$$\rho(G')(x_{v_i} - x_{v_j}) = (x_{v_j} - x_{v_i}) + (|C_i'|x_i' - x_j') \geq (x_{v_j} - x_{v_i}) + (x_i' - x_j')$$

and $\rho(G')(x_i' - x_j') = (x_j' - x_i') + (x_{v_i} - x_{v_j})$. This implies that $(\rho(G') + 1 - \frac{1}{\rho(G')+1})(x_{v_i} - x_{v_j}) \geq 0$ and hence $\rho(G^*) \geq \rho(G')$. Now assume that $\rho(G^*) = \rho(G')$, then $x_{v_i} = x_{v_j}$ and X is also the Perron vector of $D(G^*)$. Therefore, $\rho(G^*)(x_{v_i} - x_{v_j}) = (x_{v_j} - x_{v_i}) + |C_i|x_i' > 0$, a contradiction. Thus $\rho(G^*) > \rho(G')$ and the proof is completed. □

The following lemma is known as Turán's theorem (see [2]).

Lemma 2.2 *Let G be a graph on n vertices without $(\omega + 1)$-clique. Then $e(G) \leq e(T_{n,\omega})$ and the equality holds if and only if $G \cong T_{n,\omega}$, where $e(G)$ is the number of edges in G.*

Let $W(G)$ denote the Wiener index of a graph G, that is, the sum of the distances between any two vertices of G.

Lemma 2.3 ([5, 9]) *Let G be a graph on n vertices. Then $\rho(G) \geq \frac{2W(G)}{n}$ and the equality holds if and only if G is distance regular, i.e. the row sums of $D(G)$ are all equal.*

Theorem 2.4 *Let G be a graph on n vertices with clique number ω. If $\omega \mid n$, then $\rho(G) \geq \rho(T_{n,\omega})$ and the equality holds if and only if $G \cong T_{n,\omega}$.*

Proof. It is obvious that G has $e(G)$ vertex pairs at distance one and $\binom{n}{2} - e(G)$ vertex pairs at distance equal to or more than two. Suppose that $G \not\cong T_{n,\omega}$. According to Lemma 2.2,

$$W(G) \geq e(G) + 2[\binom{n}{2} - e(G)] > 2\binom{n}{2} - e(T_{n,\omega}) = W(T_{n,\omega}).$$

And by Lemma 2.3, $\rho(G) \geq \frac{2W(G)}{n} > \frac{2W(T_{n,\omega})}{n}$. On the other hand, since $D(T_{n,\omega})$ is distance regular when $\omega \mid n$, we have $\rho(T_{n,\omega}) = \frac{2W(T_{n,\omega})}{n}$. So $\rho(G) > \rho(T_{n,\omega})$. □

The following result provides the relationship between chromatic number and distance spectral radius.

Lemma 2.5 *Let G be a graph on n vertices with chromatic number $\chi(G) = \omega$. Then $\rho(G) \geq \rho(T_{n,\omega})$ and the equality holds if and only if $G \cong T_{n,\omega}$.*

Proof. We may assume that G has minimal distance spectral radius among all graphs on n vertices with chromatic number ω. It suffices to show that $G \cong T_{n,\omega}$. Since the adding of an edge decreases the distance spectral radius, G is a complete ω-partite graph. Let $V_1, V_2, \ldots, V_\omega$ be the partition of $V(G)$ (that is, $G \cong K_{|V_1|,|V_2|,\ldots,|V_\omega|}$). If $||V_i| - |V_j|| \leq 1$ for any $1 \leq i,j \leq \omega$, then $G \cong T_{n,\omega}$. Now assume without loss of generality that $|V_1| \leq |V_2| - 2$. Similarly as the proof of Theorem 2.1, one can get $\rho(G) > \rho(K_{|V_1|+1,|V_2|-1,|V_3|,\ldots,|V_\omega|})$, a contradiction. □

Lemma 2.6 ([6]) *Let G be a graph on n vertices with $\omega(G) \leq \omega$. If $\chi(G) > \omega$ and $\omega < \frac{n}{2}$, then $e(G) \leq e(T_{n,\omega}) - \lfloor \frac{n}{\omega} \rfloor + 1$.*

Theorem 2.7 *Let G be a graph on n vertices with clique number ω. Then $\rho(G) \geq \rho(T_{n,\omega})$ and the equality holds if and only if $G \cong T_{n,\omega}$.*

Proof. According to Theorems 2.1 and 2.4, the claim holds for $\omega > \frac{n}{2}$ or $\omega \mid n$. And by Lemma 2.5, the claim holds if $\chi(G) = \omega(G) = \omega$. Next suppose that $\omega < \frac{n}{2}$, $\omega \nmid n$ and $\chi(G) > \omega$. It suffices to show that $\rho(G) > \rho(T_{n,\omega})$. First we give the value of $\rho = \rho(T_{n,\omega})$. Set $k = \lfloor \frac{n}{\omega} \rfloor$, then $k \geq 2$. Note that $T_{n,\omega}$ has $n - k\omega$ partition sets of size $k+1$ and $(k+1)\omega - n$

partition sets of size k. Let X be the Perron vector of $T_{n,\omega}$ with component x_1 corresponding to the vertices of degree $n-k-1$ and x_2 corresponding to the vertices of degree $n-k$. Since $\rho X = D(T_{n,\omega})X$, we have

$$\rho x_1 = 2kx_1 + (n-k\omega-1)(k+1)x_1 + [(k+1)\omega - n]kx_2 \tag{1}$$

and

$$\rho x_2 = 2(k-1)x_2 + [(k+1)\omega - n - 1]kx_2 + (n-k\omega)(k+1)x_1.$$

Therefore, $\rho(x_1 - x_2) = (k-1)x_1 - (k-2)x_2$, that is, $x_1 = \frac{\rho-k+2}{\rho-k+1}x_2$. Applying it to (1), we have

$$[\rho - 2k - (n-k\omega-1)(k+1)](\rho-k+2) = [(k+1)\omega - n]k(\rho-k+1).$$

Straightforward calculation shows that

$$\rho(T_{n,\omega}) = \frac{1}{2}[(n+2k-3) + \sqrt{(n+2k+1)^2 - 4k(k+1)(\omega+1)}]. \tag{2}$$

