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ON SPECTRAL RADIUS OF THE DISTANCE MATRIX

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We characterize graphs with minimal spectral radius of the distance matrix in three classes of simple connected graphs with n vertices: with fixed vertex connectivity, matching number and chromatic number, respectively.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. The distance matrix of G is defined as the $n \times n$ matrix $D(G) = (d_{ij})$, where d_{ij} is the distance (i.e., the number of edges of a shortest path) between vertices v_i and v_j in G [**1**]. Denoted by $\rho(G)$ the spectral radius (the largest eigenvalue) of $D(G)$. Properties for eigenvalues of the distance matrix and especially for ρ may be found in e.g., [**2, 3, 4, 5, 6**].

In this paper, we characterize graphs with minimal spectral radius of the distance matrix in three classes of simple connected graphs with n vertices: with fixed vertex connectivity, matching number and chromatic number, respectively.

2. PRELIMINARIES

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

Lemma 1. *Let G be a connected graph with $u, v \in V(G)$ and $uv \notin E(G)$. Then $\rho(G) > \rho(G + uv)$.*

Let $J_{a\times b}$ be the $a \times b$ matrix whose entries are all equal to 1 and I_n be the $n \times n$ unit matrix. Let $J = J_{n\times n}$.

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Let $N_G(v)$ be the neighborhood of the vertex v of G. Let $G_1 \cup \cdots \cup G_k$ be the vertex-disjoint union of the graphs $G_1, \cdots, G_k$ ($k \geq 2$), and $G_1 \vee G_2$ be the graph obtained from $G_1 \cup G_2$ by joining each vertex of G_1 to each vertex of G_2. Let $x(G) = (x_1, x_2, \ldots, x_n)^T$ be a unit eigenvector of $D(G)$ corresponding to $\rho(G)$. Then

$$\rho(G)x_i = \sum_{v_j \in V(G)} d_{ij}x_j. \tag{1}$$

Lemma 2. *Let G be a connected graph, $x(G) = (x_1, x_2, \ldots, x_n)^T$ and $v_r, v_s \in V(G)$. If $N_G(v_r) \setminus \{v_s\} = N_G(v_s) \setminus \{v_r\}$, then $x_r = x_s$.*

Proof. From Eq. (1), we have

$$d_{rs}x_s + \sum_{v_t \in V(G)\setminus\{v_r,v_s\}} d_{rt}x_t = \rho(G)x_r, d_{rs}x_r + \sum_{v_t \in V(G)\setminus\{v_r,v_s\}} d_{st}x_t = \rho(G)x_s.$$

Since $N_G(v_r) \setminus \{v_s\} = N_G(v_s) \setminus \{v_r\}$, we have $d_{rt} = d_{st}$ for $v_t \in V(G) \setminus \{v_r, v_s\}$. Then

$$\begin{aligned}(\rho(G) + d_{rs})x_r &= d_{rs}(x_r + x_s) + \sum_{v_t \in V(G)\setminus\{v_r,v_s\}} d_{rt}x_t \\ &= d_{rs}(x_r + x_s) + \sum_{v_t \in V(G)\setminus\{v_r,v_s\}} d_{st}x_t = (\rho(G) + d_{rs})x_s,\end{aligned}$$

and thus $x_r = x_s$. ☐

3. GRAPHS WITH GIVEN VERTEX CONNECTIVITY

Let $G = K_s \vee (K_{n_1} \cup K_{n_2})$, where $s + n_1 + n_2 = n$. By Lemma 2, entries of $x(G)$ have the same value, say y_0, for the vertices in $V(K_s)$, y_1 for the vertices in $V(K_{n_1})$ and y_2 for the vertices in $V(K_{n_2})$.