On the other hand, by Lemmas 2.3 and 2.6, we have

$$\rho(G) \geq \frac{2W(G)}{n} \geq \frac{2[2\binom{n}{2} - e(G)]}{n} \geq \frac{2[2\binom{n}{2} - e(T_{n,\omega}) + k - 1]}{n}.$$

It is known that

$$e(T_{n,\omega}) = \binom{n-k}{2} + (\omega-1)\binom{k+1}{2}.$$

Thus we have

$$\begin{aligned} \rho(G) &\geq \frac{2}{n}[2\binom{n}{2} - \binom{n-k}{2} - (\omega-1)\binom{k+1}{2} + (k-1)] \\ &= (n+2k-1) - \frac{1}{n}[k(k+1)\omega - 2(k-1)]. \end{aligned} \tag{3}$$

To show $\rho(G) > \rho(T_{n,\omega})$, it suffices to show that the right side of (3) is more than that of (2). That is, we have to show that

$$\begin{aligned} & \frac{[k(k+1)\omega - 2(k-1)]^2}{n^2} \\ > \ & \frac{(n+2k+1)[k(k+1)\omega - 2(k-1)]}{n} - k(k+1)(\omega+1). \end{aligned} \tag{4}$$

Simplifying (4), we have

$$\begin{aligned} & 2(k-1)[(k+1)(n-k\omega) + k(n-k\omega-\omega) + n^2 + 2(k-1)] \\ > \ & -k(k+1)(n-k\omega)(n-k\omega-\omega). \end{aligned} \tag{5}$$

Let $n = k\omega + k_0$, then $0 < k_0 < \omega$. To obtain (5), it suffices to show

$$2(k-1)(n^2 - k\omega) > k(k+1)k_0\omega.$$

Note that

$$2(k-1)n^2 > 2(k-1)(k^2\omega^2 + 2kk_0\omega) > 2(k-1)k\omega + (k+1)kk_0\omega$$

for $k \geq 2$. The proof is completed. □

3 Upper bound on distance spectral radius

In this section, we give a sharp upper bound of distance spectral radius for the graphs with given clique number.

Lemma 3.1 ([7]) *Let $G_{p,q}$ be a graph obtained from G by attaching two pendent paths of length p and q at a vertex of G. If $q \geq p \geq 1$, then $\rho(G_{p-1,q+1}) > \rho(G_{p,q})$.*

Lemma 3.2 ([8]) *Let G be a graph with $uv \in E(G)$ and $G_{p,q}(u,v)$ be the graph obtained from G by attaching a pendent path of length p at u and a pendent path of length q at v. If $q > p \geq 1$, then $\rho(G_{p-1,q+1}(u,v)) > \rho(G_{p,q}(u,v))$. If $q = p \geq 1$, then either $\rho(G_{p-1,q+1}(u,v)) > \rho(G_{p,q}(u,v))$ or $\rho(G_{p+1,q-1}(u,v)) > \rho(G_{p,q}(u,v))$.*

Theorem 3.3 *Let G be a graph on n vertices with clique number ω. Then $\rho(G) \leq \rho(K_\omega^{n-w})$ and the equality holds if and only if $G \cong K_\omega^{n-w}$.*

Proof. The claim is trivial for $n = \omega$. Now let $n > \omega$. We may assume G is an extremal graph which attains the upper bound of distance spectral radius and prove that $G \cong K_\omega^{n-w}$. Let C be an ω-clique of G and $G_1, G_2, \ldots, G_k$ $(k \geq 1)$ be the components of $G - C$. Since G is connected, for each G_i there exists an edge connecting a vertex from G_i and a vertex from C. Moreover, since $\rho(G - e) > \rho(G)$ for any edge e which is not a cut edge, we can conclude that each G_i is a tree and for each G_i there is exactly one edge from it to C. We now give two claims on the structure of G.

Claim 1 Each G_i is a path with an endpoint adjacent to some $v_i \in C$.

In fact, the above discussion implies that $V_i = V(G_i) \cup \{v_i\}$ also induces a tree for each i. It suffices to show that each V_i induces a path. Assume to the contrary that for some i, u_i is a branching vertex (i.e. a vertex of degree more than two) of G_i which has the longest distance to v_i. Then the subtree of u_i consists of several paths rooted by u_i. According to Lemma 3.1, we can get a graph G' on n vertices with clique number ω such that $\rho(G') > \rho(G)$, which contradicts the maximality of $\rho(G)$.

Claim 2 There is a unique path G_i.

Suppose to the contrary that G_i and G_j are two such paths. If G_i and G_j are rooted by the same vertex of C, then by Lemma 3.1, we can get a graph G' with $\rho(G') > \rho(G)$, a contradiction. Now assume that their roots v_i and v_j are distinct. Let p_i be the length of the path G_i. Since $v_iv_j \in E(G)$, by Lemma 3.2, we can get a graph G' with $\rho(G') > \rho(G)$, also a contradiction.

Claim 1 and Claim 2 imply that $G \cong K_\omega^{n-w}$. This completes the proof. □

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