Lemma 3. *In the setup as above, if $n_2 > n_1 + 1$, then $(n_2 - 1)y_2 - n_1y_1 > 0$.*

Proof. Let $\rho = \rho(G)$. From Eq. (1), we have

$$\begin{aligned} sy_0 + (n_1 - 1)y_1 + 2n_2y_2 &= \rho y_1, \\ sy_0 + 2n_1y_1 + (n_2 - 1)y_2 &= \rho y_2. \end{aligned}$$

Then

$$\begin{aligned} n_2y_2 - n_1y_1 &= (\rho + 1)(y_1 - y_2), \\ y_1/y_2 &= (\rho + n_2 + 1)/(\rho + n_1 + 1), \end{aligned}$$

which implies that

$$\begin{aligned}(n_2-1)y_2 - n_1 y_1 &= (\rho+1)(y_1-y_2) - y_2\\ &= y_2\left[(\rho+1)\frac{y_1}{y_2} - (\rho+2)\right]\\ &= y_2\left[(\rho+1)\frac{\rho+n_2+1}{\rho+n_1+1} - (\rho+2)\right]\\ &= \frac{y_2}{\rho+n_1+1}\left[(\rho+1)(n_2-n_1-1)-n_1\right].\end{aligned}$$

Note that $n_2 - n_1 \geq 2$ and by Lemma 1, $\rho + 1 \geq \rho(K_n) + 1 = n > n_1$. Then

$$(\rho+1)(n_2-n_1-1) - n_1 > n_1(n_2-n_1-1) - n_1 = n_1(n_2-n_1-2) \geq 0.$$

Thus $(n_2-1)y_2 - n_1 y_1 > 0$. □

Recall that the vertex connectivity of the graph G is the minimum number of vertices whose deletion yields a disconnected graph.

Theorem 1. *Let G be an n-vertex connected graph with vertex connectivity s, where $1 \leq s \leq n-2$. Then $\rho(G) \geq \rho\left(K_s \vee (K_1 \cup K_{n-1-s})\right)$ with equality if and only if $G = K_s \vee (K_1 \cup K_{n-1-s})$.*

Proof. Let G be a graph with minimal spectral radius of $D(G)$ in the class of n-vertex connected graphs with vertex connectivity s. By Lemma 1, $G = K_s \vee (K_{n_1} \cup K_{n_2})$, for $n_2 \geq n_1 \geq 1$ and $s + n_1 + n_2 = n$.

Suppose that $n_1 > 1$. Let $G_1 = K_s \vee (K_{n_1-1} \cup K_{n_2+1})$ and by Lemma 2, $x(G_1)$ can be written as

$$x(G_1) = (\underbrace{y_0,\dots,y_0}_{s}, \underbrace{y_1,\dots,y_1}_{n_1-1}, \underbrace{y_2,\dots,y_2}_{n_2+1})^T.$$

Then, by minimality argument we have

$$x^T(G_1)D(G_1)x(G_1) = \rho(G_1) \geq \rho(G) \geq x^T(G_1)D(G)x(G_1),$$

i.e.,

$$x^T(G_1)D(G_1)x(G_1) - x^T(G_1)D(G)x(G_1) \geq 0. \tag{2}$$

Note that

$$D(G) = J - I_n + \begin{pmatrix} 0 & 0 & 0\\ 0 & 0 & J_{n_1\times n_2}\\ 0 & J_{n_2\times n_1} & 0\end{pmatrix},$$

$$D(G_1) = J - I_n + \begin{pmatrix} 0 & 0 & 0\\ 0 & 0 & J_{(n_1-1)\times(n_2+1)}\\ 0 & J_{(n_2+1)\times(n_1-1)} & 0\end{pmatrix}.$$

By Lemma 3, we have

$$
\begin{aligned}
&x^T(G_1)\left(D(G)-D(G_1)\right)x(G_1)\\
&=x^T(G_1)\begin{pmatrix} 0 & 0 & 0 & 0\\ 0 & 0 & -J_{(n_1-1)\times 1} & 0\\ 0 & -J_{1\times(n_1-1)} & 0 & J_{1\times n_2}\\ 0 & 0 & J_{n_2\times 1} & 0 \end{pmatrix}x(G_1)\\
&=x^T(G_1)\begin{pmatrix} 0\\ -y_2J_{(n_1-1)\times 1}\\ n_2y_2-(n_1-1)y_1\\ y_2J_{n_2\times 1} \end{pmatrix}\\
&=2\left[\left((n_2+1)-1\right)y_2-(n_1-1)y_1\right]y_2=2(n_2y_2-n_1y_1+y_1)y_2>0,
\end{aligned}
$$

which is a contradiction to (2).

Thus $n_1 = 1$, and therefore $G = K_s \vee (K_1 \cup K_{n-1-s})$. □

4. GRAPHS WITH GIVEN MATCHING NUMBER

Let $G = V(K_s \vee (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_t}))$, where $s + \sum_{i=1}^{t} n_i = n$. By Lemma 2, entries of $x(G)$ have the same value, say y_0, for the vertices in $V(K_s)$, and y_i for the vertices in $V(K_{n_i})$, where $i = 1, 2, \cdots, t$.

In a similar way as Lemma 3, we have

Lemma 4. *In the setup as above, if $n_2 > n_1 + 1$, then $(n_2 - 1)y_2 - n_1y_1 > 0$.*

A component of a graph is said to be even (odd) if it has an even (odd) number of vertices. Let G be a graph with n vertices. Let $o(G)$ be the number of odd components of G. By the Tutte-Berge formula [**8, 9**],

$$
n-2m=\max\left\{o(G-X)-|X| : X\subset V(G)\right\}.
$$

The matching number of the graph G is the number of edges in a maximum matching, denoted by $m(G)$ and if the graph G is understood, we omit the argument G and simply write m.

Theorem 2. *Let G be an n-vertex connected graphs with matching number m, where $2 \le m \le \left\lfloor \frac{n}{2} \right\rfloor$.*

(i) *If $m = \left\lfloor \frac{n}{2} \right\rfloor$, then $\rho(G) \ge n-1$ with equality if and only if $G = K_n$;*

(ii) *If $2 \le m \le \left\lfloor \frac{n}{2} \right\rfloor - 1$, then $\rho(G) \ge \rho\left(K_m \vee \overline{K_{n-m}}\right)$ with equality if and only if $G = K_m \vee \overline{K_{n-m}}$.*

Proof. Let G be a graph with minimal spectral radius of $D(G)$ in the class of n-vertex connected graphs with matching number m. By the Tutte-Berge formula, there is a vertex subset $X_0 \subset V(G)$ such that $n - 2m = \max\{o(G - X) - |X| : X \subset V(G)\} = o(G - X_0) - |X_0|$. For convenience, let $|X_0| = s$ and $o(G - X_0) = k$. Then $n - 2m = k - s$.

Suppose that $s = 0$. Then $G - X_0 = G$ and $n - 2m = k \leq 1$. If $k = 0$, then $m = \dfrac{n}{2}$, and if $k = 1$, then $m = \dfrac{n-1}{2}$. In both cases, we have by Lemma 1 that $G = K_n$.

Suppose in the following that $s \geq 1$. Then $k \geq 1$. Let $G_1, G_2, \ldots, G_k$ be all odd components of $G - X_0$. If $G - X_0$ has an even component, then by adding an edge to G between a vertex of an even component and a vertex of an odd component of $G - X_0$, we obtain a graph G', for which $n - 2m(G') \geq o(G' - x_0) = o(G - X_0)$, and then $m(G') = m(G)$. By Lemma 1, $\rho(G) > \rho(G')$, it is a contradiction to the choice of G. Thus $G - X_0$ does not have an even component. Similarly, $G_1, G_2, \ldots, G_k$ and the subgraph induced by X_0 are all complete, and any vertex of G_i $(i = 1, \ldots, k)$ is adjacent to every vertex in X_0. Thus $G = K_s \vee (K_{n_1} \cup K_{n_2} \cup \ldots \cup K_{n_k})$.

First, we show that $G - X_0$ has at most one odd component whose number of vertex is more than one. Assume that $n_2 \geq n_1 \geq 2$. Let $G_1 = K_s \vee (K_{n_1-1} \cup K_{n_2+1} \cup K_{n_3} \ldots \cup K_{n_k})$ and by Lemma 2, $x(G_1)$ may be written as

$$x(G_1) = (\underbrace{y_0, ..., y_0}_{s}, \underbrace{y_1, \ldots, y_1}_{n_1-1}, \underbrace{y_2, \ldots, y_2}_{n_2+1}, \underbrace{y_3, \ldots, y_3}_{n_3}, \ldots, \underbrace{y_k, \ldots, y_k}_{n_k})^T.$$

Then, by minimality argument we have

$$x^T D(G_1) x = \rho(G_1) \geq \rho(G) \geq x^T D(G) x,$$

i.e.,

$$x^T(G_1) D(G_1) x(G_1) - x^T(G_1) D(G) x(G_1) \geq 0. \tag{3}$$

Note that

$$D(G) = J - I_n + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & J_{n_1 \times n_2} & J_{n_1 \times n_3} & \cdots & J_{n_1 \times n_t} \\ 0 & J_{n_2 \times n_1} & 0 & J_{n_2 \times n_3} & \cdots & J_{n_2 \times n_t} \\ 0 & J_{n_3 \times n_1} & J_{n_3 \times n_2} & 0 & \cdots & J_{n_3 \times n_t} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}.$$

By Lemma 4, we have

$$\begin{aligned} & x^T(G_1) \left(D(G) - D(G_1) \right) x(G_1) \\ &= x^T(G_1) \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -J_{(n_1-1) \times 1} & 0 & 0 \\ 0 & -J_{1 \times (n_1-1)} & 0 & J_{1 \times n_2} & 0 \\ 0 & 0 & J_{n_2 \times 1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} x(G_1) \end{aligned}$$

$$= x^T(G_1) \begin{pmatrix} 0 \\ -y_2 J_{(n_1-1)\times 1} \\ n_2 y_2 - (n_1-1)y_1 \\ y_2 J_{n_2\times 1} \\ 0 \end{pmatrix} = 2(n_2y_2 - n_1y_1 + y_1)y_2 > 0,$$

which is a contradiction to (3). Thus $G - X_0$ has at most one odd component whose number of vertex is more than one.

Now, we show that G does not have the odd component with number of vertices greater than 1. By contradiction, suppose that $G = K_s \vee (\overline{K_{k-1}} \cup K_{n-s-k+1})$, where $n \geq s+k$. Let $n_1 = n - s - k + 1$ and $G_2 = K_{s+1} \vee (\overline{K_{k-1}} \cup K_{n_1-1})$, by Lemma 2, $x(G_2)$ may be written as

$$x(G_2) = (\underbrace{y_0, ..., y_0}_{s+1}, \underbrace{y_1, \ldots, y_1}_{n_1-1}, y_2, y_3, \ldots, y_k)^T.$$

Then, by minimality argument we have

$$x^T(G_2)D(G_2)x(G_2) = \rho(G_2) \geq \rho(G) \geq x^T(G_2)D(G)x(G_2),$$

i.e.,

$$x^T(G_2)D(G_2)x(G_2) - x^T(G_2)D(G)x(G_2) \geq 0. \tag{4}$$

Note that

$$D(G) = J + I_n + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & J_{n_1\times k} \\ 0 & J_{k\times n_1} & J_{k\times k} - I_k \end{pmatrix}.$$

Then we have

$$x^T(G_2)\left(D(G) - D(G_2)\right)x(G_2) = x^T(G_2) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & J_{1\times k} \\ 0 & 0 & 0 \\ 0 & J_{k\times 1} & 0 \end{pmatrix} x(G_2) > 0,$$

which is a contradiction to (4), thus $G = K_{n-k} \vee \overline{K_k} = K_m \vee \overline{K_{n-m}}$. □

5. GRAPHS WITH GIVEN CHROMATIC NUMBER

Let $G = K_{n_1,n_2,\ldots,n_r}$, where $\sum_{i=1}^{r} n_i = n$ and $n_i > 0$. By Lemma 2, entries of $x(G)$ have the same value, say y_i, for vertices in V_i $(i = 1, 2, \ldots, r)$, where V_i is a vertex partition and $|V_i| = n_i$.

Lemma 5. *In the setup as above, $n_i > n_j$ if and only if $y_i > y_j$ and $n_i = n_j$ if and only if $y_i = y_j$.*

Proof. Let $\rho = \rho(G)$. From Eq. (1), we have

$$\sum_{k=1}^{r} n_k y_k + (n_i - 2)y_i = \rho y_i,$$
$$\sum_{k=1}^{r} n_k y_k + (n_j - 2)y_j = \rho y_j.$$

Then

$$\frac{\sum_{k=1}^{r} n_k y_k}{y_i} + (n_i - 2) = \frac{\sum_{k=1}^{r} n_k y_k}{y_j} + (n_j - 2),$$

i.e.,

$$n_i - n_j = \sum_{k=1}^{r} n_k y_k \left(\frac{1}{y_j} - \frac{1}{y_i} \right),$$

which implies that

$$n_i > n_j \quad \Leftrightarrow \quad y_i > y_j,$$
$$n_i = n_j \quad \Leftrightarrow \quad y_i = y_j,$$

as desired. □

The chromatic number of a graph G is the smallest number of colors needed to color the vertices of G such that any two adjacent vertices have different colors. A subset of vertices assigned to the same color is called a color class, every such class forms an independent set. The Turán graph $T_{n,r}$ is a complete r-partite graph on n vertices for which the numbers of vertices of vertex classes are as equal as possible.

Theorem 3. *Let G be an n-vertex connected graph with chromatic number r, where $2 \le r \le n-1$. If $G \ne T_{n,r}$, then $\rho(G) > \rho(T_{n,r})$.*

Proof. Let G be the graph with minimal spectral radius of $D(G)$ in the class of n-vertex connected graph with chromatic number r. Then $V(G)$ can be partitioned into r independent sets $V_1,\ V_2, \ldots,\ V_r$, where $|V_i| = n_i$ $(i = 1, 2, \ldots, r)$ and $\sum_{i=1}^{r} n_i = n$. By Lemma 1, $G = K_{n_1,n_2,\ldots,n_r}$.

Suppose that G is not the Turán graph. Then there exist i, j such that $|n_i - n_j| > 1$. Suppose without loss of generality that $n_2 - 1 > n_1$. Let $G_1 = K_{n_1+1,n_2-1,n_3,\ldots,n_s}$ and by Lemma 2, $x(G_1)$ may be written as

$$x(G_1) = (\underbrace{y_1, \ldots, y_1}_{n_1+1}, \underbrace{y_2, \ldots, y_2}_{n_2-1}, \underbrace{y_3, \ldots, y_3}_{n_3} \ldots, \underbrace{y_r, \ldots, y_r}_{n_r})^T.$$

Then, by minimality argument we have

$$x^T(G_1)D(G_1)x(G_1) = \rho(G_1) \ge \rho(G) \ge x^T(G_1)D(G)x(G_1),$$

i.e.,

$$x^T(G_1)D(G_1)x(G_1) - x^T(G_1)D(G)x(G_1) \geq 0. \tag{5}$$

Note that

$$D(G) = J - I_n + \begin{pmatrix} J_{n_1\times n_1} - I_{n_1} & 0 & 0 & 0 \\ 0 & J_{n_2\times n_2} - I_{n_2} & 0 & 0 \\ 0 & 0 & J_{n_3\times n_3} - I_{n_3} & 0 \\ \cdots & \cdots & \cdots & \end{pmatrix}.$$

Then, by Lemma 5

$$\begin{aligned} & x^T(G_1)(D(G) - D(G_1))x(G_1) \\ & \quad = x^T(G_1) \begin{pmatrix} 0 & -J_{n_1\times 1} & 0 & 0 \\ -J_{1\times n_1} & 0 & J_{1\times(n_2-1)} & 0 \\ 0 & J_{(n_2-1)\times 1} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} x(G_1) \\ & \quad = x^T(G_1) \begin{pmatrix} -y_1 J_{n_1\times 1} \\ (n_2-1)y_2 - n_1 y_1 \\ y_2 J_{(n_2-1)\times 1} \\ 0 \end{pmatrix} \\ & \quad = y_1[(n_2-1)y_2 - n_1 y_1] + (n_2-1)y_2(y_2 - y_1) + y_1[(n_2-1)y_2 - n_1 y_1] \\ & \quad = (n_2-1){y_2}^2 + (n_2-1)y_1 y_2 - 2n_1 {y_1}^2 > 0, \end{aligned}$$

which is a contradiction to (5), and thus G is the Turán graph $T_{n,r}$. □

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